# Network Science Homework 2

# PageRank, Communities and Subgraph Patterns

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### Work can be located in here

It was use a LLM (Gemini 2.5 Pro Preview 05-06) for help to write the questions and answers in a correct format for the Jupyter Notebook

it was use also from Questions 1 to 5 in the creation of cements, and the copilot's suggestions were depending on them followed.

# Link Analysis and PageRank

### QUESTION 1.

Draw a graph with at least 6 nodes in which one node has a very **high value of PageRank**, although the same node has **low closeness and betweenness centrality** (don’t forget to point out the node).**

**Answer**:

Consider the following directed graph with 6 nodes:

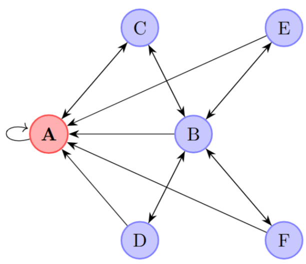



*Figure 1: Graph with Node A having high PageRank but low Closeness and Betweenness Centrality.*

The target node is **A**.

### QUESTION 2.

The **damping factor** in PageRank (parameter β, in slides) controls how of often we follow one of the links of the current node vs going to an arbitrary node on the network.

**(a) What does β = 0 mean? What would happen to the PageRank values in that case? Why?**

**Answer**:

The equation that governs if the algorithm follows the outgoing licks is

$$r_i = \sum_{i->j} \beta \frac{r_i}{d_i} + (1 - \beta) \frac{1}{n}$$

where $\beta \in [0, 1]$

In this equation the damping factor $\beta$ represents the probability of following the outgoing edges.

If $\beta = 0$ then the algorithm will always follow to a random page

**(b) What does β = 1 mean? Can you explain a possible problem with using that value?**

**Answer**:

As explain in the previous question (a) $\beta$ represents the probability of following the ou going edges, if $\beta = 1$ that means that the algorithm always follow the outgoing edges of the current page.

the problems of this implementation are:

- Dead ends : what happens if there is no more outgoing edges on the current page, if the $\beta = 1$ then the algorithm stops without traversing the entire graph.
- Spider traps : the problem of all out-link are within a group, eventually the Spider trap absorbs all importance.

## QUESTION 3.

**Implement a program** (in any programming language) for manually computing the (normalized) PageRank values of a small network using **power iterations** (the "flow" mode). Attach the program to your homework submission with a very short description on how it works.

**Answer**:

In [1]:

```
import networkx as nx
import numpy as np
import sys
import os
import random
import json
from networkx.readwrite import json_graph

parent_dir = os.path.abspath(os.path.join(os.getcwd(), '..'))
```

```
sys.path.append(parent_dir)
from homeWork1_NS.src.load_save_network import load_network_advanced, save_netwo

random.seed(42)
```

This Page Rank was created to use as input a networkx.DiGraph graph

we also create a graph to test results

In [2]:
```
def my_Page_Rank(graph: nx.DiGraph, beta=0.85, iterations=100, tolerance=1.0e-6,
    """
    Computes the PageRank values using power iterations.  (the ”flow” mode)

    Args:
        graph (nx.DiGraph): The input directed graph from NetworkX.
        beta (float): The damping factor (probability of following a link).
        iterations (int): The maximum number of iterations to perform.
        tolerance (float): The tolerance for convergence. Iteration stops if the
                           of the difference between PageRank vectors in consecu
                           iterations is less than this.
        print_iteration (bool): If True, prints the PageRank values at each iter

    Returns:
        dict: A dictionary with node IDs as keys and their normalized PageRank v

    this comment was generated by Gemini 2.5 Pro Preview 05-06
    """
    #Power iterations.  (the ”flow” mode)

    nodes = list(graph.nodes())
    N = len(nodes)

    if N == 0:
        return {}

    if beta < 0 or beta > 1:
        raise ValueError("Damping factor beta must be in the range [0, 1].")
    if iterations <= 0:
        raise ValueError("Number of iterations must be a positive integer.")
    if tolerance <= 0:
        raise ValueError("Tolerance must be a positive number.")
    if not isinstance(graph, nx.DiGraph):
        raise TypeError("Input graph must be a directed graph (nx.DiGraph).")

    # First iteration
    final_iteration = 0

    # create a page rank list pr
    pr = {node: 1.0 / N for node in nodes}


    # Ensure all nodes are added, even if isolated after edge directionality
    out_degree = dict(graph.out_degree())
    dangling_nodes = [node for node in nodes if out_degree.get(node, 0) == 0]

    if (not print_iteration) and print_check:
        print(f"Computing PageRank with {N} nodes, {len(graph.edges())} edges, a
        print(f"Total Nodes (N): {N}")
        print(f"Initial PageRank (sample): { {k: v for i, (k,v) in enumerate(pr.
```

```
        print(f"Dangling Nodes (count): {len(dangling_nodes)}")
        print(f"Damping Factor (beta): {beta}")
        print("-" * 40)

    for iteration in range(1, iterations + 1):
        new_pr = {node: 0.0 for node in nodes}
        iteration_dangling_pr_sum = 0.0

        for node in nodes:
            if node in dangling_nodes:
                # Distribute PageRank of dangling nodes evenly
                iteration_dangling_pr_sum += pr[node]
            else:
                # Calculate PageRank contribution from neighbors
                if graph.in_degree(node) > 0:
                    for neighbor in graph.successors(node):
                        new_pr[neighbor] += pr[node] / out_degree[node]
                else:
                    new_pr[node] += 0

        for node in nodes:
            dangling_contribution_to_node = iteration_dangling_pr_sum / N
            new_pr[node] = (1 - beta) / N + beta * (new_pr[node] + dangling_cont

        # Check for convergence
        diff = sum(abs(new_pr[node] - pr[node]) for node in nodes)
        pr = new_pr

        if print_iteration and print_check:
            print(f"Iteration {iteration}:")
            for node_id in sorted(pr.keys()):
                print(f"  Node {node_id}: {pr[node_id]:.8f}")
            print(f"Diff: {diff:.6e}\n")
            print("-" * 40)

        final_iteration = iteration
        if diff < tolerance:
            if print_check:
                print(f"Converged after {iteration} iterations (L1 Diff: {diff:.
            break

    # Normalize the PageRank values (final step, mostly for precision)
    total_pr = sum(pr.values())
    if total_pr > 0:
        final_pr = {node: value / total_pr for node, value in pr.items()}
    else:
        final_pr = {node: 0.0 for node in nodes} # Should not happen if N > 0

    if (not print_iteration) and print_check:
        print(f"Final PageRank (the first 3 samples): { {k: v for i, (k,v) in en
        print(f"Final PageRank Sum: {sum(final_pr.values()):.6f}")
        print("-" * 40)

    return final_pr, final_iteration
```

Creating a graph to test using watts strogatz graph and converting to a directed graph

In [3]:
```
# Generate an undirected Watts-Strogatz graph
G = nx.watts_strogatz_graph(n=30, k=4, p=0.3)
```

```
# Converting to a directed
Directed_G = nx.DiGraph()
Directed_G.add_nodes_from(G.nodes)
Directed_G.add_edges_from((u, v) if random.random() > 0.5 else (v, u) for u, v i
Directed_G.add_edges_from((a, b) if random.random() > 0.5 else (b, a) for b, a i

## start
# Ensure all nodes are added, even if isolated after edge directionality
all_original_nodes = set(G.nodes())
current_digraph_nodes = set(Directed_G.nodes())
if all_original_nodes != current_digraph_nodes:
    Directed_G.add_nodes_from(all_original_nodes - current_digraph_nodes)
## end , this code was completely generated by Gemini 2.5 Pro Preview 05-06

graph_data = json_graph.node_link_data(Directed_G)

# Save the graph using json
with open("data/directed_graph.json", "w") as file:
    json.dump(graph_data, file)

# Save the graph using my custom function for easier reading
save_network_nx(Directed_G, "data/directed_graph_nx.txt")
```

```
c:\Users\davib\AppData\Local\Programs\Python\Python312\Lib\site-packages\networkx
\readwrite\json_graph\node_link.py:142: FutureWarning:
The default value will be `edges="edges" in NetworkX 3.6.

To make this warning go away, explicitly set the edges kwarg, e.g.:

  nx.node_link_data(G, edges="links") to preserve current behavior, or
  nx.node_link_data(G, edges="edges") for forward compatibility.
  warnings.warn(
File data/directed_graph_nx.txt already exists.
```

Loading the Graph

In [4]:
```
with open("data/directed_graph.json", "r") as file:
    loaded_data = json.load(file)

Directed_G_loaded = json_graph.node_link_graph(loaded_data, directed=True)

print("Loaded Graph Nodes:", Directed_G_loaded.nodes())
print("Loaded Graph Edges:", Directed_G_loaded.edges())
```

```
Loaded Graph Nodes: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 1
7, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29]
Loaded Graph Edges: [(0, 1), (0, 2), (0, 28), (1, 3), (1, 0), (1, 26), (2, 4),
(2, 6), (3, 5), (3, 23), (3, 20), (4, 5), (4, 7), (5, 3), (5, 4), (5, 7), (5, 1
3), (6, 12), (7, 5), (7, 9), (7, 4), (8, 1), (8, 6), (8, 9), (8, 10), (9, 8), (9,
10), (9, 11), (10, 8), (10, 11), (10, 12), (11, 13), (11, 9), (11, 12), (12, 11),
(12, 13), (12, 6), (13, 5), (13, 14), (13, 16), (13, 11), (14, 13), (14, 16), (1
4, 18), (15, 13), (15, 17), (15, 25), (16, 7), (16, 14), (17, 18), (18, 14), (18,
24), (18, 29), (19, 21), (19, 20), (20, 3), (20, 16), (20, 19), (20, 22), (21, 2
3), (21, 22), (22, 21), (22, 23), (22, 24), (23, 1), (23, 2), (23, 3), (23, 17),
(23, 25), (23, 21), (23, 22), (24, 18), (24, 22), (24, 25), (24, 26), (25, 24),
(25, 27), (25, 15), (26, 1), (26, 24), (26, 25), (26, 27), (27, 14), (27, 28), (2
7, 29), (28, 0), (28, 29), (29, 0), (29, 27), (29, 28)]
```

```
c:\Users\davib\AppData\Local\Programs\Python\Python312\Lib\site-packages\networkx
\readwrite\json_graph\node_link.py:287: FutureWarning:
The default value will be changed to `edges="edges" in NetworkX 3.6.

To make this warning go away, explicitly set the edges kwarg, e.g.:

  nx.node_link_graph(data, edges="links") to preserve current behavior, or
  nx.node_link_graph(data, edges="edges") for forward compatibility.
  warnings.warn(
```

In [5]:
```python
final_pr, final_iteration = my_Page_Rank(Directed_G_loaded, beta=0.85, iteration
```

```
Computing PageRank with 30 nodes, 90 edges, and damping factor 0.85.
Total Nodes (N): 30
Initial PageRank (sample): {0: 0.03333333333333333, 1: 0.03333333333333333, 2: 0.
03333333333333333}
Dangling Nodes (count): 0
Damping Factor (beta): 0.85
----------------------------------------
Converged after 34 iterations (L1 Diff: 8.102533e-07).
Final PageRank (the first 3 samples): {0: 0.03850978495054025, 1: 0.0287701814581
89277, 2: 0.01975812477323785}
Final PageRank Sum: 1.000000
----------------------------------------
```

test our results are similar to the official implementation

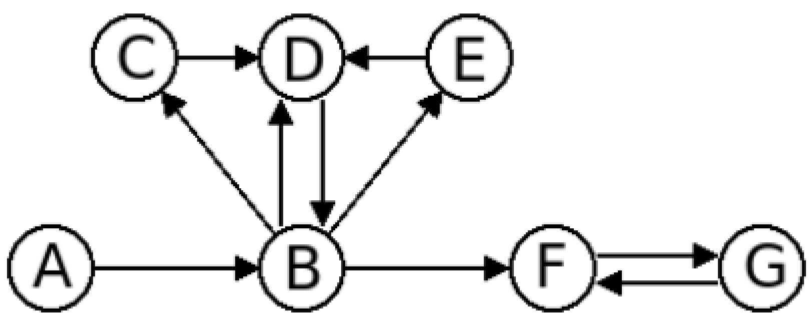
In [6]:
```python
n_compare = 5
results = nx.pagerank(Directed_G_loaded, alpha=0.85, max_iter=100, tol=1.0e-6)
for i in range(n_compare):
    print(f"Node {i}: My PageRank = {final_pr[i]:.8f}, NetworkX PageRank = {resu
```

```
Node 0: My PageRank = 0.03850978, NetworkX PageRank = 0.03851562
Node 1: My PageRank = 0.02877018, NetworkX PageRank = 0.02877240
Node 2: My PageRank = 0.01975812, NetworkX PageRank = 0.01976067
Node 3: My PageRank = 0.03375210, NetworkX PageRank = 0.03375269
Node 4: My PageRank = 0.04081663, NetworkX PageRank = 0.04081693
```

## QUESTION 4.

Use your program to **compute the PageRank values** of the following network (with β = 0.85).

