GraphLearning_CodingAssignment

June 25, 2024

1 Coding Assignment - "Graph Learning"

1.1 1. Preparation

1.1.1 1.1 Libraries

1.1.2 1.2 Helper functions

```
plt.plot([coords[edge[0],1],coords[edge[1],1]],__
 →[coords[edge[0],0],coords[edge[1],0]], linestyle='-', color='gray', alpha=0.
 ⇒5)
    plt.xlabel('longitude')
    plt.ylabel('latitude')
    plt.title('FMI stations')
    plt.show()
# The function below extracts a feature and label from each row
# of dataframe df. Each row is expected to hold a FMI weather
# measurement with cols "Latitude", "Longitude", "temp", "Timestamp".
# Returns numpy arrays X, y.
def ExtractFeatureMatrixLabelVector(data):
    nrfeatures = 7
    nrdatapoints = len(data)
    # We build the feature matrix X (each of its rows hold the features of a_{\sqcup}
 \hookrightarrow data point)
    # and the label vector y (whose entries hold the labels of data points).
    X = np.zeros((nrdatapoints, nrfeatures))
    y = np.zeros((nrdatapoints, 1))
    # Iterate over all rows in dataframe and create corresponding feature_
 ⇔vector and label.
    for ind in range(nrdatapoints):
        # Latitude of FMI station, normalized by 100.
        lat = float(data['Latitude'].iloc[ind])/100
        # Longitude of FMI station, normalized by 100.
        lon = float(data['Longitude'].iloc[ind])/100
        # Temperature value of the data point.
        tmp = data['temp'].iloc[ind]
        # Read the date and time of the temperature measurement.
        date_object = datetime.strptime(data['Timestamp'].iloc[ind], '%Y-%m-%du
 →%H:%M:%S')
        # Extract year, month, day, hour, and minute. Normalize these values
        # to ensure that the features are in range [0,1].
        year = float(date object.year)/2025
        month = float(date_object.month)/13
        day = float(date_object.day)/32
        hour = float(date_object.hour)/25
        minute = float(date_object.minute)/61
        # Store the data point's features and a label.
        X[ind,:] = [lat, lon, year, month, day, hour, minute]
        y[ind,:] = tmp
```

```
return X, y
```

1.2 2. Data

1.2.1 2.1 Dataset

```
[]: # Import the weather measurements.
data = pd.read_csv('Assignment_MLBasicsData.csv')

# We consider each temperature measurement (=a row in dataframe) as a
# separate data point.
# Get the numbers of data points and the unique stations.
num_stations = len(data.name.unique())
num_datapoints = len(data)
```

1.2.2 2.2 Features and labels

```
[]: # We next build the feature matrix X (each of its rows hold the features of audata point)

# and the label vector y (whose entries hold the labels of data points).

X, y = ExtractFeatureMatrixLabelVector(data)

print(f"The created feature matrix contains {np.shape(X)[0]} entries of {np.

shape(X)[1]} features each.")

print(f"The created label vector contains {np.shape(y)[0]} measurements.")
```

1.2.3 2.3 Empirical graph

```
[]: # Create a networkX graph
G_FMI = nx.Graph()

# Add a one node per station
G_FMI.add_nodes_from(range(0, num_stations))

for i, station in enumerate(data.name.unique()):
    # Extract data of a certain station
    station_data = data[data.name==station]

# Extract features and labels
    X_node, y_node = ExtractFeatureMatrixLabelVector(station_data)

localsamplesize = len(y_node)
    G_FMI.nodes[i]['samplesize'] = localsamplesize # The number of measurements_u
    of the i-th weather station
    G_FMI.nodes[i]['name'] = station # The name of the i-th weather station
```

```
G_FMI.nodes[i]['coord'] = np.array([station_data.Latitude.unique()[0],__
station_data.Longitude.unique()[0]]) # The coordinates of the i-th weather__
station

G_FMI.nodes[i]['X'] = X_node # The feature matrix for local dataset at node__

G_FMI.nodes[i]['y'] = y_node # The label vector for local dataset at node__

G_FMI.nodes[i]['z'] = None # The representation vector for local dataset at__
node i

# Visualize the empirical graph.
plotFMI(G_FMI)
```

