Graph Neural Network to solve Au=b

In [1]:
```
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim
from torch_geometric.data import Data
from torch_geometric.nn import GCNConv
from torch_geometric.transforms import AddSelfLoops
from torch_geometric.data import Data, DataLoader

from scipy.sparse import coo_matrix, csr_matrix
from torch_sparse import coalesce, SparseTensor
from sklearn.model_selection import train_test_split

import matplotlib.pyplot as plt
import numpy as np
```

```
C:\Users\soha9\anaconda3\envs\torch\lib\site-packages\tqdm\auto.py:22: TqdmWa
rning: IProgress not found. Please update jupyter and ipywidgets. See http
s://ipywidgets.readthedocs.io/en/stable/user_install.html (https://ipywidget
s.readthedocs.io/en/stable/user_install.html)
  from .autonotebook import tqdm as notebook_tqdm
```

In [2]:
```
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
```

Load sparse matrix A in coo format

A: m x n

b: n x 1

x: m x 1

In [3]:
```
#Load the data
A_matrix_path = "data/A_ex9.txt"
A_info = np.loadtxt(A_matrix_path)

# Extract the row, column, and value arrays from the data
row_A = A_info[:, 0].astype(int)
col_A = A_info[:, 1].astype(int)
val_A = A_info[:, 2]

# Create the sparse matrix using COO format
A = coo_matrix((val_A, (row_A, col_A)))
num_nodes = A.shape[0]

print('Number of nodes: ', num_nodes)
print('A shape: ', A.shape)
```

```
Number of nodes:  36865
A shape:  (36865, 36865)
```

Load u

In [4]:
```
# # Load u
# u_vector_path = "data/u_ex9.txt"
# u = np.loadtxt(u_vector_path)
# print('u shape: ', u.shape)
```

Compute b

In [5]:
```
# Convert A to PyTorch SparseTensor
indices = torch.from_numpy(np.vstack((A.row, A.col))).long()
values = torch.from_numpy(A.data).float()
shape = torch.Size(A.shape)
A = torch.sparse.FloatTensor(indices, values, shape)

u = torch.FloatTensor(np.random.rand(num_nodes, 1))
b = A.matmul(u)

print(b.shape)
print(u.shape)
print(A.shape)
```

```
torch.Size([36865, 1])
torch.Size([36865, 1])
torch.Size([36865, 36865])
```

In [6]:
```
A
```

Out[6]:
```
tensor(indices=tensor([[    1,     1,     1,  ..., 36864, 36864, 36864],
                       [    1,     2,     3,  ..., 36862, 36863, 36864]]),
       values=tensor([ 8.8577e-06,  3.3011e-06, -3.3011e-06,  ...,
                      -3.3005e-06,  3.2999e-06,  8.8583e-06]),
       size=(36865, 36865), nnz=662016, layout=torch.sparse_coo)
```

In [7]:
```
u
```

Out[7]:
```
tensor([[0.6212],
        [0.1044],
        [0.0266],
        ...,
        [0.1812],
        [0.3843],
        [0.7157]])
```

In [8]:
```
b
```

Out[8]:
```
tensor([[ 0.0000e+00],
        [-1.5544e-06],
        [-5.1648e-06],
        ...,
        [ 5.9315e-06],
        [ 1.0078e-05],
        [ 1.1225e-05]])
```

Edge Index

In graph neural networks, edge_index is a commonly used term that refers to a matrix or tensor that represents the edges of a graph. It is a two-dimensional matrix with two rows, where each column represents an edge of the graph. The first row of the matrix contains the index of the source nodes of each edge, while the second row contains the index of the destination nodes.

For example, let's say we have a simple undirected graph with 4 nodes and 3 edges, where the edges are (0,1), (1,2), and (2,3). We can represent this graph using the following edge_index matrix:

```
edge_index = [
  [0, 1, 1, 2],
  [1, 0, 2, 3]
]
```

Here, the first row of edge_index represents the source nodes of each edge, and the second row represents the destination nodes. For example, the first edge (0,1) has source node 0 and destination node 1.

The edge_index matrix is typically used in conjunction with node feature matrices to define the input to a graph neural network. The node feature matrix contains features for each node in the graph, while the edge_index matrix describes the edges that connect the nodes. By combining these two matrices, a graph neural network can learn to operate on the graph structure and its associated features.

Edge Weights

In graph neural networks, edge_weights are values associated with the edges of a graph, which can be used to represent the strength, importance or similarity between connected nodes. edge_weights can be used in a variety of ways, such as during message passing, graph convolutions or pooling operations.

edge_weights can be represented as a tensor or an array, with one value per edge. If the edges are unweighted, i.e., all edges are equally important, then the edge_weights can be represented as an array of ones. However, if the edges have different weights, then the edge_weights can be assigned accordingly.