**Show the values of all nodes for each iteration** until the computation converges.




**Answer**:

In [7]:
```
newG = nx.DiGraph()
newG.add_nodes_from(['A', 'B', 'C', 'D', 'E', 'F', 'G'])
newG.add_edges_from([
    ('A', 'B'),
    ('B', 'C'), ('B', 'D'), ('B', 'E'), ('B', 'F'),
    ('C', 'D'),
    ('D', 'B'),
    ('E', 'D'),
    ('F', 'G'),
    ('G', 'F'),
])
print("Nodes in newG:", newG.nodes())
print("Edges in newG:", newG.edges())
```

```
Nodes in newG: ['A', 'B', 'C', 'D', 'E', 'F', 'G']
Edges in newG: [('A', 'B'), ('B', 'C'), ('B', 'D'), ('B', 'E'), ('B', 'F'), ('C',
'D'), ('D', 'B'), ('E', 'D'), ('F', 'G'), ('G', 'F')]
```

In [8]:
```
final_page, final_iteration = my_Page_Rank(newG, beta=0.85, iterations=100, tole
```

```
Iteration 1:
  Node A: 0.02142857
  Node B: 0.14285714
  Node C: 0.05178571
  Node D: 0.29464286
  Node E: 0.05178571
  Node F: 0.17321429
  Node G: 0.14285714
Diff: 4.857143e-01

----------------------------------------
Iteration 2:
  Node A: 0.02142857
  Node B: 0.27187500
  Node C: 0.05178571
  Node D: 0.13982143
  Node E: 0.05178571
  Node F: 0.17321429
  Node G: 0.16866071
Diff: 3.096429e-01

----------------------------------------
Iteration 3:
  Node A: 0.02142857
  Node B: 0.14027679
  Node C: 0.07920201
  Node D: 0.16723772
  Node E: 0.07920201
  Node F: 0.22256362
  Node G: 0.16866071
Diff: 2.631964e-01

----------------------------------------
Iteration 4:
  Node A: 0.02142857
  Node B: 0.16358064
  Node C: 0.05123739
  Node D: 0.18588080
  Node E: 0.05123739
  Node F: 0.19459900
  Node G: 0.21060765
Diff: 1.677877e-01

----------------------------------------
Iteration 5:
  Node A: 0.02142857
  Node B: 0.17942725
  Node C: 0.05618946
  Node D: 0.14329302
  Node E: 0.05618946
  Node F: 0.23520595
  Node G: 0.18683772
Diff: 1.327154e-01

----------------------------------------
Iteration 6:
  Node A: 0.02142857
  Node B: 0.14322764
  Node C: 0.05955686
  Node D: 0.15507894
```

```
  Node E: 0.05955686
  Node F: 0.21836892
  Node G: 0.22135363
Diff: 1.060733e-01

----------------------------------------
Iteration 7:
  Node A: 0.02142857
  Node B: 0.15324567
  Node C: 0.05186444
  Node D: 0.15311111
  Node E: 0.05186444
  Node F: 0.24001503
  Node G: 0.20704216
Diff: 6.332829e-02

----------------------------------------
Iteration 8:
  Node A: 0.02142857
  Node B: 0.15157302
  Node C: 0.05399328
  Node D: 0.14216283
  Node E: 0.05399328
  Node F: 0.22997911
  Node G: 0.22544135
Diff: 4.531371e-02

----------------------------------------
Iteration 9:
  Node A: 0.02142857
  Node B: 0.14226698
  Node C: 0.05363784
  Node D: 0.14542641
  Node E: 0.05363784
  Node F: 0.24526298
  Node G: 0.21691081
Diff: 3.709490e-02

----------------------------------------
Iteration 10:
  Node A: 0.02142857
  Node B: 0.14504102
  Node C: 0.05166030
  Node D: 0.14284463
  Node E: 0.05166030
  Node F: 0.23603450
  Node G: 0.22990211
Diff: 3.153067e-02

----------------------------------------
Iteration 11:
  Node A: 0.02142857
  Node B: 0.14284650
  Node C: 0.05224979
  Node D: 0.14007230
  Node E: 0.05224979
  Node F: 0.24766658
  Node G: 0.22205789
Diff: 2.562210e-02
```

```
----------------------------------------
Iteration 12:
  Node A: 0.02142857
  Node B: 0.14049003
  Node C: 0.05178345
  Node D: 0.14060809
  Node E: 0.05178345
  Node F: 0.24053266
  Node G: 0.23194516
Diff: 2.084612e-02

----------------------------------------
Iteration 13:
  Node A: 0.02142857
  Node B: 0.14094545
  Node C: 0.05128270
  Node D: 0.13931457
  Node E: 0.05128270
  Node F: 0.24843609
  Node G: 0.22588133
Diff: 1.671770e-02

----------------------------------------
Iteration 14:
  Node A: 0.02142857
  Node B: 0.13984596
  Node C: 0.05137948
  Node D: 0.13856007
  Node E: 0.05137948
  Node F: 0.24337861
  Node G: 0.23259925
Diff: 1.382294e-02

----------------------------------------
Iteration 15:
  Node A: 0.02142857
  Node B: 0.13920463
  Node C: 0.05114584
  Node D: 0.13849095
  Node E: 0.05114584
  Node F: 0.24885520
  Node G: 0.22830039
Diff: 1.095317e-02

----------------------------------------
Iteration 16:
  Node A: 0.02142857
  Node B: 0.13914588
  Node C: 0.05100956
  Node D: 0.13795748
  Node E: 0.05100956
  Node F: 0.24506489
  Node G: 0.23295549
Diff: 9.310196e-03

----------------------------------------
Iteration 17:
  Node A: 0.02142857
  Node B: 0.13869243
  Node C: 0.05099707
```

```
  Node D: 0.13771332
  Node E: 0.05099707
  Node F: 0.24900924
  Node G: 0.22973373
Diff: 7.888696e-03

----------------------------------------
Iteration 18:
  Node A: 0.02142857
  Node B: 0.13848489
  Node C: 0.05090071
  Node D: 0.13759573
  Node E: 0.05090071
  Node F: 0.24617438
  Node G: 0.23308642
Diff: 6.705392e-03

----------------------------------------
Iteration 19:
  Node A: 0.02142857
  Node B: 0.13838495
  Node C: 0.05085661
  Node D: 0.13738782
  Node E: 0.05085661
  Node F: 0.24898007
  Node G: 0.23067680
Diff: 5.611379e-03

----------------------------------------
Iteration 20:
  Node A: 0.02142857
  Node B: 0.13820822
  Node C: 0.05083537
  Node D: 0.13729161
  Node E: 0.05083537
  Node F: 0.24691065
  Node G: 0.23306163
Diff: 4.769672e-03

----------------------------------------
Iteration 21:
  Node A: 0.02142857
  Node B: 0.13812644
  Node C: 0.05079782
  Node D: 0.13721795
  Node E: 0.05079782
  Node F: 0.24890021
  Node G: 0.23130262
Diff: 3.979113e-03

----------------------------------------
Iteration 22:
  Node A: 0.02142857
  Node B: 0.13806383
  Node C: 0.05078044
  Node D: 0.13713673
  Node E: 0.05078044
  Node F: 0.24738767
  Node G: 0.23299375
Diff: 3.382246e-03
```

```
----------------------------------------
Iteration 23:
  Node A: 0.02142857
  Node B: 0.13799479
  Node C: 0.05076714
  Node D: 0.13709388
  Node E: 0.05076714
  Node F: 0.24881182
  Node G: 0.23170809
Diff: 2.848300e-03

----------------------------------------
Iteration 24:
  Node A: 0.02142857
  Node B: 0.13795837
  Node C: 0.05075246
  Node D: 0.13705659
  Node E: 0.05075246
  Node F: 0.24770434
  Node G: 0.23291862
Diff: 2.421055e-03

----------------------------------------
Iteration 25:
  Node A: 0.02142857
  Node B: 0.13792668
  Node C: 0.05074473
  Node D: 0.13702392
  Node E: 0.05074473
  Node F: 0.24872555
  Node G: 0.23197726
Diff: 2.042418e-03

----------------------------------------
Iteration 26:
  Node A: 0.02142857
  Node B: 0.13789890
  Node C: 0.05073799
  Node D: 0.13700402
  Node E: 0.05073799
  Node F: 0.24791866
  Node G: 0.23284529
Diff: 1.736055e-03

----------------------------------------
Iteration 27:
  Node A: 0.02142857
  Node B: 0.13788199
  Node C: 0.05073209
  Node D: 0.13698667
  Node E: 0.05073209
  Node F: 0.24865058
  Node G: 0.23215944
Diff: 1.463842e-03

----------------------------------------
Iteration 28:
  Node A: 0.02142857
  Node B: 0.13786724
```

```
  Node C: 0.05072849
  Node D: 0.13697304
  Node E: 0.05072849
  Node F: 0.24806401
  Node G: 0.23278157
Diff: 1.244265e-03

----------------------------------------
Iteration 29:
  Node A: 0.02142857
  Node B: 0.13785566
  Node C: 0.05072536
  Node D: 0.13696380
  Node E: 0.05072536
  Node F: 0.24858969
  Node G: 0.23228298
Diff: 1.051357e-03

----------------------------------------
Iteration 30:
  Node A: 0.02142857
  Node B: 0.13784780
  Node C: 0.05072290
  Node D: 0.13695601
  Node E: 0.05072290
  Node F: 0.24816344
  Node G: 0.23272981
Diff: 8.936535e-04

----------------------------------------
Iteration 31:
  Node A: 0.02142857
  Node B: 0.13784118
  Node C: 0.05072123
  Node D: 0.13695016
  Node E: 0.05072123
  Node F: 0.24854157
  Node G: 0.23236749
Diff: 7.562666e-04

----------------------------------------
Iteration 32:
  Node A: 0.02142857
  Node B: 0.13783621
  Node C: 0.05071982
  Node D: 0.13694591
  Node E: 0.05071982
  Node F: 0.24823219
  Node G: 0.23268890
Diff: 6.428266e-04

----------------------------------------
Iteration 33:
  Node A: 0.02142857
  Node B: 0.13783260
  Node C: 0.05071877
  Node D: 0.13694246
  Node E: 0.05071877
  Node F: 0.24850433
  Node G: 0.23242593
```

```
Diff: 5.442879e-04

----------------------------------------
Iteration 34:
  Node A: 0.02142857
  Node B: 0.13782967
  Node C: 0.05071800
  Node D: 0.13693990
  Node E: 0.05071800
  Node F: 0.24828004
  Node G: 0.23265726
Diff: 4.626447e-04

----------------------------------------
Iteration 35:
  Node A: 0.02142857
  Node B: 0.13782749
  Node C: 0.05071738
  Node D: 0.13693797
  Node E: 0.05071738
  Node F: 0.24847604
  Node G: 0.23246661
Diff: 3.920019e-04

----------------------------------------
Iteration 36:
  Node A: 0.02142857
  Node B: 0.13782585
  Node C: 0.05071691
  Node D: 0.13693645
  Node E: 0.05071691
  Node F: 0.24831353
  Node G: 0.23263321
Diff: 3.332016e-04

----------------------------------------
Iteration 37:
  Node A: 0.02142857
  Node B: 0.13782455
  Node C: 0.05071656
  Node D: 0.13693531
  Node E: 0.05071656
  Node F: 0.24845479
  Node G: 0.23249507
Diff: 2.825254e-04

----------------------------------------
Iteration 38:
  Node A: 0.02142857
  Node B: 0.13782359
  Node C: 0.05071629
  Node D: 0.13693445
  Node E: 0.05071629
  Node F: 0.24833710
  Node G: 0.23261514
Diff: 2.401466e-04

----------------------------------------
Iteration 39:
  Node A: 0.02142857
```

```
  Node B: 0.13782285
  Node C: 0.05071608
  Node D: 0.13693378
  Node E: 0.05071608
  Node F: 0.24843896
  Node G: 0.23251511
Diff: 2.037145e-04

----------------------------------------
Iteration 40:
  Node A: 0.02142857
  Node B: 0.13782228
  Node C: 0.05071593
  Node D: 0.13693327
  Node E: 0.05071593
  Node F: 0.24835377
  Node G: 0.23260168
Diff: 1.731573e-04

----------------------------------------
Iteration 41:
  Node A: 0.02142857
  Node B: 0.13782185
  Node C: 0.05071581
  Node D: 0.13693288
  Node E: 0.05071581
  Node F: 0.24842724
  Node G: 0.23252927
Diff: 1.469408e-04

----------------------------------------
Iteration 42:
  Node A: 0.02142857
  Node B: 0.13782152
  Node C: 0.05071571
  Node D: 0.13693259
  Node E: 0.05071571
  Node F: 0.24836560
  Node G: 0.23259172
Diff: 1.248996e-04

----------------------------------------
Iteration 43:
  Node A: 0.02142857
  Node B: 0.13782127
  Node C: 0.05071564
  Node D: 0.13693236
  Node E: 0.05071564
  Node F: 0.24841861
  Node G: 0.23253933
Diff: 1.060247e-04

----------------------------------------
Iteration 44:
  Node A: 0.02142857
  Node B: 0.13782108
  Node C: 0.05071559
  Node D: 0.13693219
  Node E: 0.05071559
  Node F: 0.24837402
```

```
  Node G: 0.23258439
Diff: 9.012099e-05

----------------------------------------
Iteration 45:
  Node A: 0.02142857
  Node B: 0.13782093
  Node C: 0.05071555
  Node D: 0.13693206
  Node E: 0.05071555
  Node F: 0.24841228
  Node G: 0.23254649
Diff: 7.652152e-05

----------------------------------------
Iteration 46:
  Node A: 0.02142857
  Node B: 0.13782082
  Node C: 0.05071552
  Node D: 0.13693195
  Node E: 0.05071552
  Node F: 0.24838003
  Node G: 0.23257901
Diff: 6.504329e-05

----------------------------------------
Iteration 47:
  Node A: 0.02142857
  Node B: 0.13782073
  Node C: 0.05071550
  Node D: 0.13693188
  Node E: 0.05071550
  Node F: 0.24840765
  Node G: 0.23255160
Diff: 5.523908e-05

----------------------------------------
Iteration 48:
  Node A: 0.02142857
  Node B: 0.13782067
  Node C: 0.05071548
  Node D: 0.13693182
  Node E: 0.05071548
  Node F: 0.24838434
  Node G: 0.23257508
Diff: 4.695322e-05

----------------------------------------
Iteration 49:
  Node A: 0.02142857
  Node B: 0.13782062
  Node C: 0.05071546
  Node D: 0.13693177
  Node E: 0.05071546
  Node F: 0.24840428
  Node G: 0.23255526
Diff: 3.988245e-05

----------------------------------------
Iteration 50:
```

```
  Node A: 0.02142857
  Node B: 0.13782058
  Node C: 0.05071545
  Node D: 0.13693174
  Node E: 0.05071545
  Node F: 0.24838742
  Node G: 0.23257221
Diff: 3.390008e-05

----------------------------------------
Iteration 51:
  Node A: 0.02142857
  Node B: 0.13782055
  Node C: 0.05071544
  Node D: 0.13693171
  Node E: 0.05071544
  Node F: 0.24840182
  Node G: 0.23255788
Diff: 2.879892e-05

----------------------------------------
Iteration 52:
  Node A: 0.02142857
  Node B: 0.13782053
  Node C: 0.05071544
  Node D: 0.13693169
  Node E: 0.05071544
  Node F: 0.24838964
  Node G: 0.23257012
Diff: 2.447908e-05

----------------------------------------
Iteration 53:
  Node A: 0.02142857
  Node B: 0.13782051
  Node C: 0.05071543
  Node D: 0.13693168
  Node E: 0.05071543
  Node F: 0.24840004
  Node G: 0.23255976
Diff: 2.079780e-05

----------------------------------------
Iteration 54:
  Node A: 0.02142857
  Node B: 0.13782050
  Node C: 0.05071543
  Node D: 0.13693167
  Node E: 0.05071543
  Node F: 0.24839123
  Node G: 0.23256860
Diff: 1.767813e-05

----------------------------------------
Iteration 55:
  Node A: 0.02142857
  Node B: 0.13782049
  Node C: 0.05071543
  Node D: 0.13693166
  Node E: 0.05071543
```

```
  Node F: 0.24839874
  Node G: 0.23256112
Diff: 1.502091e-05

----------------------------------------
Iteration 56:
  Node A: 0.02142857
  Node B: 0.13782048
  Node C: 0.05071543
  Node D: 0.13693165
  Node E: 0.05071543
  Node F: 0.24839237
  Node G: 0.23256750
Diff: 1.276777e-05

----------------------------------------
Iteration 57:
  Node A: 0.02142857
  Node B: 0.13782048
  Node C: 0.05071542
  Node D: 0.13693165
  Node E: 0.05071542
  Node F: 0.24839780
  Node G: 0.23256209
Diff: 1.084941e-05

----------------------------------------
Iteration 58:
  Node A: 0.02142857
  Node B: 0.13782047
  Node C: 0.05071542
  Node D: 0.13693164
  Node E: 0.05071542
  Node F: 0.24839320
  Node G: 0.23256670
Diff: 9.221995e-06

----------------------------------------
Iteration 59:
  Node A: 0.02142857
  Node B: 0.13782047
  Node C: 0.05071542
  Node D: 0.13693164
  Node E: 0.05071542
  Node F: 0.24839712
  Node G: 0.23256279
Diff: 7.836830e-06

----------------------------------------
Iteration 60:
  Node A: 0.02142857
  Node B: 0.13782047
  Node C: 0.05071542
  Node D: 0.13693164
  Node E: 0.05071542
  Node F: 0.24839379
  Node G: 0.23256612
Diff: 6.661305e-06

----------------------------------------
```

```
Iteration 61:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693164
  Node E: 0.05071542
  Node F: 0.24839662
  Node G: 0.23256329
Diff: 5.661021e-06

----------------------------------------
Iteration 62:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839422
  Node G: 0.23256570
Diff: 4.811868e-06

----------------------------------------
Iteration 63:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839627
  Node G: 0.23256366
Diff: 4.089454e-06

----------------------------------------
Iteration 64:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839453
  Node G: 0.23256540
Diff: 3.476036e-06

----------------------------------------
Iteration 65:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839601
  Node G: 0.23256392
Diff: 2.954261e-06

----------------------------------------
Iteration 66:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
```

```
  Node E: 0.05071542
  Node F: 0.24839475
  Node G: 0.23256518
Diff: 2.511122e-06

----------------------------------------
Iteration 67:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839582
  Node G: 0.23256411
Diff: 2.134238e-06

----------------------------------------
Iteration 68:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839491
  Node G: 0.23256502
Diff: 1.814102e-06

----------------------------------------
Iteration 69:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839568
  Node G: 0.23256425
Diff: 1.541862e-06

----------------------------------------
Iteration 70:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839503
  Node G: 0.23256490
Diff: 1.310582e-06

----------------------------------------
Iteration 71:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839559
  Node G: 0.23256435
Diff: 1.113922e-06
```

```
----------------------------------------
Iteration 72:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839511
  Node G: 0.23256482
Diff: 9.468336e-07

----------------------------------------
Iteration 73:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839552
  Node G: 0.23256442
Diff: 8.047659e-07

----------------------------------------
Iteration 74:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839517
  Node G: 0.23256476
Diff: 6.840510e-07

----------------------------------------
Iteration 75:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839546
  Node G: 0.23256447
Diff: 5.814185e-07

----------------------------------------
Iteration 76:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839522
  Node G: 0.23256472
Diff: 4.942057e-07

----------------------------------------
Iteration 77:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
```

```
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839543
  Node G: 0.23256451
Diff: 4.200604e-07

----------------------------------------
Iteration 78:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839525
  Node G: 0.23256468
Diff: 3.570513e-07

----------------------------------------
Iteration 79:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839540
  Node G: 0.23256453
Diff: 3.034852e-07

----------------------------------------
Iteration 80:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839527
  Node G: 0.23256466
Diff: 2.579624e-07

----------------------------------------
Iteration 81:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839538
  Node G: 0.23256455
Diff: 2.192631e-07

----------------------------------------
Iteration 82:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839529
  Node G: 0.23256465
Diff: 1.863737e-07
```

```
----------------------------------------
Iteration 83:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839537
  Node G: 0.23256457
Diff: 1.584147e-07

----------------------------------------
Iteration 84:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839530
  Node G: 0.23256463
Diff: 1.346525e-07

----------------------------------------
Iteration 85:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839536
  Node G: 0.23256458
Diff: 1.144530e-07

----------------------------------------
Iteration 86:
  Node A: 0.02142857
  Node B: 0.13782046
  Node C: 0.05071542
  Node D: 0.13693163
  Node E: 0.05071542
  Node F: 0.24839531
  Node G: 0.23256462
Diff: 9.728503e-08

----------------------------------------
Converged after 86 iterations (L1 Diff: 9.728503e-08).
```

