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1. These imports load PyTorch, PyG Data container, GraphSAGE layer and common neural network functions needed to build and train a graph model.

```
import torch
from torch_geometric.data import Data
from torch_geometric.nn import SAGEConv
import torch.nn.functional as F
```

2.

```
[3] 0s  x = torch.tensor(
    [
        [1.0, 0.0],
        [1.0, 0.0],
        [1.0, 0.0],
        [0.0, 1.0],
        [0.0, 1.0],
        [0.0, 1.0]
    ],
    dtype=torch.float,
)
```

- We define a feature matrix x that contains one row per node (6 rows total).
- Each row is a 2-dimensional feature vector describing whether the node is benign or malicious.
- Benign nodes (0, 1, 2) are assigned the feature $[1.0, 0.0]$, meaning benign = 1, malicious = 0.
- Malicious nodes (3, 4, 5) are assigned $[0.0, 1.0]$, meaning benign = 0, malicious = 1.

```
[4] 0s  edge_index = (
    torch.tensor(
        [
            [0, 1],
            [1, 0],
            [1, 2],
            [2, 1],
            [0, 2],
            [2, 0],
            [3, 4],
            [4, 3],
            [4, 5],
            [5, 4],
            [3, 5],
            [5, 3],
            [2, 3],
            [3, 2],
        ],
        dtype=torch.long,
    ).t()
    .contiguous()
)
```

- We define all graph connections where each row represents one directed edge between two nodes.
- PyTorch Geometric only works with directed edges. So to represent an undirected connection, we write it twice ($0 \rightarrow 1$ and $1 \rightarrow 0$) to make sure both nodes can exchange information during message passing.
- Nodes 0, 1, and 2 are fully connected to each other, forming a small benign subgraph and Nodes 3, 4, and 5 are also fully connected, forming the malicious subgraph.

```
[5] 0s
y = torch.tensor([0, 0, 0, 1, 1, 1], dtype=torch.long)
data = Data(x=x, edge_index=edge_index, y=y)
```

- y stores the true class label for each node: 0 for benign nodes (0, 1, 2) and 1 for malicious nodes (3, 4, 5).
- The Data object bundles everything into one graph structure:
 - $x \rightarrow$ node features
 - $\text{edge_index} \rightarrow$ the graph's connections
 - $y \rightarrow$ node labels

```
[6] 0s
class GraphSAGENet(torch.nn.Module):
    def __init__(self, in_channels, hidden_channels, out_channels):
        super(GraphSAGENet, self).__init__()
        self.conv1 = SAGEConv(in_channels, hidden_channels)
        self.conv2 = SAGEConv(hidden_channels, out_channels)

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

- The forward function describes how data flows through the model every time the graph is passed into it.
- The first layer conv1 takes the original 2-dimensional node features and transforms them into 4-dimensional embeddings (conv1: $2 \rightarrow 4$).
- A ReLU activation is applied to help the model learn more complex patterns.
- The second layer conv2 receives the 4-dimensional vectors and maps them to 2 output values per node one for each class (benign or malicious) (conv2: $4 \rightarrow 2$).
- log_softmax converts these two output scores into log-probabilities so the network can correctly learn which class each node belongs to.

```
[7] 0s
model = GraphSAGENet(in_channels=2, hidden_channels=4, out_channels=2)
```

- This line creates an instance of the GraphSAGENet model and specifies the size of each layer.
- $\text{in_channels}=2$ tells the model that each node has 2 input features.
- $\text{hidden_channels}=4$ sets the hidden layer to produce 4-dimensional embeddings.
- $\text{out_channels}=2$ means the final layer outputs 2 class scores for each node (benign vs malicious).

```
[9] 0s
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)
model.train()
for epoch in range(50):
    optimizer.zero_grad()
    out = model(data.x, data.edge_index)
    loss = F.nll_loss(out, data.y)
    loss.backward()
    optimizer.step()
```

- We create an Adam optimizer to update the model's weights with a learning rate of 0.01.
- `model.train()` -> we are in training mode.
- The loop runs for 50 epochs, meaning we train the model 50 times over the same graph.
- `optimizer.zero_grad()` -> clears old gradients from the previous step.
- `out = model(data.x, data.edge_index)` -> runs the model to get the predicted class scores for each node.
- `loss = F.nll_loss(out, data.y)` -> compares the predictions to the true labels and computes how wrong the model is.
- `loss.backward()` -> computes the corrections needed for each model weight by showing how much each one contributed to the prediction error.
- `optimizer.step()` -> updates the model's weights to reduce the loss on the next iteration.

```
[10] ✓ 0s
  model.eval()
  pred = model(data.x, data.edge_index).argmax(dim=1)
  print("Predicted labels:", pred.tolist())
...
... Predicted labels: [0, 0, 0, 1, 1, 1]
```

Switch the model to evaluation mode, run it on the graph and take the class with the highest score for each node using `argmax`.