1.3 3. The discrepancy measure

1.3.1 3.1 Helper function

```
[]:  # Inputs:
         1. graph FMI (class: networkx.classes.graph.Graph) - a graph to which the
     ⇔edges will be added.
     # 2. node_degree (class: int) - the minimum number of neighbors (the minimum_
      ⇔node degree).
     # Outputs:
         1. graph (class: networkx.classes.graph.Graph) - a graph with added edges.
     def add_edges(graph_FMI, node_degree):
         graph = graph_FMI.copy()
         for node in graph.nodes:
             # TODO: Extract the representation vector of the node.
             \# z node =
             raise NotImplementedError
             # Create storages for discrepancies and the corresponding neighbors.
             d_mins = np.full(shape=node_degree, fill_value=1e10)
             edges = np.full(shape=(node_degree, 2), fill_value=(node, -1))
             for potential_neighbor in graph.nodes:
                 if potential_neighbor != node:
                     # TODO: Extract the representation vecotr of the potential
      \rightarrowneighbor.
                     \# z_neighbor =
                     raise NotImplementedError
                     # TODO: Calculate the discrepancy.
                     \# d =
```

```
raise NotImplementedError
            # TODO: Find the max discrepancy so far.
                    Also, find its index to access the
                   corresponding neighbor later.
            \# d_max_idx =
            \# d max =
            raise NotImplementedError
            if d < d_max:</pre>
                # TODO: Store the calculated discrepancy and
                       the corresponding neighbor.
                \# d_mins[d_max_idx] =
                \# edges[d_max_idx][1] =
                raise NotImplementedError
    # Add edges from the given pairs of connected nodes.
    graph.add_edges_from(edges)
return graph
```

1.3.2 3.2 Student task #1 - The average temperature

1.3.3 3.3 Student task #2 - The difference in GMM parameters

```
[]: def add_edges_GMM_param(graph_FMI, GMM_seed, n_neighbors):
    # Copy the nodes to a new graph.
    graph = graph_FMI.copy()

# Define the number components for the GMM.
    n_components = 2
```

1.3.4 3.4 Student task #3 - The gradient of the average squared error loss

```
[]: def add_edges_gradient_loss(graph_FMI, n_neighbors):
        # Copy the nodes to a new graph.
        graph = graph_FMI.copy()
        # TODO: 1. Create the representation vector for each node (see "NOTE").
               2. Add the edges based on the representation vectors.
        # NOTE: 1. Fit a linear regression to the whole dataset
                  and extract the model's parameters.
               2. Calculate the gradient of the average squared error loss for
      ⇔each node
                  according to the Section 7.5 in the Lecture Notes .
        raise NotImplementedError
        # Add edges.
        graph = add_edges(graph, n_neighbors)
        return graph
    # Visualize an example graph.
    plotFMI(add_edges_gradient_loss(G_FMI, 1))
```

1.4 4. Model

1.4.1 4.1 FedGD (TODO)

```
[]: def FedGD(graph FMI, split seed):
         graph = graph_FMI.copy()
         # Define hyperparameters.
         max_iter = 1000 # The number of gradient steps.
         alpha = 0.5 # Alpha parameter.
         1_rate = 0.1 # The learning rate.
         # Create the storages for the training and validation errors.
         num_stations = len(graph.nodes)
         train_errors = np.zeros(num_stations)
         val_errors = np.zeros(num_stations)
         # TODO: Use your previous implementation of
                 the FedGD algorithm.
                 See coding assignment "FL Algorithms".
         # HINT: 1. Split the local datasets into training and validation sets.
                 2. Initialize all weight vectors with zeros.
                 3. Perform FedGD on the local training sets.
                 4. Compute and store the training and validation errors
                    for each node.
        raise NotImplementedError
         # Output the average training and validation errors.
         return np.mean(train_errors), np.mean(val_errors)
```