## QUESTION 5.

Use the program to do computations varying the β parameter from 0.0 to 1.0 in steps of 0.05 and:

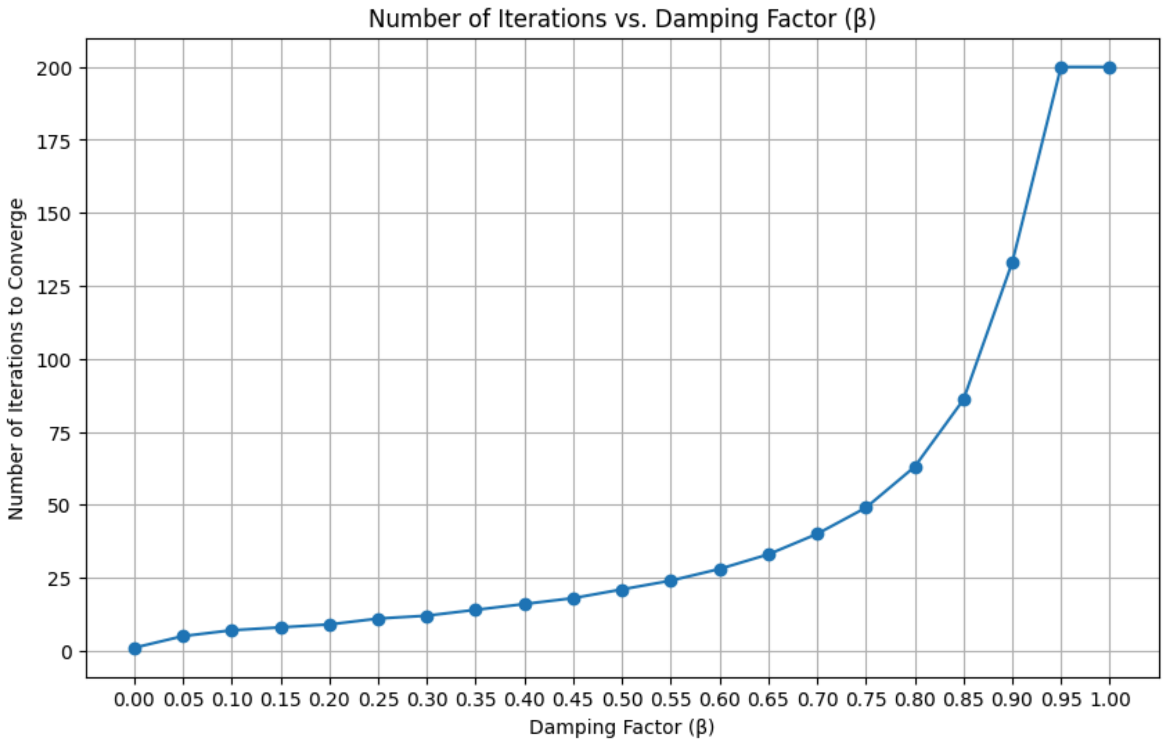
In [9]:
```
import matplotlib.pyplot as plt
beta_values = np.arange(0.0, 1.05, 0.05) # from 0.0 to 1.0 inclusive, step 0.05
```

- **(a)** Show in a plot the **number of iterations needed until convergence is reached as you change** β. Can you explain what is happening?

