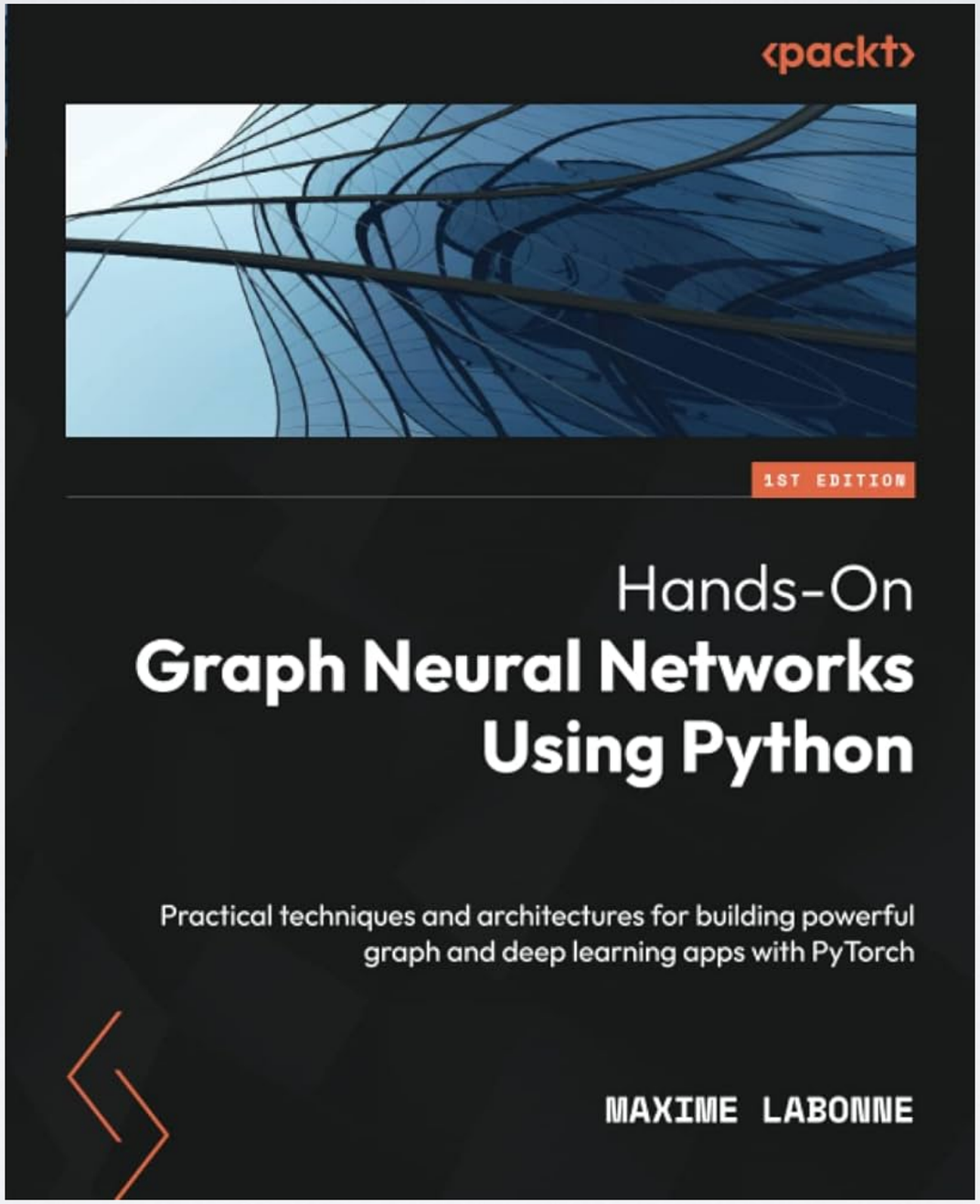
GNN WITH PYTORCH

REFERENCE


packt
1ST EDITION
Hands-On
Graph Neural Networks
Using Python
Practical techniques and architectures for building powerful
graph and deep learning apps with PyTorch
MAXIME LABONNE