1.4.2 4.2 Test connectivity

```
# Define the random seed for
# add_edges_GMM_param function.
seed = 4740

for num_neighbors in range(1, 11):
    G_FMI_1 = add_edges_avg_temp(G_FMI, num_neighbors)
    G_FMI_2 = add_edges_GMM_param(G_FMI, seed, num_neighbors)
    G_FMI_3 = add_edges_gradient_loss(G_FMI, num_neighbors)

# Print the results.
print(f"The minimum number of neighbors is {num_neighbors}")
print(f"G_FMI_1 is connected: {nx.is_connected(G_FMI_1)}")
print(f"G_FMI_2 is connected: {nx.is_connected(G_FMI_2)}")
print(f"G_FMI_3 is connected: {nx.is_connected(G_FMI_3)}\n")
```

1.4.3 **4.3** FedGD errors

```
[]: # Define the random seed for
     # add_edges_GMM_param and FedGD functions.
     seed = 4740
     # The minimum number of neighbors to connect with.
     num_neighbors = 1
     # Add edges.
     G_FMI_1 = add_edges_avg_temp(G_FMI, num_neighbors)
     G_FMI_2 = add_edges_GMM_param(G_FMI, seed, num_neighbors)
     G_FMI_3 = add_edges_gradient_loss(G_FMI, num_neighbors)
     # Apply the FedGD algorithm.
     G FMI 1 train error, G FMI 1 val error = FedGD(G FMI 1, seed)
     G_FMI_2_train_error, G_FMI_2_val_error = FedGD(G_FMI_2, seed)
     G_FMI_3_train_error, G_FMI_3_val_error = FedGD(G_FMI_3, seed)
     # Print the results.
     print(f"The seed is {seed}")
     print(f"The average training error for G_FMI_1: {G_FMI_1_train_error}\nThe_\
      →average validation error for G_FMI_1: {G_FMI_1_val_error}\n")
     print(f"The average training error for G_FMI_2: {G_FMI_2_train_error}\nThe_\_
      →average validation error for G_FMI_2: {G_FMI_2_val_error}\n")
     print(f"The average training error for G_FMI_3: {G_FMI_3_train_error}\nThe_\_
      →average validation error for G_FMI_3: {G_FMI_3_val_error}\n\n")
```

[]:

GraphLearning_RefSol

June 25, 2024

1 Reference Solution for Coding Assignment "Graph Learning"

1.1 1. Preparation

1.1.1 1.1 Libraries

1.1.2 1.2 Helper functions

```
plt.plot([coords[edge[0],1],coords[edge[1],1]],__
 →[coords[edge[0],0],coords[edge[1],0]], linestyle='-', color='gray', alpha=0.
 ⇒5)
    plt.xlabel('longitude')
    plt.ylabel('latitude')
    plt.title('FMI stations')
    plt.show()
# The function below extracts a feature and label from each row
# of dataframe df. Each row is expected to hold a FMI weather
# measurement with cols "Latitude", "Longitude", "temp", "Timestamp".
# Returns numpy arrays X, y.
def ExtractFeatureMatrixLabelVector(data):
    nrfeatures = 7
    nrdatapoints = len(data)
    # We build the feature matrix X (each of its rows hold the features of a_{\sqcup}
 \hookrightarrow data point)
    # and the label vector y (whose entries hold the labels of data points).
    X = np.zeros((nrdatapoints, nrfeatures))
    y = np.zeros((nrdatapoints, 1))
    # Iterate over all rows in dataframe and create corresponding feature_
 ⇔vector and label.
    for ind in range(nrdatapoints):
        # Latitude of FMI station, normalized by 100.
        lat = float(data['Latitude'].iloc[ind])/100
        # Longitude of FMI station, normalized by 100.
        lon = float(data['Longitude'].iloc[ind])/100
        # Temperature value of the data point.
        tmp = data['temp'].iloc[ind]
        # Read the date and time of the temperature measurement.
        date_object = datetime.strptime(data['Timestamp'].iloc[ind], '%Y-%m-%du
 →%H:%M:%S')
        # Extract year, month, day, hour, and minute. Normalize these values
        # to ensure that the features are in range [0,1].
        year = float(date object.year)/2025
        month = float(date_object.month)/13
        day = float(date_object.day)/32
        hour = float(date_object.hour)/25
        minute = float(date_object.minute)/61
        # Store the data point's features and a label.
        X[ind,:] = [lat, lon, year, month, day, hour, minute]
        y[ind,:] = tmp
```

```
return X, y
```