**Answer**:

In [10]:
```
iteration_counts = []

for values in beta_values:
    # We don't need verbose output for each iteration here, just the count
    _, final_iteration = my_Page_Rank(newG, beta=values, iterations=200, toleran
    iteration_counts.append(final_iteration)
    print(f"Beta = {values:.2f} took {final_iteration} iterations.")

# Plotting
plt.figure(figsize=(10, 6))
plt.plot(beta_values, iteration_counts, marker='o', linestyle='-')
plt.title('Number of Iterations vs. Damping Factor (β)')
plt.xlabel('Damping Factor (β)')
plt.ylabel('Number of Iterations to Converge')
plt.xticks(beta_values)
plt.grid(True)
plt.show()
```

```
Beta = 0.00 took 1 iterations.
Beta = 0.05 took 5 iterations.
Beta = 0.10 took 7 iterations.
Beta = 0.15 took 8 iterations.
Beta = 0.20 took 9 iterations.
Beta = 0.25 took 11 iterations.
Beta = 0.30 took 12 iterations.
Beta = 0.35 took 14 iterations.
Beta = 0.40 took 16 iterations.
Beta = 0.45 took 18 iterations.
Beta = 0.50 took 21 iterations.
Beta = 0.55 took 24 iterations.
Beta = 0.60 took 28 iterations.
Beta = 0.65 took 33 iterations.
Beta = 0.70 took 40 iterations.
Beta = 0.75 took 49 iterations.
Beta = 0.80 took 63 iterations.
Beta = 0.85 took 86 iterations.
Beta = 0.90 took 133 iterations.
Beta = 0.95 took 200 iterations.
Beta = 1.00 took 200 iterations.
```




- When β is low (close to 0.0), the random jump component dominates
- When β is high (close to 1.0), the algorithm relies more heavily on the link structure
- β close to 1.0 can be problematic. If there are dangling nodes (pages with no out-links), PageRank "leaks" out of the system unless handled. If there are spider traps, they can absorb all the PageRank. The `my_Page_Rank` function handles dangling nodes by redistributing their PageRank, which mitigates complete leakage for β=1,
- `my_Page_Rank` doesn't accept 0 or 1

Conclusion:

Since there are spider traps and dangling nodes in the graph ex F and G we can state that the less the random jump component of the equation is prevalent the more interactions are needed to converge

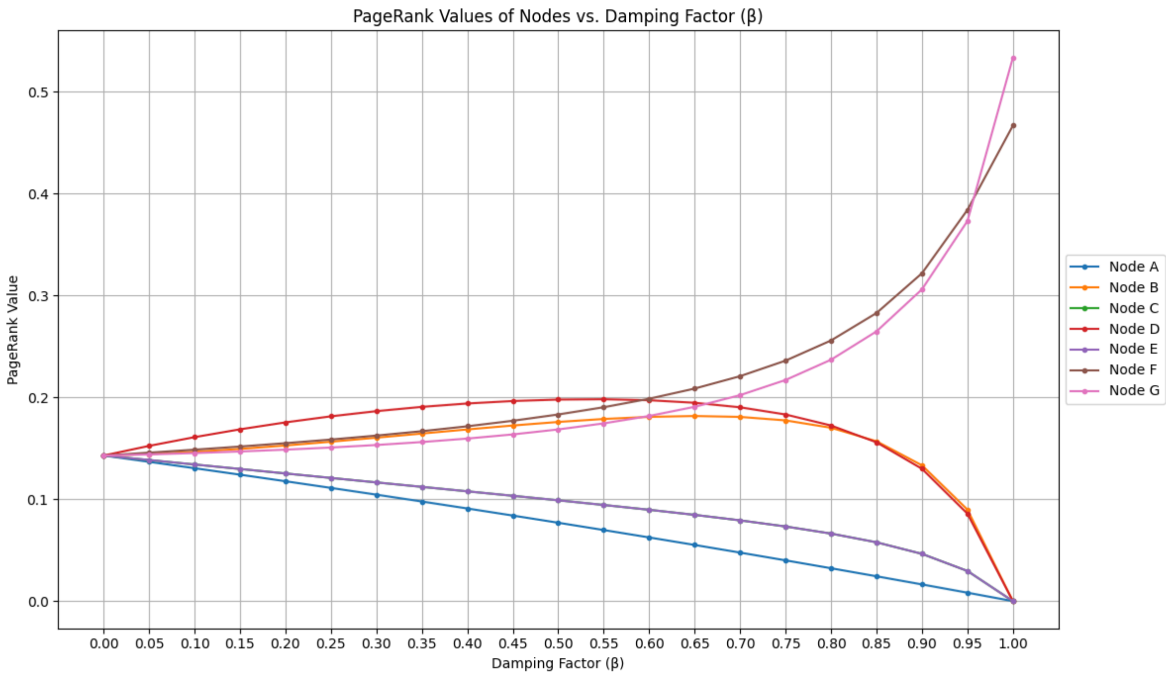
- **(b)** Show in a plot the different **PageRank values of all nodes as your change** β. Can you divide the nodes into different curve behaviors? Can you explain what is happening?

**Answer**:

In [11]:
```
pageRank_results = {node: [] for node in newG.nodes()}

for values in beta_values:
    pr_dict, _ = my_Page_Rank(newG, beta=values, iterations=200, tolerance=1.0e-
    for node in newG.nodes():
        pageRank_results[node].append(pr_dict.get(node, 0.0))
    print(f"PageRanks for beta = {values:.2f} (sample A, B, C, D, E, F, G): A={p

# Plotting
```

```
plt.figure(figsize=(12, 7))
for node_id in sorted(pageRank_results.keys()): # sorted for consistent legend o
    plt.plot(beta_values, pageRank_results[node_id], marker='.', linestyle='-',

plt.title('PageRank Values of Nodes vs. Damping Factor (β)')
plt.xlabel('Damping Factor (β)')
plt.ylabel('PageRank Value')
plt.xticks(beta_values)
plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
plt.grid(True)
plt.tight_layout()
plt.show()
```

```
PageRanks for beta = 0.00 (sample A, B, C, D, E, F, G): A=0.143, B=0.143, C=0.14
3, D=0.143, E=0.143, F=0.143, G=0.143
PageRanks for beta = 0.05 (sample A, B, C, D, E, F, G): A=0.137, B=0.144, C=0.13
8, D=0.152, E=0.138, F=0.146, G=0.144
PageRanks for beta = 0.10 (sample A, B, C, D, E, F, G): A=0.130, B=0.147, C=0.13
4, D=0.161, E=0.134, F=0.149, G=0.145
PageRanks for beta = 0.15 (sample A, B, C, D, E, F, G): A=0.124, B=0.149, C=0.13
0, D=0.169, E=0.130, F=0.152, G=0.147
PageRanks for beta = 0.20 (sample A, B, C, D, E, F, G): A=0.118, B=0.153, C=0.12
5, D=0.175, E=0.125, F=0.155, G=0.149
PageRanks for beta = 0.25 (sample A, B, C, D, E, F, G): A=0.111, B=0.156, C=0.12
1, D=0.181, E=0.121, F=0.159, G=0.151
PageRanks for beta = 0.30 (sample A, B, C, D, E, F, G): A=0.104, B=0.160, C=0.11
7, D=0.186, E=0.117, F=0.162, G=0.153
PageRanks for beta = 0.35 (sample A, B, C, D, E, F, G): A=0.098, B=0.164, C=0.11
2, D=0.191, E=0.112, F=0.167, G=0.156
PageRanks for beta = 0.40 (sample A, B, C, D, E, F, G): A=0.091, B=0.168, C=0.10
8, D=0.194, E=0.108, F=0.172, G=0.160
PageRanks for beta = 0.45 (sample A, B, C, D, E, F, G): A=0.084, B=0.172, C=0.10
3, D=0.196, E=0.103, F=0.177, G=0.164
PageRanks for beta = 0.50 (sample A, B, C, D, E, F, G): A=0.077, B=0.176, C=0.09
9, D=0.198, E=0.099, F=0.183, G=0.168
PageRanks for beta = 0.55 (sample A, B, C, D, E, F, G): A=0.070, B=0.179, C=0.09
4, D=0.198, E=0.094, F=0.190, G=0.174
PageRanks for beta = 0.60 (sample A, B, C, D, E, F, G): A=0.062, B=0.181, C=0.09
0, D=0.197, E=0.090, F=0.199, G=0.182
PageRanks for beta = 0.65 (sample A, B, C, D, E, F, G): A=0.055, B=0.182, C=0.08
5, D=0.195, E=0.085, F=0.209, G=0.191
PageRanks for beta = 0.70 (sample A, B, C, D, E, F, G): A=0.048, B=0.181, C=0.07
9, D=0.190, E=0.079, F=0.221, G=0.202
PageRanks for beta = 0.75 (sample A, B, C, D, E, F, G): A=0.040, B=0.177, C=0.07
3, D=0.183, E=0.073, F=0.236, G=0.217
PageRanks for beta = 0.80 (sample A, B, C, D, E, F, G): A=0.032, B=0.170, C=0.06
6, D=0.172, E=0.066, F=0.256, G=0.237
PageRanks for beta = 0.85 (sample A, B, C, D, E, F, G): A=0.024, B=0.157, C=0.05
8, D=0.156, E=0.058, F=0.283, G=0.265
PageRanks for beta = 0.90 (sample A, B, C, D, E, F, G): A=0.016, B=0.133, C=0.04
6, D=0.130, E=0.046, F=0.322, G=0.306
PageRanks for beta = 0.95 (sample A, B, C, D, E, F, G): A=0.008, B=0.090, C=0.03
0, D=0.086, E=0.030, F=0.384, G=0.373
PageRanks for beta = 1.00 (sample A, B, C, D, E, F, G): A=0.000, B=0.000, C=0.00
0, D=0.000, E=0.000, F=0.467, G=0.533
```




- **When β = 0.0:** All nodes have (or are very close to) the same PageRank value, equal to 1/N (where N is the number of nodes). This is because the random surfer always teleports to a random page, ignoring the link structure.
- **As β increases towards 1.0:** The link structure becomes more prevalent in the Page Rank calculation.
  - Nodes that are "important" according to the link structure ( many incoming links from other important pages, or part of a structure that accumulates rank) will see their PageRank values increase.
  - Nodes that are less "important" ( few incoming links, or primarily link out to non-reciprocating structures) will see their PageRank values decrease relative to the more important nodes.

In this graph we can also observe the absorption of "importance" by spider trap (F,G),forcing the other nodes to have a lower page rank the more "importance" the spider trap has.

# Community Discovery

### QUESTION 6

For this exercise you will be asked to analyze a set of undirected networks depicting the **”social networks”** (character co-occurrences in a scene) of **movies**.

You should download the following zip file: movies.zip. It contains:

- Nodes and edges (csv format) for 773 different movies from 1915 to 2012
- a movies.csv file with meta data, indicating which movie name, IMDB id, release year, number of nodes and edges
- A readme file describing the original source of the dataset

Start by opening the files on a text editor to see how they internally look like.

In [12]:
```
from networkx.algorithms.community.quality import modularity
import networkx as nx
from task6.src import utils, modularity_utils
import pandas as pd
```

In [13]:
```
%load_ext autoreload
%autoreload 2
```

- **QUESTION (a)**

Select any six networks of the dataset and using Gephi, networkx or any other platform/library, you should run **Louvain Algorithm** to find the best possible communities and **create a table showing**: id of the dataset, name of the movie, number of nodes and edges, number of communities found and modularity for those communities. Give a brief comment on which networks seem to present **community structure**, and why.