PYTORCH GEOMETRIC

- Pytorch Geometric (PyG) is an official library built on top of PyTorch to deal with graphs neural networks (and other types of structured data)
- https://pytorch-geometric.readthedocs.io/

PYTORCH GEOMETRIC

Implements most
Well-known GNN layers

Graph Neural Network Operators

Name	`SparseTensor`	`edge_weight`	`edge_attr`	bipartite	static	lazy
`SimpleConv`	✓	✓		✓	✓	
`GCNConv` (Paper)	✓	✓			✓	✓
`ChebConv` (Paper)		✓			✓	✓
`SAGEConv` (Paper)	✓			✓	✓	✓
`CuGraphSAGEConv` (Paper)					✓	
`GraphConv` (Paper)	✓	✓		✓	✓	✓
`GatedGraphConv` (Paper)	✓	✓			✓	
`ResGatedGraphConv` (Paper)	✓		✓	✓	✓	✓
`GATConv` (Paper)	✓		✓	✓		✓
`CuGraphGATConv` (Paper)					✓	
`FusedGATConv` (Paper)					✓	
`GATv2Conv` (Paper)	✓		✓	✓		✓
`TransformerConv` (Paper)	✓		✓	✓		✓
`AGNNConv` (Paper)	✓				✓	
`TAGConv` (Paper)	✓	✓			✓	✓
`GINConv` (Paper)	✓			✓	✓	
`GINEConv` (Paper)	✓		✓	✓	✓	

PYTORCH GEOMETRIC

```
import torch
import torch.nn.functional as F
from torch_geometric.nn import GCNConv
```

PYTORCH GEOMETRIC

```
class GCN(torch.nn.Module):
    """Graph Convolutional Network"""
    def __init__(self, dim_in, dim_h, dim_out):
        super().__init__()
        self.gcn1 = GCNConv(dim_in, dim_h)
        self.gcn2 = GCNConv(dim_h, dim_out)
```

Creating a torch module

PYTORCH GEOMETRIC

```
class GCN(torch.nn.Module):
    """Graph Convolutional Network"""
    def __init__(self, dim_in, dim_h, dim_out):
        super().__init__()
        self.gcn1 = GCNConv(dim_in, dim_h)
        self.gcn2 = GCNConv(dim_h, dim_out)
```

```
def forward(self, x, edge_index):
    h = self.gcn1(x, edge_index)
    h = torch.relu(h)
    h = self.gcn2(h, edge_index)
    return F.log_softmax(h, dim=1)
```

Adjacency matrix (A)
As an edge list (2 x N matrix)

PYTORCH GEOMETRIC

```
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        super().__init__()
        self.gcn1 = GCNConv(dim_in, dim_h)
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```

```
def forward(self, x, edge_index):
    h = self.gcn1(x, edge_index)
    h = torch.relu(h)
    h = self.gcn2(h, edge_index)
    return F.log_softmax(h, dim=1)
```

```
    def fit(self, data, epochs):
        criterion = torch.nn.CrossEntropyLoss()
        optimizer = torch.optim.Adam(self.parameters(),
                                     lr=0.01,
                                     weight_decay=5e-4)
        self.train()
        for epoch in range(epochs+1):
            optimizer.zero_grad()
            out = self(data.x, data.edge_index)
            loss = criterion(out[data.train_mask],
data.y[data.train_mask])
            acc = accuracy(out[data.train_mask].
argmax(dim=1), data.y[data.train_mask])
            loss.backward()
            optimizer.step()
```

Module in training mode

Reset gradient at each step

call forward

Mask to use only some nodes for training

train_mask = [True, True, True, False, False]

PYTORCH GEOMETRIC

No gradient computation in this function

```
    @torch.no_grad()
    def test(self, data):
        self.eval()
        out = self(data.x, data.edge_index)
        acc = accuracy(out.argmax(dim=1)[data.test_mask],
data.y[data.test_mask])
        return acc
```

Module in evaluation mode

PYTORCH GEOMETRIC

```
class GCN(torch.nn.Module):
    """Graph Convolutional Network"""
    def __init__(self, dim_in, dim_h, dim_out):
        super().__init__()
        self.gcn1 = GCNConv(dim_in, dim_h)
        self.gcn2 = GCNConv(dim_h, dim_out)
```

