## Markov Chain

March 4, 2025

```
[15]: import numpy as np import matplotlib.pyplot as plt import networkx as nx
```

In this notebook, you'll determine the relation between mixing time and the number of nodes in a graph.

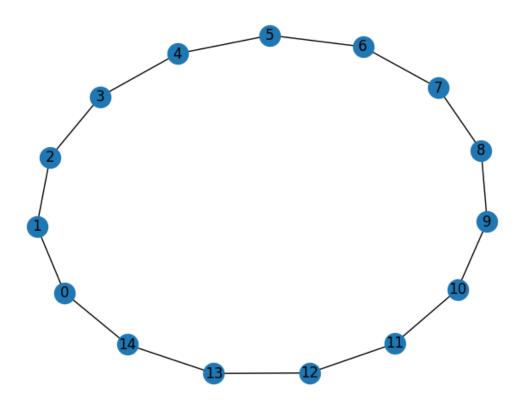
#### 0.1 networkx

The first task to get some familiarity with networkx. For all of the tasks below, use the networkx library.

- 1. Create a cycle graph with 15 vertices.
- 2. Draw the graph.
- 3. Print its number of nodes, number of edges, the adjacency matrix.
- 4. Plot the eigenvalues of the normalized Laplacian matrix in increasing order. You'll need to use todense() to convert the sparse matrix produced by networkx.normalized\_laplacian\_matrix() to a dense matrix.

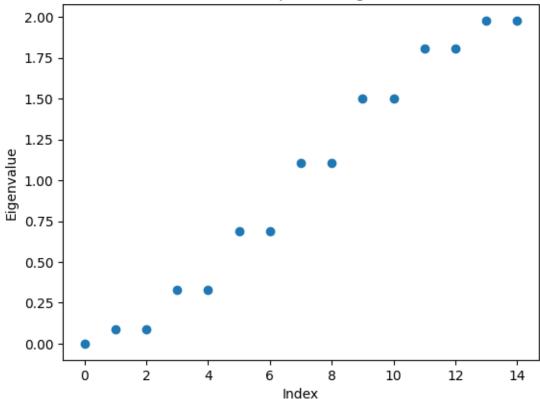
```
[16]: # Test the networkx library
    G: nx.Graph = nx.cycle_graph(15)
    nx.draw(G, with_labels=True)
    plt.title('Cycle Graph')
    plt.show()
    print("Number of nodes =", len(G.nodes))
    print("Number of edges =", len(G.edges))
    print("Adjacency matrix = \n", nx.adjacency_matrix(G).todense())
    lap_adj_matrix = nx.normalized_laplacian_matrix(G).todense()
    eigvals = sorted(np.linalg.eigvals(lap_adj_matrix))
    plt.plot(eigvals, 'o')
    plt.title('Normalized Laplacian Eigenvalues')
    plt.xlabel('Index')
    plt.ylabel('Eigenvalue')
    plt.show()
```

# Cycle Graph



```
Number of nodes = 15
Number of edges = 15
Adjacency matrix =
 [[0 1 0 0 0 0 0 0 0 0 0 0 0 1]
 [1 0 1 0 0 0 0 0 0 0 0 0 0 0 0]
 [0 1 0 1 0 0 0 0 0 0 0 0 0 0 0]
 [0 0 1 0 1 0 0 0 0 0 0 0 0 0 0]
 [0 0 0 1 0 1 0 0 0 0 0 0 0 0 0]
 [0 0 0 0 1 0 1 0 0 0 0 0 0 0 0]
 [0 0 0 0 0 1 0 1 0 0 0 0 0 0 0]
 [0 0 0 0 0 0 1 0 1 0 0 0 0 0 0]
 [0 0 0 0 0 0 0 1 0 1 0 0 0 0 0]
 [0 0 0 0 0 0 0 0 1 0 1 0 0 0 0]
 [0 0 0 0 0 0 0 0 0 1 0 1 0 0 0]
 [0 0 0 0 0 0 0 0 0 0 1 0 1 0 0]
 [0 0 0 0 0 0 0 0 0 0 0 1 0 1 0]
 [0 0 0 0 0 0 0 0 0 0 0 0 1 0 1]
 [1 0 0 0 0 0 0 0 0 0 0 0 1 0]]
```