**Answer**:

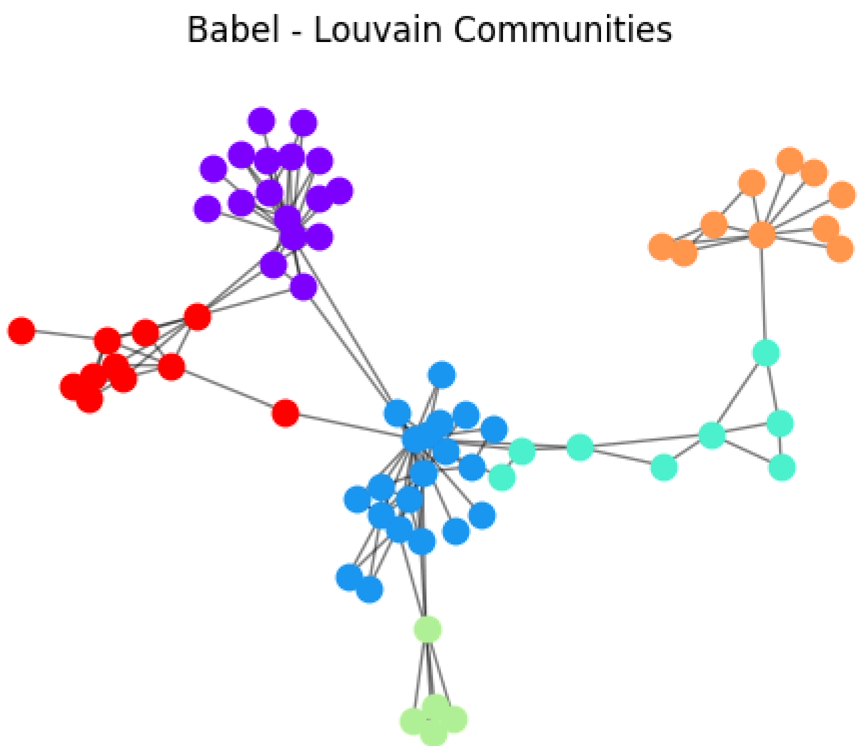
In [14]:
```
movies_data = pd.read_csv("./task6/movies/movies/movies.csv")

table_data = []
table_columns = ['ID', 'Movie Title', 'Nodes', 'Edges', 'Communities', 'Modulari

# Create a DataFrame to store the results
for index, row in movies_data.iterrows():

    id = row['ID']
    # print(f"Processing {id}...")
    name = row['Title']
    num_nodes = row['Characters'] # This is the number of nodes
    num_edges = row['Edges']
    nodes_df, edges_df = utils.get_network_dataframe(id)

    # print(f'nodes columns: {nodes_df.columns}')
    # print(f'edges columns: {edges_df.columns}')
    G = utils.create_graph_from_dataframes(nodes_df, edges_df)
    communities, community_data = utils.compute_louvain_communities(G, edges_df)
    # print(f"Number of communities: {community_data['n_communities']}")
    # print(f"Modularity: {community_data['modularity_score']:.4f}")

    num_communities = community_data['n_communities']
    modularity_score = community_data['modularity_score']
    # Create a new row with the data
    row = (id, name, num_nodes, num_edges, num_communities, modularity_score)
    table_data.append(row)
    # print(row)

# Create a DataFrame from the list of rows
table_df = pd.DataFrame(table_data, columns=table_columns)

table_df.sort_values(by='Modularity', ascending=False, inplace=True)
```

```
top_6 = table_df.head(6)
top_6
```

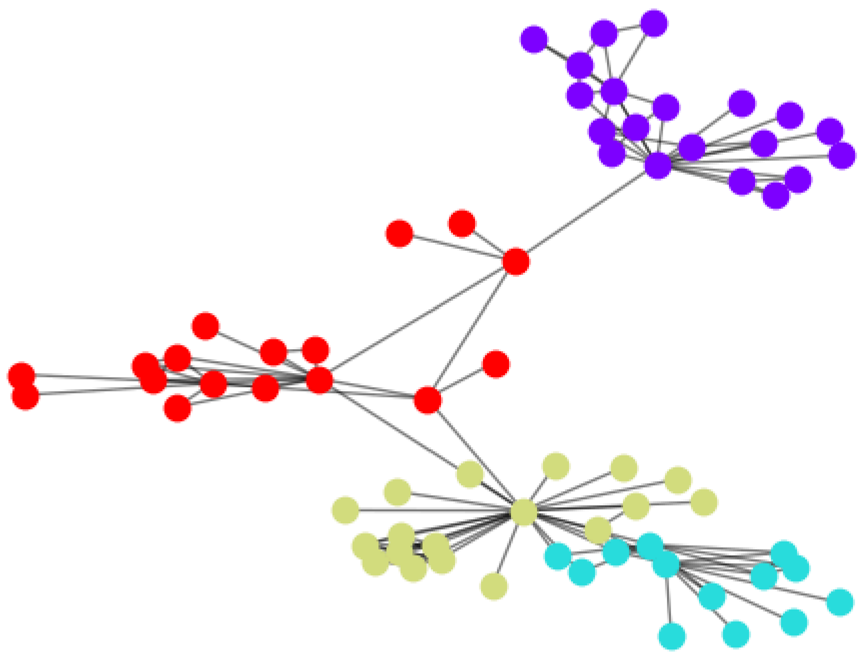
Out[14]:

| | ID | Movie Title | Nodes | Edges | Communities | Modularity |
|---|---|---|---|---|---|---|
| **74** | 92 | Babel | 71 | 154 | 6 | 0.690504 |
| **711** | 837 | Traffic | 68 | 131 | 4 | 0.668580 |
| **447** | 523 | Magnolia | 82 | 239 | 8 | 0.662979 |
| **342** | 402 | Highlander | 59 | 108 | 5 | 0.606953 |
| **328** | 386 | He's Just Not That Into You | 51 | 114 | 4 | 0.603339 |
| **88** | 110 | Batman Returns | 51 | 124 | 6 | 0.579572 |

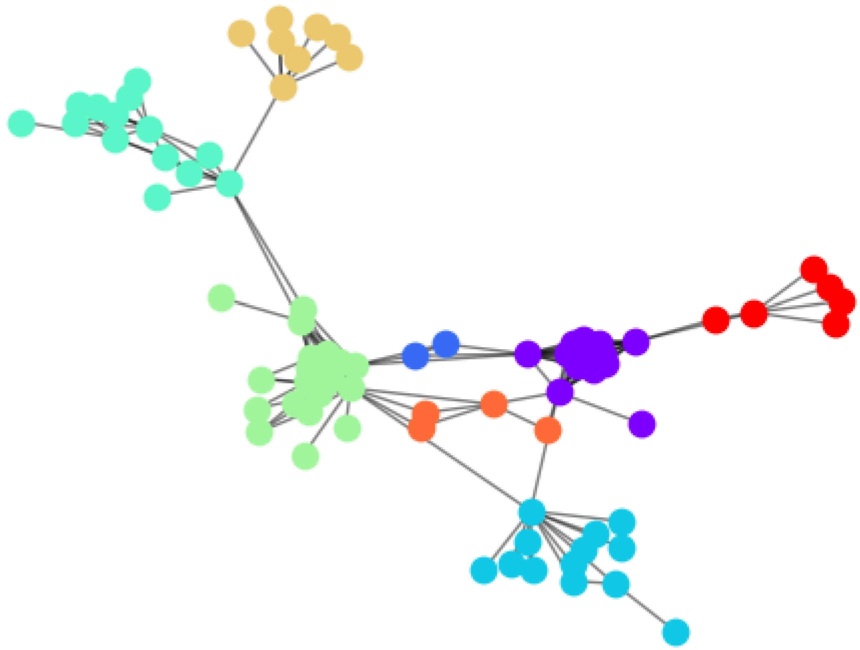
In [15]:
```
for index, row in top_6.iterrows():
    id = row['ID']
    # print(f"Processing {id}...")
    name = row['Movie Title']
    num_nodes = row['Nodes']
    num_edges = row['Edges']
    nodes_df, edges_df = utils.get_network_dataframe(id)

    # print(f'nodes columns: {nodes_df.columns}')
    # print(f'edges columns: {edges_df.columns}')
    G = utils.create_graph_from_dataframes(nodes_df, edges_df)
    communities, community_data = utils.compute_louvain_communities(G, edges_df)
    # print(f"Number of communities: {community_data['n_communities']}")
    # print(f"Modularity: {community_data['modularity_score']:.4f}")
    utils.visualize_communities(G, communities, name)
```