1.2 2. Data

1.2.1 2.1 Dataset

```
[3]: # Import the weather measurements.
data = pd.read_csv('Assignment_MLBasicsData.csv')

# We consider each temperature measurement (=a row in dataframe) as a
# separate data point.
# Get the numbers of data points and the unique stations.
num_stations = len(data.name.unique())
num_datapoints = len(data)
```

1.2.2 2.2 Features and labels

```
[4]: # We next build the feature matrix X (each of its rows hold the features of a

data point)

# and the label vector y (whose entries hold the labels of data points).

X, y = ExtractFeatureMatrixLabelVector(data)

print(f"The created feature matrix contains {np.shape(X)[0]} entries of {np.

shape(X)[1]} features each.")

print(f"The created label vector contains {np.shape(y)[0]} measurements.")
```

The created feature matrix contains 19768 entries of 7 features each. The created label vector contains 19768 measurements.

1.2.3 2.3 Empirical graph

```
[5]: # Create a networkX graph
G_FMI = nx.Graph()

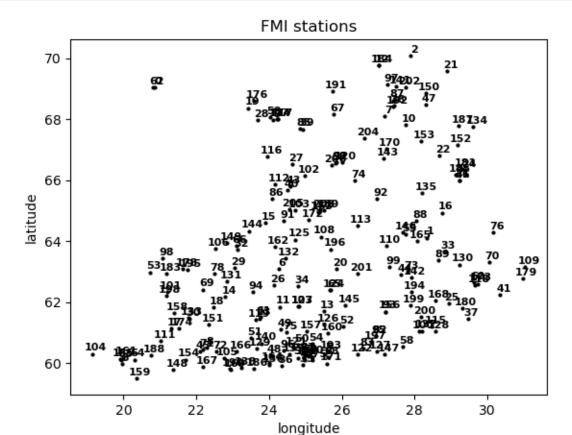
# Add a one node per station
G_FMI.add_nodes_from(range(0, num_stations))

for i, station in enumerate(data.name.unique()):
    # Extract data of a certain station
    station_data = data[data.name==station]

# Extract features and labels
X_node, y_node = ExtractFeatureMatrixLabelVector(station_data)

localsamplesize = len(y_node)
    G_FMI.nodes[i]['samplesize'] = localsamplesize # The number of measurements_
    of the i-th weather station
```

```
G_FMI.nodes[i]['name'] = station # The name of the i-th weather station
G_FMI.nodes[i]['coord'] = np.array([station_data.Latitude.unique()[0],___
station_data.Longitude.unique()[0]]) # The coordinates of the i-th weather__
station
G_FMI.nodes[i]['X'] = X_node # The feature matrix for local dataset at node___
i
G_FMI.nodes[i]['y'] = y_node # The label vector for local dataset at node___
si
G_FMI.nodes[i]['z'] = None # The representation vector for local dataset at___
snode i
# Visualize the empirical graph.
plotFMI(G_FMI)
```



1.3 3. The discrepancy measure

1.3.1 3.1 Helper function

```
[6]: def add_edges(graph_FMI, node_degree):
         graph = graph_FMI.copy()
         for node in graph.nodes:
             z_node = graph.nodes[node]['z']
             # Create storages for discrepancies and the corresponding neighbors.
             d_mins = np.full(shape=node_degree, fill_value=1e10)
             edges = np.full(shape=(node_degree, 2), fill_value=(node, -1))
             for potential_neighbor in graph.nodes:
                 if potential_neighbor != node:
                     z_neighbor = graph.nodes[potential_neighbor]['z']
                     d = LA.norm(z_node - z_neighbor)
                     # Find the max discrepancy so far.
                     d_max_idx = np.argmax(d_mins)
                     d_max = d_mins[d_max_idx]
                     if d < d_max:</pre>
                         d_{mins}[d_{max_idx}] = d
                         edges[d_max_idx][1] = potential_neighbor
             # print(f"Node {node} has neighbors {[edges[neighbor][1] for neighbor_
      →in range(node_degree)]}")
             graph.add_edges_from(edges)
         return graph
```