### 0.2 GraphMC

Define the following methods for the class GraphMC. Instead of finding the mixing\_time over all possible distributions, we'll simply find the mixing time from a given initial distribution.

```
class GraphMC(nx.Graph):
    def __init__(self, graph):
        super().__init__(graph) # Initialize from an existing graph
        self.trans_matrix = nx.adjacency_matrix(self).todense() / np.sum(nx.
    adjacency_matrix(self), axis=1)

def transition_probabilities(self, start_node, end_node):
    assert start_node in self.nodes, "Start node must be in the graph"
    assert end_node in self.nodes, "End node must be in the graph"
    return self.trans_matrix[start_node, end_node]

def stationary_distribution(self):
    eigvals, eigvecs = np.linalg.eig(self.trans_matrix.T)
    idx = np.argmin(np.abs(eigvals - 1.0))
    stat_dist = np.abs(eigvecs[:, idx])
```

```
return stat_dist / np.sum(stat_dist)
  def update(self, distribution, num_steps=1):
      assert len(distribution) == len(self.nodes), "Distribution length must_
⇒match number of nodes"
      return distribution @ np.linalg.matrix power(self.trans matrix,

    um_steps)

  def total_variational_distance(self, distribution):
      assert len(distribution) == len(self.nodes), "Distribution length must_
→match number of nodes"
      stationary dist = self.stationary distribution()
      return 0.5 * np.sum(np.abs(stationary_dist - distribution))
  def mixing_time(self, starting_distribution, epsilon=0.25, max_steps=1000):
      assert len(starting distribution) == len(self.nodes), "Distribution⊔
⇒length must match number of nodes"
      steps = 0
      x = starting_distribution.copy()
      while self.total variational distance(x) > epsilon and steps <=_1
→max_steps:
          x = self.update(x)
          steps += 1
      return steps
```

#### 0.3 Test 1

Test your class on a cycle graph with 15 vertices. Start with the distribution where all the probability is concentrated on a single node.

- 1. Run the markov chain for 100 steps and compute the total variation distance between the distribution and the stationary distribution.
- 2. Plot the total variation distance as a function of the number of steps.
- 3. Mark the threshold  $\epsilon = 0.25$  on the plot.
- 4. Print the mixing time.

```
[18]: # Test 1
    G: nx.Graph = nx.cycle_graph(15)
    mc = GraphMC(G)
    eps = 0.25
    num_steps = 100

    x = np.zeros(len(G.nodes))
    x[0] = 1
    dist = [None] * (num_steps + 1)
    dist[0] = x
```

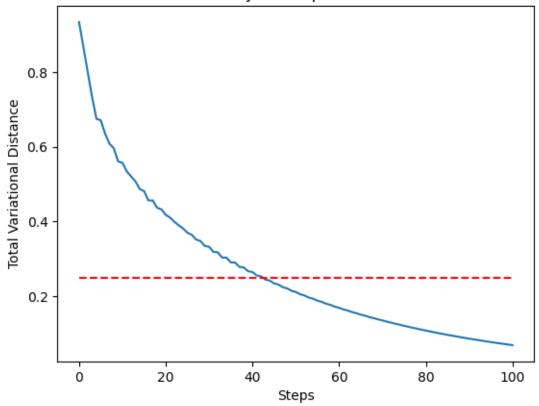
```
for i in range(0, num_steps):
    dist[i+1] = mc.update(dist[i], 1)
var_dist = [mc.total_variational_distance(d) for d in dist]

print(f"Final TVD = {var_dist[-1]:.4f}")
print("Mixing time =", mc.mixing_time(x, epsilon=eps))

plt.plot(var_dist)
plt.title('TVD in Cycle Graph of Size 15')
plt.xlabel('Steps')
plt.ylabel('Total Variational Distance')
plt.plot([eps] * len(var_dist), 'r--')
plt.show()
```

Final TVD = 0.0700 Mixing time = 43





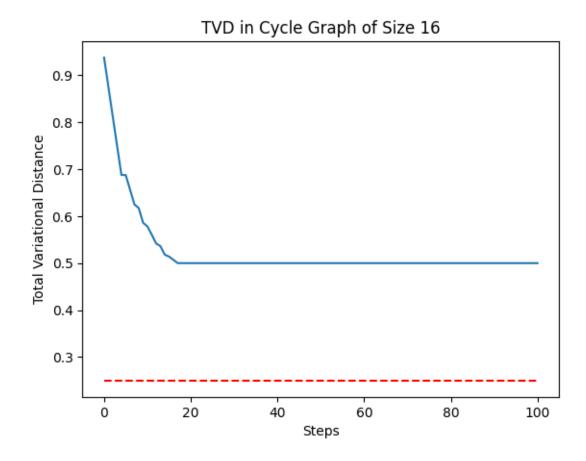
#### 0.4 Test 2

Test your class on a cycle graph with 16 vertices. Start with the distribution where all the probability is concentrated on a single node.