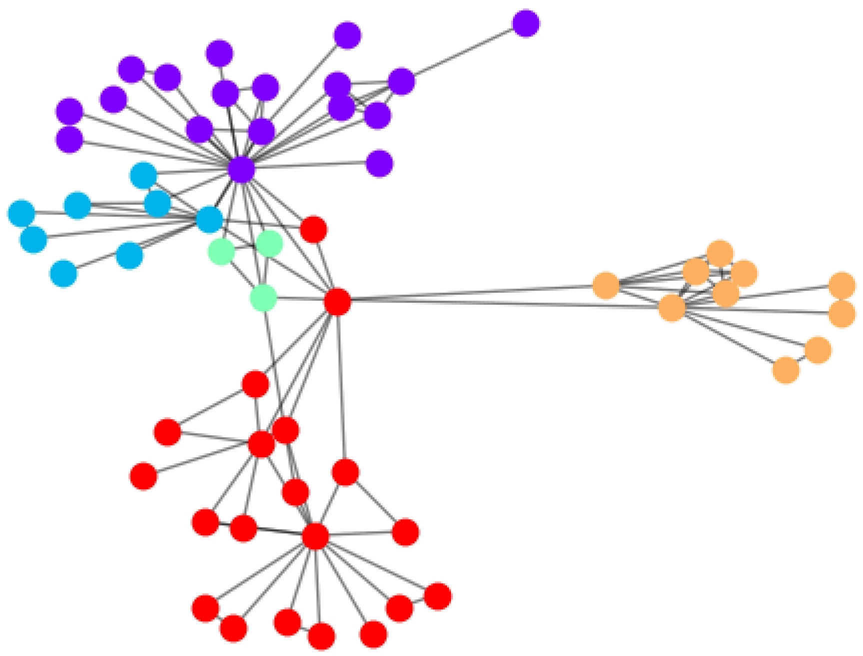
Traffic - Louvain Communities



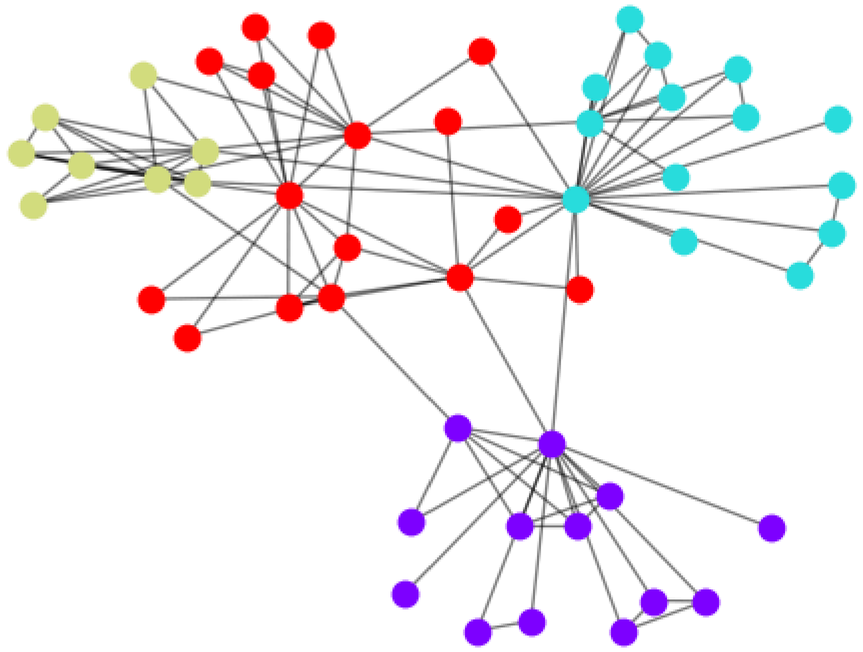
Magnolia - Louvain Communities

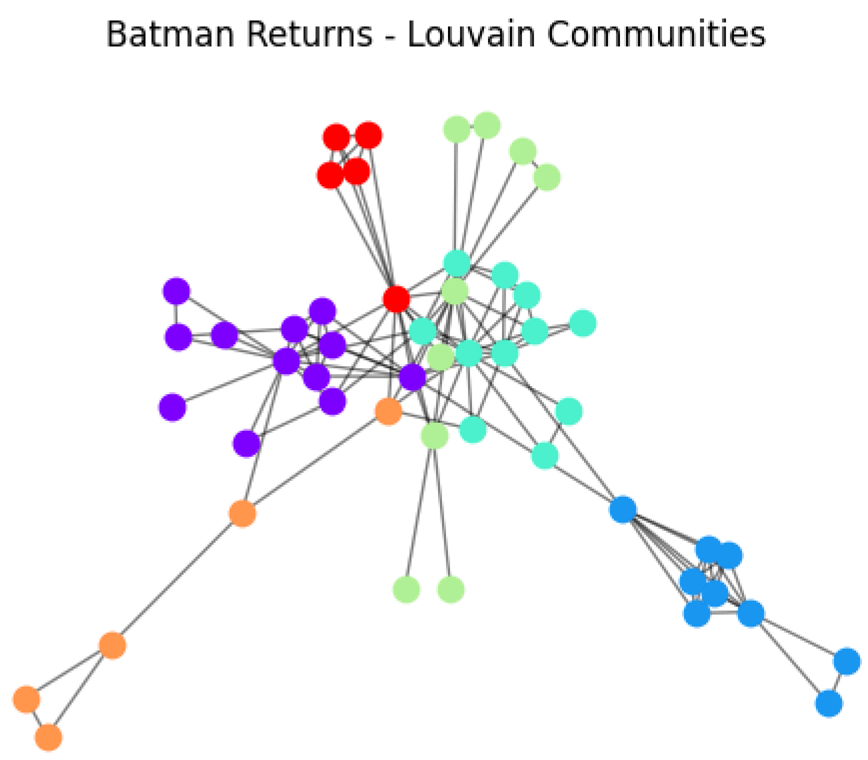


## Highlander - Louvain Communities



## He's Just Not That Into You - Louvain Communities






**R:** We approached the problem by applying the Louvain Algorithm to all the networks and sorting them by descending modularity. The top 6 modularity scores are for "Babel", "Traffic", "Magnolia", "Highlander", "He's Just Not That Into You" and "Batman Returns" ordered by higher modularity to lower. When analyzing the networks we can see community structure mainly for the 3 networks, since the nodes are clearly well connected and separated from the other clusters exposing the community structures. For the last 3 as the modularity decreases, harder is to notice the community structures. In these last cases we have more separated nodes without clear clustering or aggregation in general. In some cases there are clusters or defined communities but not at entire network level.

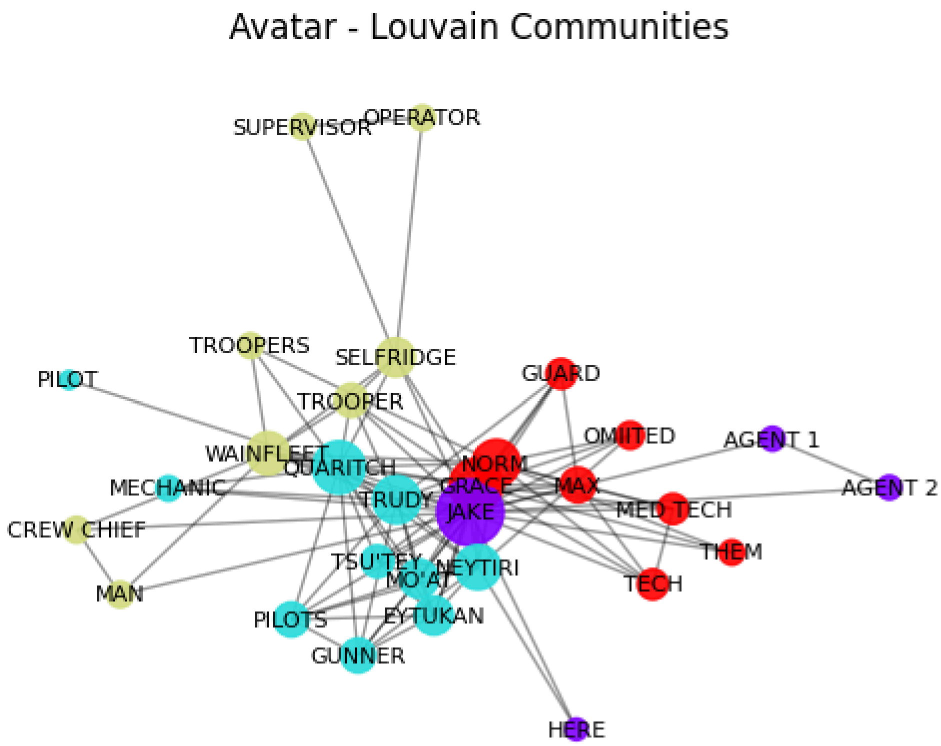
- **QUESTION (b)**

Choose **any two of the movies** (that are not different chapters of the same universe) and produce **visualizations for the networks**, labeling the nodes with their character names, using colors to represent communities and the size of the nodes to represent PageRank values. Try to make the picture as **aesthetically pleasing** as possible, reinforcing the community structure (and explain how you created the layout). Give a brief **informal description on the meaning of the communities** in the context of the movie (are they what you were expecting? are they meaningful? choose movies that you are familiar with and that you believe should have community structure).

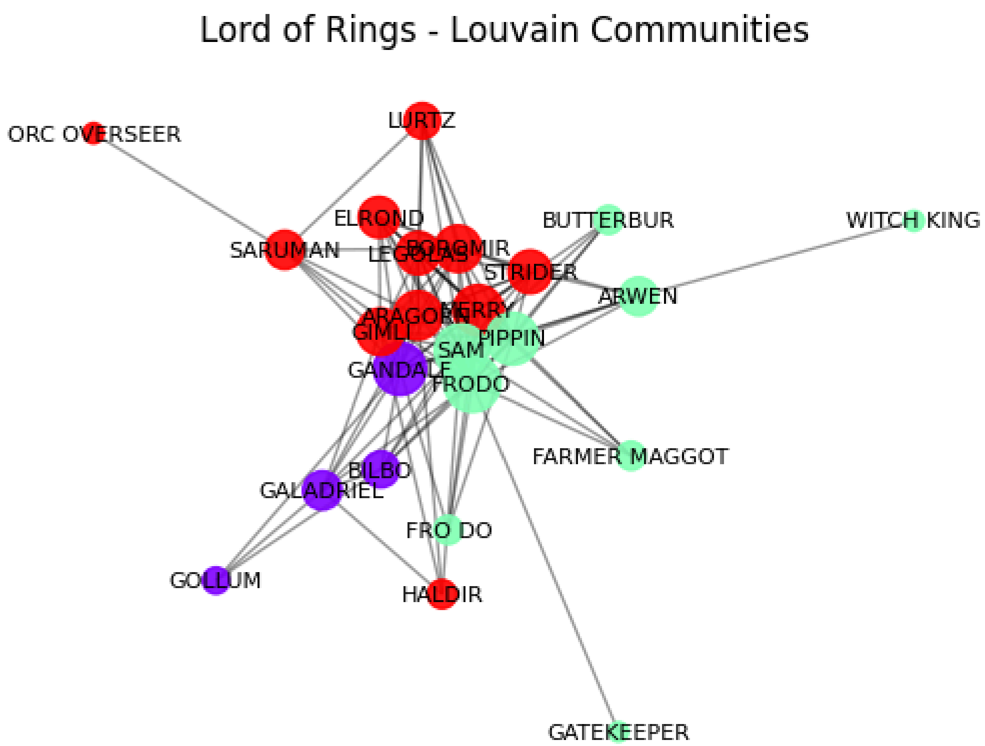
**Answer**:

In [16]:
```
nodes_df, edges_df = utils.get_network_dataframe(88)
G = utils.create_graph_from_dataframes(nodes_df, edges_df)
communities, _ = utils.compute_louvain_communities(G, edges_df)
pagerank_scores = utils.compute_pagerank(G, edges_df)
```

```
labels = {node: G.nodes[node].get('label') for node in G.nodes()}
# print(labels)
utils.visualize_communities_pgrank(G, communities, title="Avatar", pagerank_scor
```




In [17]:
```
nodes_df, edges_df = utils.get_network_dataframe(512)
G = utils.create_graph_from_dataframes(nodes_df, edges_df)
communities, _ = utils.compute_louvain_communities(G, edges_df)
pagerank_scores = utils.compute_pagerank(G, edges_df)
labels = {node: G.nodes[node].get('label') for node in G.nodes()}
# print(labels)
utils.visualize_communities_pgrank(G, communities, title="Lord of Rings", pagera
```




**R:** For this task the network was constructed using the node labels, the pagerank value obtained by NetworkX.pagerank function, the colors for the nodes were determined using community ids generated by the Louvain Algorithm. We selected the films Avatar (88) - node degree 0.27 - and The Lord of Rings (512) - node degree 0.11.

For Avatar we can notice some understandable community aggregations in terms of colors, but they are not well separated. For example we have the scientists (Grace, Norm, Max...) aggregated in the same community. Jake is the central point of the history and have high betweenes in the network. He is classified in a separated community and makes sense because of his dynamic role in the history construction. The Na'vi characters (Tsu'Tey, Neytiri, Mo'At..) a are also aggregated in the same community. We don't have for any of these communities a clear community structure.

For Lord of the Rings network we also don't findclear community structure defined. However, in the communities we can notice the representation aggregations that are reflected in the film history. The hobbities are classified in the same community (Sam, Pippin, Frodo). They are closelly linked to Gandlaf, which belongs to same community of Galladriel. In other hand there is a aggregation of knights (Gimli, Aragorn, Legolas, Boromir) but having in the same community the Saruman. This community reflects some ambiguity and not clear definition.

- **QUESTION (c)**

**Implement a program** (in any programming language) for manually computing the (normalized) **modularity of a network when given a partition**. Test it on one movie of your choice and the on the partitions you produced on the previous questions (and report if the value seems ok). Attach the program to your homework submission with a very short description on how it works and how I could run it.

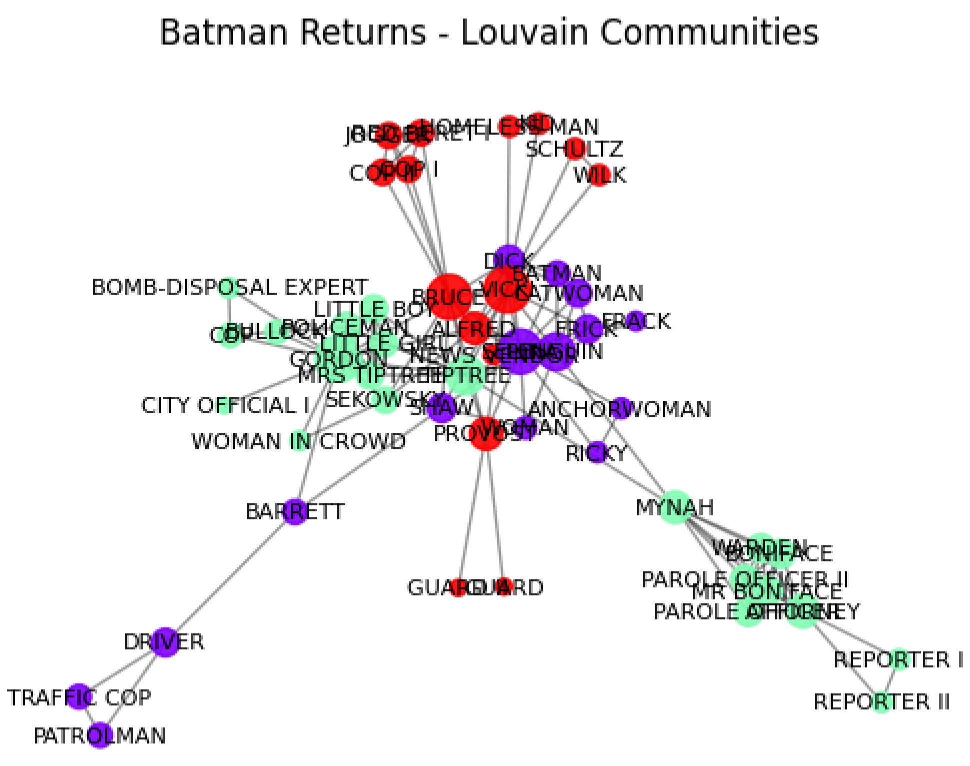
The modularity can be computed as:

$$Modularity = \frac{1}{2m}\left(\sum_{i,j \in V}\left(A_{ij} - \frac{K_i K_j}{2m}\right)\delta\left(C_i, C_j\right)\right)$$

Where A is the adjacency matrix of the graph, Ci is the community to which node i belongs, ki is the degree of node i, m is the total number of edges and V is the set of nodes.