In [9]:
```
# Assuming A_sp is a PyTorch SparseTensor
A_coo = A.coalesce()
edge_index = A_coo.indices()
edge_weights = A_coo.values()

# Convert edge indices to PyTorch LongTensor
edge_index = edge_index.long()
```

In [10]:
```
print('====== Edge Index =====')
print('edge_index shape: ',edge_index.shape)
print(edge_index)
print('====== Edge Weights =====')
print('edge_weights shape: ',edge_weights.shape)
print(edge_weights)
```

```
====== Edge Index =====
edge_index shape:  torch.Size([2, 662016])
tensor([[    1,     1,     1,  ..., 36864, 36864, 36864],
        [    1,     2,     3,  ..., 36862, 36863, 36864]])
====== Edge Weights =====
edge_weights shape:  torch.Size([662016])
tensor([ 8.8577e-06,  3.3011e-06, -3.3011e-06,  ..., -3.3005e-06,
         3.2999e-06,  8.8583e-06])
```

Create data object for input to GNN

The Data object has the following attributes:

- **'x'**: a tensor of node features with shape **'[36865, 1]'**. This means there are 36865 nodes in the graph, each with 1 feature.
- **'edge_index'**: a tensor of shape **'[2, 662016]'** representing the edge index of the graph. The first row contains the source nodes and the second row contains the destination nodes. There are 662016 edges in the graph.
- **'edge_attr'**: a tensor of edge weights with shape **'[662016]'**. This means there is one weight for each edge in the graph.

- **'num_nodes'**: an integer value of **36865** representing the total number of nodes in the graph.

In [12]:
```
# Create a Data object from edge_index, edge_weights, and node features
data = Data(x=b, edge_index=edge_index, edge_attr=edge_weights, num_nodes=num_
data = data.to(device)

# Print the Data object
print(data)
```

```
Data(x=[36865, 1], edge_index=[2, 662016], edge_attr=[662016], y=[36865, 1],
num_nodes=36865)
```

Graph Neural Network model

The given model is a graph convolutional network (GCN) that consists of 4 graph convolutional layers.

- First layer, the model takes a feature vector of size 1 for each node and applies the GCNConv operation with 128 output channels. The output of this layer is then passed through a rectified linear unit (ReLU) activation function.
- Last layer applies the GCNConv operation with a single output channel, which is the predicted value for each node.

The model takes the input data **'x'** and **'edge_index'** and returns the predicted values for each node.

In [13]:
```
class GCN(torch.nn.Module):
    def __init__(self):
        super(GCN, self).__init__()
        self.conv1 = GCNConv(1, 128)
        self.conv2 = GCNConv(128, 64)
        self.conv3 = GCNConv(64, 16)
        self.conv4 = GCNConv(16, 1)

    def forward(self, x, edge_index):
        x = self.conv1(x, edge_index)
        x = F.relu(x)
        x = self.conv2(x, edge_index)
        x = F.relu(x)
        x = self.conv3(x, edge_index)
        x = F.relu(x)
        x = self.conv4(x, edge_index)
        return x
```