1.3.2 3.2 Student task #1 - The average temperature

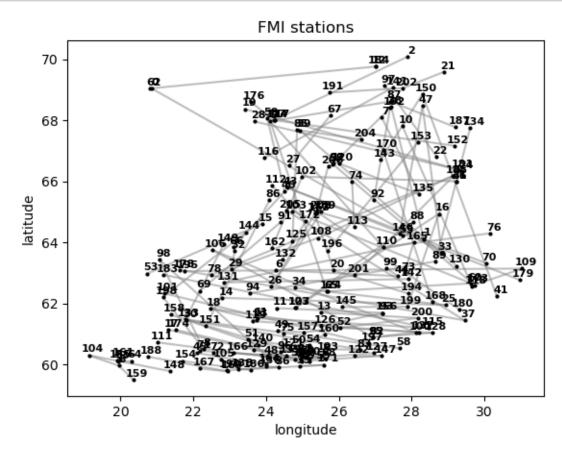
```
[7]: def add_edges_avg_temp(graph_FMI, n_neighbors):
    # Copy the nodes to a new graph.
    graph = graph_FMI.copy()

# Create the representation vector for each node.
for node in graph.nodes:
    avg_temp = np.mean(graph.nodes[node]['y'])
    graph.nodes[node]['z'] = avg_temp

# Add edges.
graph = add_edges(graph, n_neighbors)
```

```
return graph

# Visualize an example graph.
plotFMI(add_edges_avg_temp(G_FMI, 1))
```



1.3.3 3.3 Student task #2 - The difference in GMM parameters

```
[8]: def add_edges_GMM_param(graph_FMI, GMM_seed, n_neighbors):
    # Copy the nodes to a new graph.
    graph = graph_FMI.copy()

# Define the number components for the GMM.
    n_components = 2

# Fit the nodes to the GMM model and extract the model's parameters.
    for node in graph.nodes():

# Extract node's features.
    node_X = graph.nodes[node]['X']
```

```
# Fit GMM.
    gmm = GaussianMixture(n_components=n_components, random_state = GMM_seed)
    gmm.fit(node_X)

# Get the parameters of the GMM (mean vectors, covariance matricies, GMM_seed)
    gmm_params = np.concatenate((np.concatenate((gmm.means_.ravel(), gmm.GOVARIANCES_.ravel())), gmm.weights_))

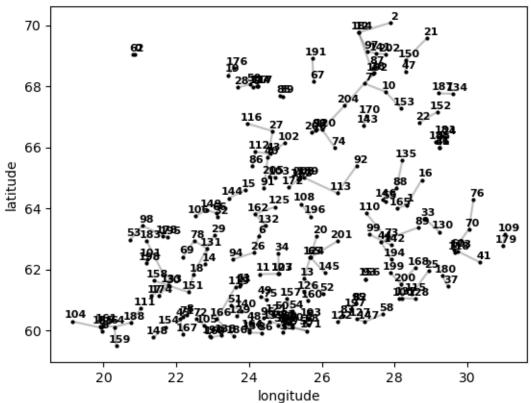
# Assign GMM parameters to the node.
    graph.nodes[node]['z'] = gmm_params

# Add edges.
    graph = add_edges(graph, n_neighbors)

return graph

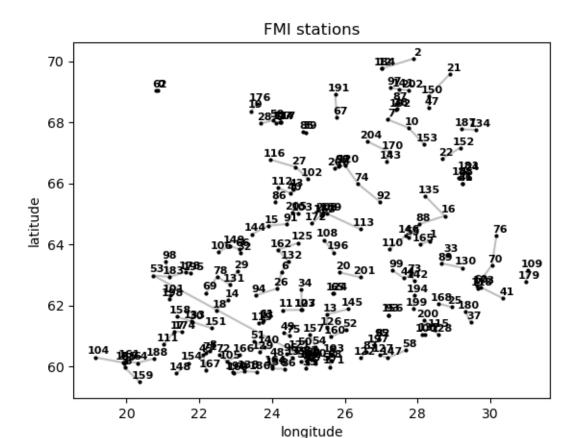
# Visualize an example graph.
plotFMI(add_edges_GMM_param(G_FMI, 4740, 1))
```