**Answer**:

In [18]:
```
nodes_df, edges_df = utils.get_network_dataframe(110)
G = utils.create_graph_from_dataframes(nodes_df, edges_df)
comm_2, progress_scores = modularity_utils.greedy_agglomerative(G)
pagerank_scores = utils.compute_pagerank(G, edges_df)
labels = {node: G.nodes[node].get('label') for node in G.nodes()}
# print(labels)
utils.visualize_communities_pgrank(G, comm_2, title="Batman Returns", pagerank_s
modularity_local_implementation = sum(modularity_utils.get_intra_community_modul
print(f"Modularity (local implementation): {modularity_local_implementation:.4f}
# Example usage of the networkx modularity function
communities, community_data = utils.compute_louvain_communities(G, edges_df)
modularity_score = modularity(G, communities)
print(f"Modularity (networkx): {modularity_score:.4f}")
```




```
Modularity (local implementation): 0.4822
Modularity (networkx): 0.4749
```

**R:** We found similar results for modularity but not the same values. At the end it impacted also in the communities composition. In this example we had 0.48 as modularity result whereas the NetworkX implementation found 0.57. To execute the program it is needed to:

1. execute the ./task6/src/main.py using the "python main.py" command. The program will ask inputs and output the modularity results of self implemented algorithm

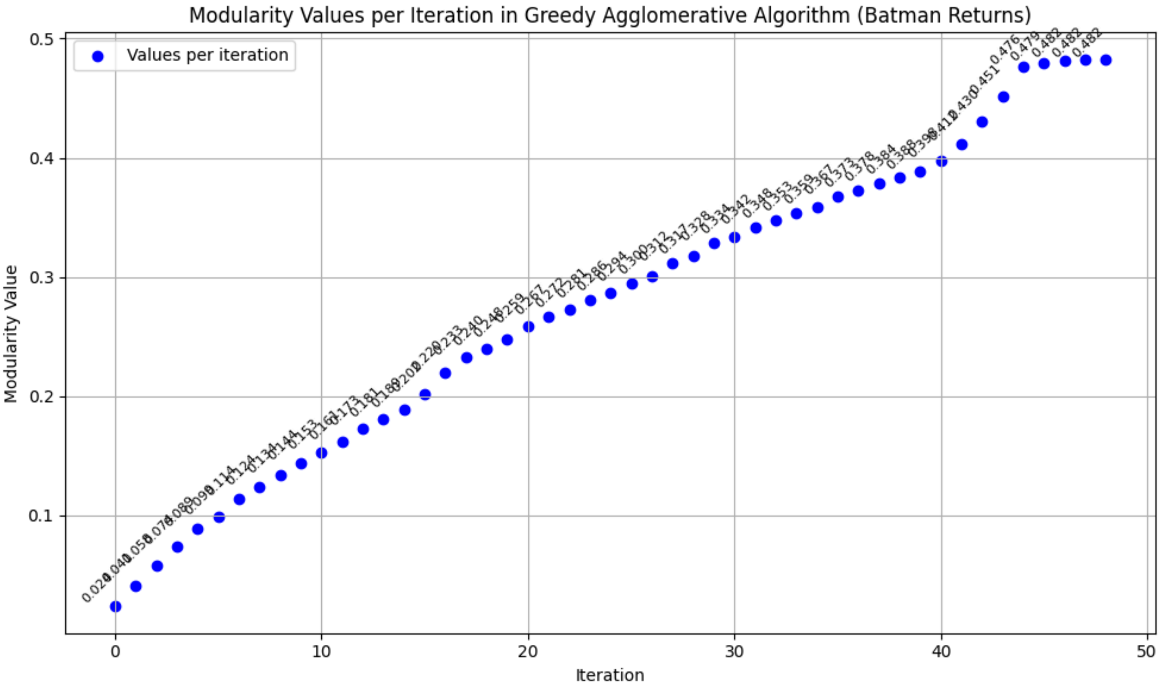
- **QUESTION (d)**

**Implement** (in any programming language) a **simple greedy agglomerative algorithm**: start with each node being a separated community and then do successive iterations in which you try all possible changes for one node (that is, for each node i ∈ V , try changing its community to all possible communities j ∈ C), and apply the change that produces the best gain in modularity (if there is ties, choose any possible). Attach the program to your homework submission with a very short description on how it works.

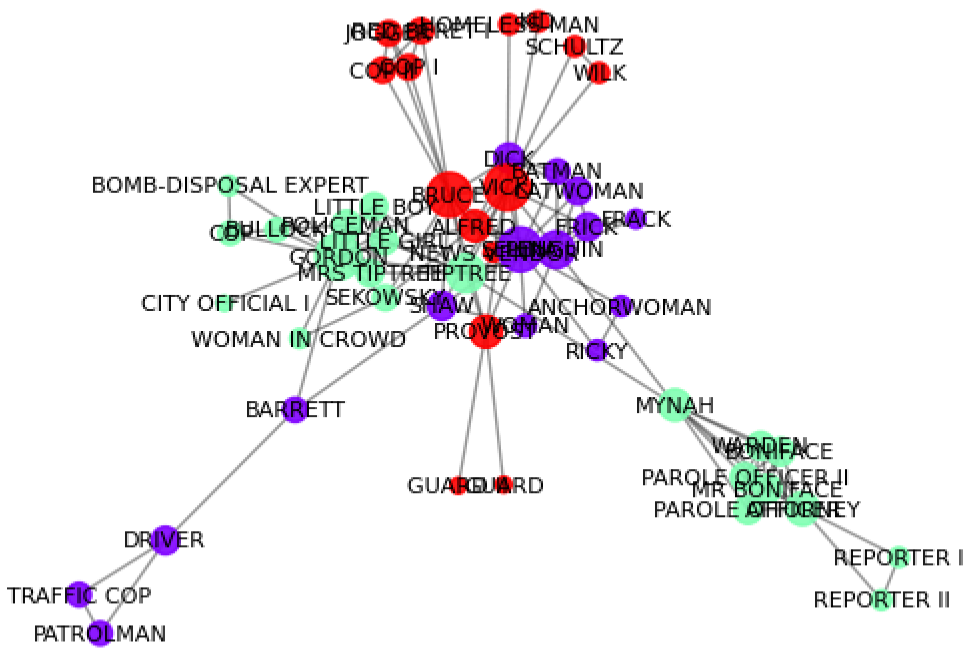
Using one of the movies from from the previous questions, make a **plot showing the modularity increase** as you are making more iterations until you reach you a "local maximum", and report the communities you found (as a visualization), comparing them to the communities found previously.

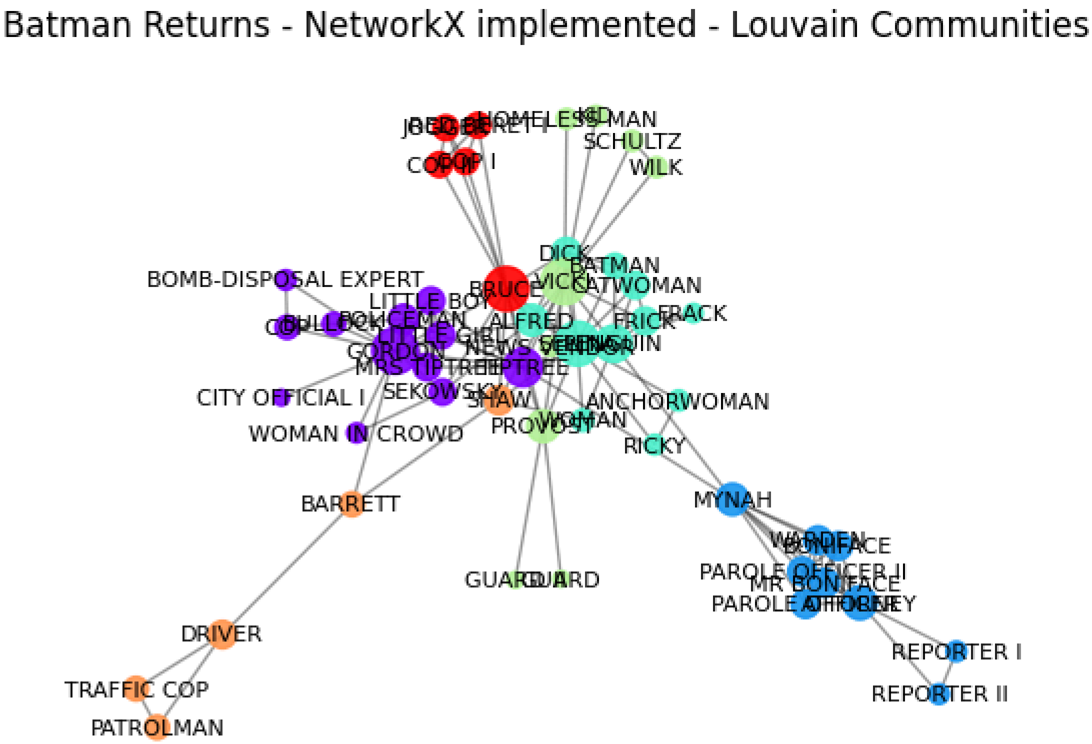
**Answer**:

In [19]:
```
# print(progress_scores)
# Create iteration index
iterations = list(range(len(progress_scores)))

# Plot
plt.figure(figsize=(10, 6))
plt.scatter(iterations, progress_scores, color='blue', label='Values per iterati

# Add labels
for i, val in enumerate(progress_scores):
    plt.text(i, val, f"{val:.3f}", fontsize=8, ha='right', va='bottom', rotation

plt.title('Modularity Values per Iteration in Greedy Agglomerative Algorithm (Ba
plt.xlabel('Iteration')
plt.ylabel('Modularity Value')
plt.grid(True)
plt.legend()
plt.tight_layout()
plt.show()

utils.visualize_communities_pgrank(G, comm_2, title="Batman Returns - self imple
utils.visualize_communities_pgrank(G, communities, title="Batman Returns - Netwo
```




Batman Returns - self implemented - Louvain Communities






**R**: To execute the program use the command "python task6/src/main.py". It will ask for inputs, for example to the user to indicate the relative path to src folder. Afterwards it requires input to enter a example ID of movie to calculate the communities using Louvain greedy algorithm. It outputs the score of self-implemented modularity and also NetworkX implemented modularity. The program displays both (self-implemented and NetworkX implementation) networks of communities and the plot of modularity increase in Greedy Algorithm iterations. About the results, as previously mentioned we did not find exactly the same results for modularity, what at the end impacted the communities discovery. But we still possible to generate the communities in several cases.

- **QUESTION (e)**

Using your previous program as a basis, explain how could you obtain a **larger quantity of communities**? And how could you obtain **less communities**?

**Answer**:

**R**: Since in the Louvain algorithm we have an agglomerative approach, we start with the each node of network being one community. As the iterations goes on, the communities are merged and the number of communities in the network reduces. To have larger quantity of communities we should do an early stop. In other hand, to have less communities we should do a late stop, ending with more communities merged (even without improve of modularity).