- 1. Run the markov chain for 100 steps and compute the total variation distance between the distribution and the stationary distribution.
- 2. Plot the total variation distance as a function of the number of steps.
- 3. Mark the threshold  $\epsilon = 0.25$  on the plot.

What do you observe? Why is this case different from the previous one?

```
[19]: # Test 2
      G: nx.Graph = nx.cycle_graph(16)
      mc = GraphMC(G)
      eps = 0.25
      num_steps = 100
      x = np.zeros(len(G.nodes))
      x[0] = 1
      dist = [None] * (num_steps + 1)
      dist[0] = x
      for i in range(0, num_steps):
          dist[i+1] = mc.update(dist[i], 1)
      var_dist = [mc.total_variational_distance(d) for d in dist]
      plt.plot(var_dist)
      plt.title('TVD in Cycle Graph of Size 16')
      plt.xlabel('Steps')
      plt.ylabel('Total Variational Distance')
      plt.plot([eps] * len(var_dist), 'r--')
      plt.show()
```



While the previous graph has a TVD that keeps decreasing to approach 0, here the TVD levels off at 0.5. Even-sized cycle graphs like this one are bipartite, meaning that any random walk will always alternate between "red-colored" and "blue-colored" nodes. As the number of steps approaches infinity, the Markov chain's probability distribution approaches an oscillation between uniform across even-indexed nodes, and uniform across odd-indexed nodes. Since these distributions have an absolute fractional error of 1 at each node and the sum of a distribution is 1, the TVD approaches 0.5.

### 0.5 Mixing time as a function of cycle length and spectral gap

Now vary the length of the cycle graph over odd numbers from 3 to 51.

- 1. Compute the mixing time for each cycle graph with the initial distribution where all the probability is concentrated on a single node.
- 2. Compute the spectral gap for each cycle graph. The spectral gap is the second smallest eigenvalue of the normalized Laplacian matrix.
- 3. Plot the mixing time vs the cycle length on a log-log scale. Find the rate of growth of the mixing time as a function of the number of nodes i.e. find  $\alpha$  in the relation  $mixing\_time = O(n^{\alpha})$ .
- 4. Plot the mixing time vs the spectral gap on a log-log scale. Find the rate of growth of the mixing time as a function of the spectral gap i.e. find  $\beta$  in the relation mixing time =

### $O(gap^{\beta})$ .

```
[20]: # Mixing time as a function of cycle length and spectral gap
      num_nodes = np.arange(3, 51, 2)
      mixing_time = np.zeros(len(num_nodes))
      spectral_gap = np.zeros(len(num_nodes))
      for i, n in enumerate(num_nodes):
          G: nx.Graph = nx.cycle_graph(n)
          mc = GraphMC(G)
          x = np.zeros(len(G.nodes))
          x[0] = 1
          mixing_time[i] = mc.mixing_time(x, epsilon=0.25)
          norm_lap = nx.normalized_laplacian_matrix(G).todense()
          eigvals = sorted(np.abs(np.linalg.eigvals(norm_lap)))
          spectral_gap[i] = eigvals[1]
      reg mixing time = np.polyfit(np.log(num_nodes), np.log(mixing_time), 1)
      reg_spectral_gap = np.polyfit(np.log(num_nodes), np.log(spectral_gap), 1)
      a, b = reg_mixing_time[0], reg_spectral_gap[0]
      print(f"Mixing time order: O(n^{a:.2f}), a = a:.2f")
      print(f"Spectral gap order: O(n^{b:.2f}), b = \{b:.2f\}")
      plt.plot(num_nodes, mixing_time)
      plt.xscale('log')
      plt.yscale('log')
      plt.title('Mixing Time vs Cycle Length')
      plt.xlabel('Cycle Length (log)')
      plt.ylabel('Mixing Time (log)')
      plt.show()
      plt.plot(num_nodes, spectral_gap)
      plt.xscale('log')
      plt.yscale('log')
     plt.title('Spectral Gap vs Cycle Length')
      plt.xlabel('Cycle Length (log)')
      plt.ylabel('Spectral Gap (log)')
     plt.show()
```

Mixing time order:  $O(n^1.97)$ , a = 1.97 Spectral gap order:  $O(n^{-1.92})$ , b = -1.92