1.3.4 3.4 Student task #3 - The gradient of the average squared error loss

```
[9]: def add_edges_gradient_loss(graph_FMI, n_neighbors):
         # Copy the nodes to a new graph.
         graph = graph_FMI.copy()
         # Define and fit the Linear regression.
         linear_reg = LinearRegression()
         linear_reg.fit(X, y)
         # Extract the weight vector.
         w_hat = linear_reg.coef_
         # Calculate the average squared error loss.
         for node in graph.nodes:
             node_X = graph.nodes[node]['X']
             node_y = graph.nodes[node]['y']
             m = graph.nodes[node]['samplesize']
             loss = (-2/m) * node_X.T.dot(node_y - node_X.dot(w_hat.T))
             graph.nodes[node]['z'] = loss
         # Add edges.
         graph = add_edges(graph, n_neighbors)
         return graph
     # Visualize an example graph.
     plotFMI(add_edges_gradient_loss(G_FMI, 1))
```



1.4 4. Model

1.4.1 FedGD

```
graph.nodes[node]['y_val'] = y_val # The training label vector for_
\hookrightarrow local dataset at node i
  # Initialize all weight vectors with zeros
  for station in graph.nodes:
      graph.nodes[station]['weights'] = np.zeros((7, 1))
  # Define hyperparameters.
  max_iter = 1000
  alpha = 0.5
  1_rate = 0.1
  num_stations = len(graph.nodes)
  for i in range(max_iter):
      # Iterate over all nodes.
      for current_node in graph.nodes:
           # Extract the training data from the current node.
          X_train = graph.nodes[current_node]['X_train']
          y_train = graph.nodes[current_node]['y_train']
           w current = graph.nodes[current node]['weights']
           training_size = len(y_train)
           # Compute the first term of the Equation 5.9.
           term_1 = (2/training_size) * X_train.T.dot(y_train - X_train.

dot(w_current))
           # Compute the second term of the Equation 5.9
           # by receiving neighbors' weight vectors.
           term 2 = 0
          neighbors = list(graph.neighbors(current_node))
          for neighbor in neighbors:
               w_neighbor = graph.nodes[neighbor]['weights']
               term_2 += w_neighbor - w_current
           term 2 *= 2*alpha
           # Equation 5.8
           w_updated = w_current + l_rate * (term_1 + term_2)
           # Update the current weight vector but do not overwrite the
           # "weights" attribute as we need to do all updates synchronously, i.
⇔е.,
           # using the previous local params
          graph.nodes[current_node]['newweights'] = w_updated
       # after computing the new localparmas for each node, we now update
       # the node attribute 'weights' for all nodes
      for node_id in graph.nodes:
```

```
graph.nodes[node_id]['weights'] = graph.nodes[node_id]['newweights']
# Create the storages for the training and validation errors.
train_errors = np.zeros(num_stations)
val_errors = np.zeros(num_stations)
# Iterate over all nodes.
for station in graph.nodes:
    # Extract the data of the current node.
   X_train = graph.nodes[station]['X_train']
    y train = graph.nodes[station]['y train']
   X_val = graph.nodes[station]['X_val']
   v val = graph.nodes[station]['v val']
   w = graph.nodes[station]['weights']
    # Compute and store the training and validation errors.
    train_errors[station] = mean_squared_error(y_train, X_train.dot(w))
    val_errors[station] = mean_squared_error(y_val, X_val.dot(w))
# Output the average training and validation errors.
return np.mean(train_errors), np.mean(val_errors)
```