```
    def fit(self, data, epochs):
        criterion = torch.nn.CrossEntropyLoss()
        optimizer = torch.optim.Adam(self.parameters(),
                                     lr=0.01,
                                     weight_decay=5e-4)
        self.train()
        for epoch in range(epochs+1):
            optimizer.zero_grad()
            out = self(data.x, data.edge_index)
            loss = criterion(out[data.train_mask],
data.y[data.train_mask])
            acc = accuracy(out[data.train_mask].
argmax(dim=1), data.y[data.train_mask])
            loss.backward()
            optimizer.step()
```

```
gcn = GCN(dataset.num_features, 16, dataset.num_classes)
print(gcn)
gcn.fit(data, epochs=100)
```

A MORE ADVANCED EXAMPLE

EXAMPLE 2

```
class GCN(torch.nn.Module):
    def __init__(self, dim_in, dim_h, dim_out):
        super().__init__()
        self.gcn1 = GCNConv(dim_in, dim_h*4)
        self.gcn2 = GCNConv(dim_h*4, dim_h*2)
        self.gcn3 = GCNConv(dim_h*2, dim_h)
        self.linear = torch.nn.Linear(dim_h, dim_out)
```

EXAMPLE 2

```
class GCN(torch.nn.Module):
    def __init__(self, dim_in, dim_h, dim_out):
        super().__init__()
        self.gcn1 = GCNConv(dim_in, dim_h*4)
        self.gcn2 = GCNConv(dim_h*4, dim_h*2)
        self.gcn3 = GCNConv(dim_h*2, dim_h)
        self.linear = torch.nn.Linear(dim_h, dim_out)
```

```
def forward(self, x, edge_index):
    h = self.gcn1(x, edge_index)
    h = torch.relu(h)
    h = F.dropout(h, p=0.5, training=self.training)
    h = self.gcn2(h, edge_index)
    h = torch.relu(h)
    h = F.dropout(h, p=0.5, training=self.training)
    h = self.gcn3(h, edge_index)
    h = torch.relu(h)
    h = self.linear(h)
    return h
```

EXAMPLE 2

```
h = F.dropout(h, p=0.5, training=self.training)
```

- Dropout: Implicit Regularization technique
  - Lasso: explicit regularization
  - Dropout: implicit
    - We do not control how to penalize weights

- Principe: put a fraction p of input matrix elements to 0.
  - Hide some information about some nodes

- It makes overfitting harder
  - The NN cannot rely too much on one particular information piece

- training=self.training
  - We want to do it only during training

VGAE

VGAE

```
from torch_geometric.nn import GCNConv, VGAE
```

VGAE reconstruct the graph using the dot product of embeddings.
Any encoder can be used to obtain the embeddings.
Remember: end-to-end, all weights trained simultaneously!

```
model = VGAE(Encoder(dataset.num_features, 16)).
to(device)
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)
```

VGAE

```
class Encoder(torch.nn.Module):
    def __init__(self, dim_in, dim_out):
        super().__init__()
        self.conv1 = GCNConv(dim_in, 2 * dim_out)
        self.conv_mu = GCNConv(2 * dim_out, dim_out)
        self.conv_logstd = GCNConv(2 * dim_out, dim_out)

    def forward(self, x, edge_index):
        x = self.conv1(x, edge_index).relu()
        return self.conv_mu(x, edge_index), self.conv_
logstd(x, edge_index)
```

Our encoder compute and returns 2 objects: centroids and variance

VGAE

```
def train():
    model.train()
    optimizer.zero_grad()
    z = model.encode(train_data.x, train_data.edge_index)
    loss = model.recon_loss(z, train_data.pos_edge_label_
index) + (1 / train_data.num_nodes) * model.kl_loss()
    loss.backward()
    optimizer.step()
    return float(loss)
```

VGAE traditionnally use a combination of 2 loss:
-recon_loss: binary cross entropy
-KL divergence between parameters and priors
=>priors are that centers are at 0 and variance=1, tend to force to concentrate in the center