

## 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  $(6 \times 2)$  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.

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## 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.