1.4.2 4.2 Test connectivity

```
# Define the random seed for
# add_edges_GMM_param function.
seed = 4740

for num_neighbors in range(1, 11):
    G_FMI_1 = add_edges_avg_temp(G_FMI, num_neighbors)
    G_FMI_2 = add_edges_GMM_param(G_FMI, seed, num_neighbors)
    G_FMI_3 = add_edges_gradient_loss(G_FMI, num_neighbors)

# Print the results.
print(f"The minimum number of neighbors is {num_neighbors}")
print(f"G_FMI_1 is connected: {nx.is_connected(G_FMI_1)}")
print(f"G_FMI_2 is connected: {nx.is_connected(G_FMI_2)}")
print(f"G_FMI_3 is connected: {nx.is_connected(G_FMI_3)}\n")
```

```
The minimum number of neighbors is 1 G_FMI_1 is connected: False G_FMI_2 is connected: False G_FMI_3 is connected: False

The minimum number of neighbors is 2 G_FMI_1 is connected: False G_FMI_2 is connected: False
```

G_FMI_3 is connected: False

The minimum number of neighbors is 3

G_FMI_1 is connected: False
G_FMI_2 is connected: False
G_FMI_3 is connected: False

The minimum number of neighbors is 4

G_FMI_1 is connected: False G_FMI_2 is connected: False G_FMI_3 is connected: True

The minimum number of neighbors is 5

G_FMI_1 is connected: True
G_FMI_2 is connected: False
G_FMI_3 is connected: True

The minimum number of neighbors is 6

G_FMI_1 is connected: True
G_FMI_2 is connected: False
G_FMI_3 is connected: True

The minimum number of neighbors is 7

G_FMI_1 is connected: True
G_FMI_2 is connected: False
G_FMI_3 is connected: True

The minimum number of neighbors is 8

G_FMI_1 is connected: True
G_FMI_2 is connected: False
G_FMI_3 is connected: True

The minimum number of neighbors is 9

G_FMI_1 is connected: True
G_FMI_2 is connected: False
G_FMI_3 is connected: True

The minimum number of neighbors is 10

G_FMI_1 is connected: True
G_FMI_2 is connected: False
G_FMI_3 is connected: True

1.4.3 4.3 FedGD errors

```
[14]: # Define the random seed for
      # add_edges_GMM_param and FedGD functions.
      seed = 4740
      # The minimum number of neighbors to connect with.
      num_neighbors = 1
      # Add edges.
      G_FMI_1 = add_edges_avg_temp(G_FMI, num_neighbors)
      G_FMI_2 = add_edges_GMM_param(G_FMI, seed, num_neighbors)
      G_FMI_3 = add_edges_gradient_loss(G_FMI, num_neighbors)
      # Apply the FedGD algorithm.
      G FMI 1 train error, G FMI 1 val error = FedGD(G FMI 1, seed)
      G_FMI_2_train_error, G_FMI_2_val_error = FedGD(G_FMI_2, seed)
      G_FMI_3_train_error, G_FMI_3_val_error = FedGD(G_FMI_3, seed)
      # Print the results.
      print(f"The seed is {seed}")
      print(f"The average training error for G_FMI_1: {G_FMI_1_train_error}\nThe_\times_1
       average validation error for G FMI_1: {G_FMI_1_val_error}\n")
      print(f"The average training error for G FMI 2: {G FMI 2 train error}\nThe,
       →average validation error for G_FMI_2: {G_FMI_2_val_error}\n")
      print(f"The average training error for G FMI 3: {G FMI 3 train error}\nThe,
       →average validation error for G_FMI_3: {G_FMI_3_val_error}\n\n")
```

```
The seed is 4740

The average training error for G_FMI_1: 20.68635695529578

The average validation error for G_FMI_1: 21.386552008386015

The average training error for G_FMI_2: 20.201786964135945

The average validation error for G_FMI_2: 20.892958171150042

The average training error for G_FMI_3: 20.052132233485334

The average validation error for G_FMI_3: 20.64577295712873
```

[]: