

1. Environment Setup and Library Imports

The initial cell prepares the computational environment:

- **!pip install torch_geometric**
Installs the PyTorch Geometric (PyG) library required for graph neural network (GNN) operations.
 - **import torch**
Loads the core PyTorch framework.
 - **from torch_geometric.data import Data**
Provides the Data container for representing graph structures.
 - **from torch_geometric.nn import SAGEConv**
Imports the GraphSAGE convolution operator.
 - **import torch.nn.functional as F**
Grants access to PyTorch's functional utilities such as activation functions and loss computations.
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2. Graph Construction

A small six-node graph is defined using PyTorch tensors:

- **Node features (x)**
A tensor of size (6×2) encodes two numerical attributes per node.
- **Edge indices (edge_index)**
A tensor of shape $(2 \times E)$ describes graph connectivity via the COO (coordinate) format:
 - Row 0: source node indices
 - Row 1: target node indices
- **Node labels (y)**
A one-dimensional tensor of length 6 assigns a class label to each node.

Data object creation

```
data = Data(x=x, edge_index=edge_index, y=y)
```

- This encapsulates the graph structure and associated information into a PyG-compatible format.
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3. Model Definition: GraphSAGE Network

A custom neural network class is declared:

Model architecture

- **SAGEConv(2, 4)**
First GraphSAGE layer transforming 2 input features to 4 hidden features.
- **SAGEConv(4, 2)**
Second GraphSAGE layer generating 2 output features (corresponding to 2 possible classes).

Forward propagation sequence

1. Apply the first GraphSAGE convolution.
2. Use ReLU activation.
3. Apply the second GraphSAGE convolution.
4. Produce log-probabilities via `log_softmax` along the feature dimension.

Instantiation and Optimization

- `model = Net()`
- `optimizer = Adam(model.parameters(), lr=0.01)`

The Adam optimizer is selected with a learning rate of 0.01.

4. Training Procedure

A training loop executes for 200 iterations:

1. **`optimizer.zero_grad()`**
Resets gradient accumulators.
 2. **Forward pass**
`out = model(data.x, data.edge_index)`
 3. **Produces log-probability outputs of size (6 × 2).**
 4. **Loss computation**
`loss = F.nll_loss(out, data.y)`
 5. **Uses negative log-likelihood loss appropriate for log-softmax outputs.**
 6. **Gradient computation**
`loss.backward()`
 7. **Parameter update**
`optimizer.step()`
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5. Evaluation and Prediction

Inference is performed after training:

- **`model.eval()`**
Switches the network into evaluation mode.
- **Prediction**
`pred = model(data.x, data.edge_index).argmax(dim=1)`

- The `argmax` operation extracts the predicted class index for each node.
- **Output**
Predicted node classes are printed as a Python list.