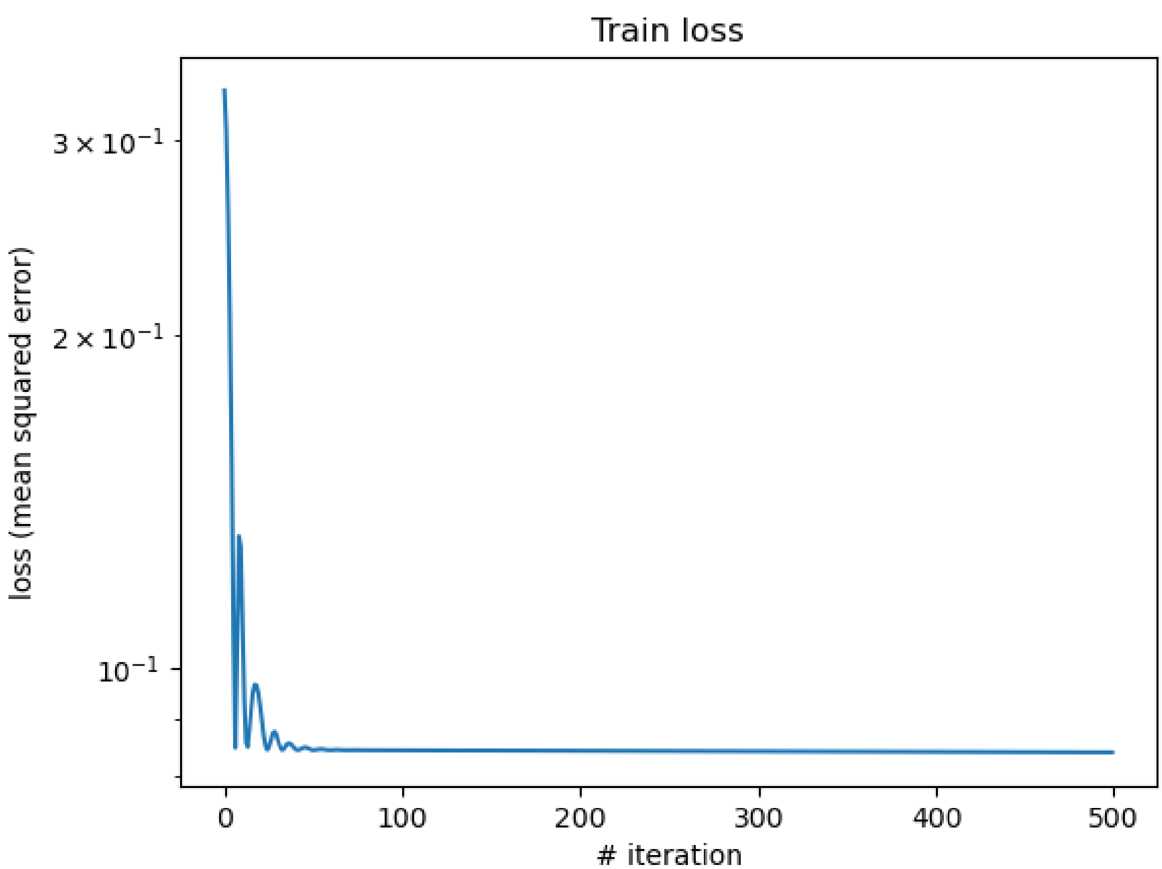
Train Graph Convolutional Network

In [14]:
```
model = GCN().to(device)
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)

# Define the loss function
criterion = torch.nn.MSELoss()

# Define the training loop
def train(model, data, optimizer, criterion, device):
    model.train()

    # Move the data to the device
    data = data.to(device)

    # Zero the gradients
    optimizer.zero_grad()

    # Compute the model output
    out = model(data.x, data.edge_index)

    # Compute the loss
    loss = criterion(out, data.y)

    # Backpropagate the gradients
    loss.backward()
    optimizer.step()

    return loss.item()

# Train the model
loss_list = []
for epoch in range(500):
    loss = train(model, data, optimizer, criterion, device)
    loss_list.append(loss)
    print('Epoch {}, Loss: {}'.format(epoch, loss))
```

```
Epoch 480, Loss: 0.08392050862512517
Epoch 481, Loss: 0.08391961455345154
Epoch 482, Loss: 0.08391872048377991
Epoch 483, Loss: 0.08391781896352768
Epoch 484, Loss: 0.08391693234443665
Epoch 485, Loss: 0.08391603827476501
Epoch 486, Loss: 0.08391514420509338
Epoch 487, Loss: 0.08391425013542175
Epoch 488, Loss: 0.08391335606575012
Epoch 489, Loss: 0.08391247689723969
Epoch 490, Loss: 0.08391158282756805
Epoch 491, Loss: 0.08391068875789642
Epoch 492, Loss: 0.08390980958938599
Epoch 493, Loss: 0.08390892297029495
Epoch 494, Loss: 0.08390803635120392
Epoch 495, Loss: 0.08390714973211288
Epoch 496, Loss: 0.08390626311302185
Epoch 497, Loss: 0.08390536904335022
Epoch 498, Loss: 0.08390448987483978
Epoch 499, Loss: 0.08390360325574875
```

In [15]:

```
plt.figure(1)
plt.plot(loss_list, label = 'train loss')
plt.xlabel('# iteration')
plt.ylabel('loss (mean squared error)')
plt.yscale('log')
plt.title('Train loss')
plt.show()
```



In [16]:
```
data.edge_index
```

Out[16]:
```
tensor([[    1,     1,     1,  ..., 36864, 36864, 36864],
        [    1,     2,     3,  ..., 36862, 36863, 36864]], device='cuda:0')
```

In [17]:
```
# Compute predicted u and residual error
model.eval()
predicted_u = model(data.x, data.edge_index)
```

In [18]:
```
predicted_u
```

Out[18]:
```
tensor([[0.4953],
        [0.4888],
        [0.4888],
        ...,
        [0.4827],
        [0.4827],
        [0.5119]], device='cuda:0', grad_fn=<AddBackward0>)
```

In [19]:
```
u
```

Out[19]:
```
tensor([[0.6212],
        [0.1044],
        [0.0266],
        ...,
        [0.1812],
        [0.3843],
        [0.7157]])
```

Residual Error

The residual error can be interpreted as the sum of the squared distances between the predicted values Au and the true values b. It is a measure of how well the solution u fits the original matrix equation Au = b. A lower residual error indicates a better fit of the solution to the equation.

$$error = \sum(||Au - b||^2)$$

In [20]:
```
residual = (torch.mm(A.to(device), predicted_u) - b.to(device))
residual
```

Out[20]:
```
tensor([[ 0.0000e+00],
        [ 7.4996e-06],
        [ 3.4891e-05],
        ...,
        [ 2.3305e-05],
        [ 1.9381e-05],
        [-5.0572e-06]], device='cuda:0', grad_fn=<SubBackward0>)
```

In [21]:
```
residual_error = torch.sum(torch.square(torch.mm(A.to(device), predicted_u) -
print(f'Residual error is: {residual_error}')
```

```
Residual error is: 4.600614192895591e-05
```