# Network Motifs

**QUESTION 7.**

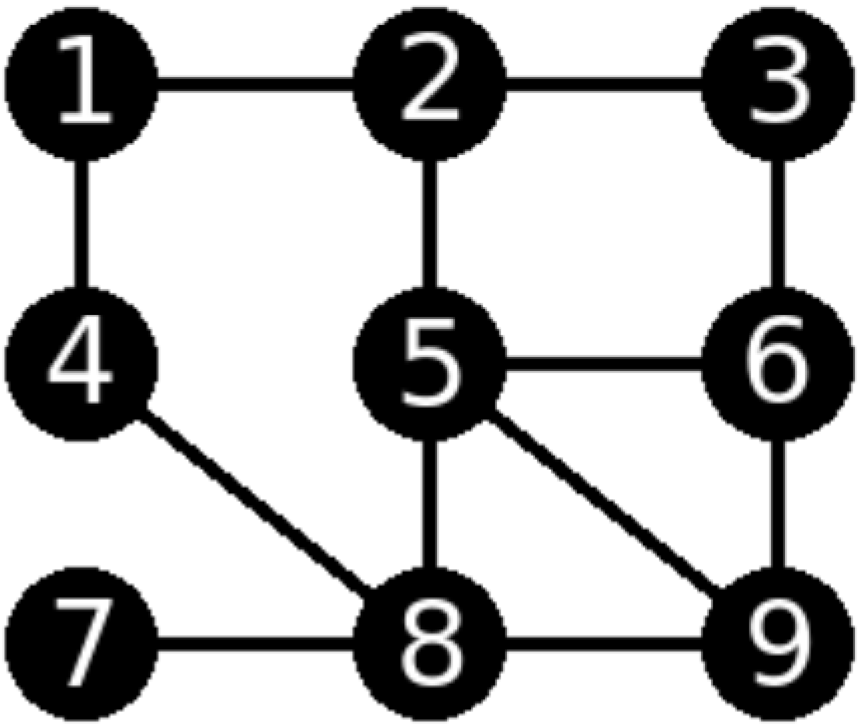
For this part of your homework it is highly advisable that you use the gtrieScanner tool. You should download, unzip and compile this version: gtrieScanner_src_01.zip (it is the same as the version online with a newly added "-raw" option to help you on the homework plus some pre-computed g-tries)

Your first task is to be able to compile the source code. You will need a C++ compiler and make tools. If you have Linux you can simply use g++ and make available on any common distribution. If you use Windows we suggest you use WSL or Cygwin to have a shell with Linux-like functionality.

## Counting subgraphs

- **QUESTION (a)**

Consider the following undirected network:




The frequency (number of occurrences of size 3) of subgraphs of size 3 in this network is:

| Subgraph | Frequency |
|---|---|
|  | 18 |
|  | 2 |

You could obtain these results by running (for instance) one of the following commands:

```
./gtrieScanner -s 3 -m esu -g network.txt -f simple
./gtrieScanner -s 3 -m gtrie undir3.gt -g network.txt -f simple
```

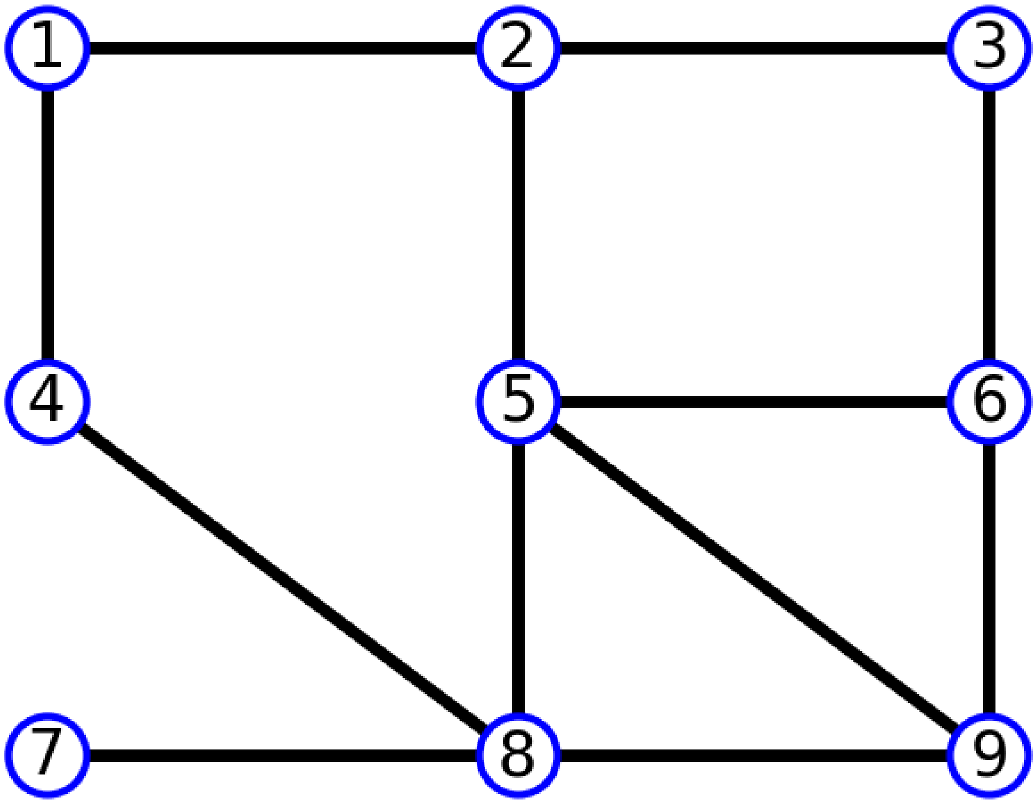
supposing that **network.txt** is a text file containing the description of the network as an adjacency list: one line per edge, each line containing two integers separated by a space, the endpoints of the respective edge (the file should have 12 lines, the first of which could be 1 2, for example).

**Your task here is to determine the number of occurrences of all subgraphs of size 4 in this network.** You should put in the report a table like the one shown above (the html version of the output is "broken", so you should produce your own images of the subgraphs)

**Answer**:

In [20]:
```
import networkx as nx

# Step 1: Create an undirected graph with no parallel edges
G = nx.Graph()

# Add the nodes and edges
G.add_nodes_from([1,9])
G.add_edges_from([(1,2),(1,4),
                  (2,1), (2,5), (2,3),
                  (3,2), (3,6),
                  (4,1), (5,2), (5,6), (5,8), (5,9),
                  (6,3), (6,5), (6,9),
                  (7,8), (8,4), (8,5), (8,9)])

# Position like the image:
pos = {
    7: (0, 0), 8: (1, 0), 9: (2, 0),
    4: (0, 1), 5: (1, 1), 6: (2, 1),
    1: (0, 2), 2: (1, 2), 3: (2, 2)
}

options = {
    "with_labels": True,
    "font_size": 25,
    "node_size": 1000,
    "node_color": "white",
    "edgecolors": "blue",
    "linewidths": 3,
    "width": 5,
}

# Show the nodes and edges
print(G.nodes)
print(G.edges)

# Draw the graph
nx.draw(G, pos, **options)
```

```
[1, 9, 2, 4, 5, 3, 6, 8, 7]
[(1, 2), (1, 4), (9, 5), (9, 6), (9, 8), (2, 5), (2, 3), (4, 8), (5, 6), (5, 8),
(3, 6), (8, 7)]
```




In [21]:
```
#  Write to file in gtrieScanner-compatible format
with open("network.txt", "w") as f:
    for u, v in G.edges():
        f.write(f"{u} {v}\n")
```

In [22]:
```
import matplotlib.pyplot as plt
import numpy as np
import os

adj_matrix_1 = np.array([
    [0, 1, 1, 0],
    [1, 0, 0, 1],
    [1, 0, 0, 0],
    [0, 1, 0, 0]
]) # freq = 21

adj_matrix_2 = np.array([
    [0, 1, 1, 1],
    [1, 0, 1, 0],
    [1, 1, 0, 0],
    [1, 0, 0, 0]
]) # freq = 5

adj_matrix_3 = np.array([
    [0, 1, 1, 1],
    [1, 0, 0, 0],
    [1, 0, 0, 0],
    [1, 0, 0, 0]
]) # freq = 4

adj_matrix_4 = np.array([
    [0, 1, 1, 0],
```

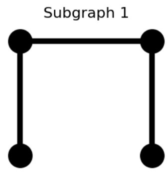
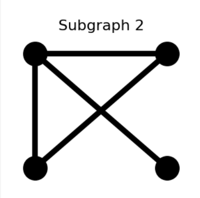
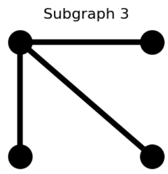
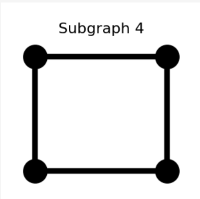
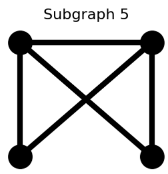
```
    [1, 0, 0, 1],
    [1, 0, 0, 1],
    [0, 1, 1, 0]
]) # freq = 1

adj_matrix_5 = np.array([
    [0, 1, 1, 1],
    [1, 0, 1, 1],
    [1, 1, 0, 0],
    [1, 1, 0, 0]
]) # freq = 1


pos1 = {
    2: (0, 1), 3: (1, 1),
    0: (0, 2), 1: (1, 2),
}

options2 = {
    "with_labels": False,
    "node_size": 150,
    "node_color": "black",
    "edgecolors": "black",
    "width": 3,
}

adj_matrices = [adj_matrix_1, adj_matrix_2, adj_matrix_3, adj_matrix_4, adj_matr

# Create output directory if it doesn't exist
output_dir = "subgraph_images"
os.makedirs(output_dir, exist_ok=True)

# Draw all graphs
for i, mat in enumerate(adj_matrices, 1):
    G = nx.from_numpy_array(mat)
    plt.figure(figsize=(1.5,1.5))
    plt.title(f"Subgraph {i}", fontsize=8)
    nx.draw(G, pos1, **options2)
    plt.axis("off")             # Hide axis
    plt.tight_layout()
    filepath = os.path.join(output_dir, f"subgraph{i}.png")
    plt.savefig(filepath, dpi=200)
    plt.close()
```

To generate the subgraphs, we plotted the network and saved its adjacency list to a `.txt` file containing 12 lines, each representing a pair of connected nodes (as shown in the code above). After generating the file, we ran the following command in the shell to search for subgraphs of size 4 within the network:

`gtrieScanner -s 4 -m esu -g network.txt -f simple`

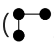
We got 5 subgraphs as shown in the table below:

## Subgraphs Table:

| Subgraph | Frequency |
|---|---|
|   | 21 |
|   | 5 |
|   | 4 |
|   | 1 |
|   | 1 |

### A bit of math: subgraphs in purely random networks

- **QUESTION (b)**

Imagine you have a $G_{np}$ undirected Erd˝os–R´enyi random network. What is its expected number of triangles ( )? And what about the expected number of chains ()? Justify your answer.

Note that you can test your theory by generating Erd˝os–R´enyi networks and counting the subgraphs using gtrieScanner, but your answer should be stated as formulas involving $n$ and $p$.

**Answer**:

## 📊 Expected Subgraph Counts in Erdős–Rényi Graph ( G(n, p) )

- **Expected number of triangles**:

$$\mathbb{E}[\text{Triangles}] = \binom{n}{3} \cdot p^3 = \frac{n(n-1)(n-2)}{6} \cdot p^3$$

- **Expected number of 3-node chains (Path of length 2)**:

$$\mathbb{E}[\text{Chains}] = \binom{n}{3} \cdot 3p^2(1-p) = \frac{n(n-1)(n-2)}{2} \cdot p^2(1-p)$$

For testing the hypothesis we generated 2 networks containing 500 nodes and 1000 nodes and evaluated the error (%). After creating the networks, we used `Gtrie` to count the subgraphs with 3 nodes (chains and triangles), using the code below (example for the file with 1000 nodes):

`gtrieScanner -s 3 -m esu -g Expected1000_p0.1.txt -f simple`

In [23]:
```
from IPython.display import Markdown

def generate_erdos_renyi_and_save(n, p, filename):
    G = nx.erdos_renyi_graph(n, p)
    # Save as edge list (one edge per line, undirected)
    with open(f"{filename}.txt", "w") as f:
        for u, v in G.edges():
            f.write(f"{u+1} {v+1}\n")

def expected_triangles(n, p):
    return (n * (n - 1) * (n - 2) / 6) * (p ** 3)

def expected_chains(n, p):
    return (n * (n - 1) * (n - 2) / 2) * (p ** 2) * (1 - p)
```

Lets try 500 nodes

In [24]:
```
n = 500

# Generate the adjency files (Only load the next cell when necessary!!!)
#for p in [0.01, 0.05, 0.1]:
    #generate_erdos_renyi_and_save(500, p, f"Teste_Expected500_p{p}")

# Calculate the expected frequencies
expected_triangles_1 = expected_triangles(n, 0.01)
expected_chains_1 = expected_chains(n, 0.01)

expected_triangles_2 = expected_triangles(n, 0.05)
expected_chains_2 = expected_chains(n, 0.05)

expected_triangles_3 = expected_triangles(n, 0.1)
expected_chains_3 = expected_chains(n, 0.1)

# Real frequencies (calculated by Gtrie)
real1_triangles = 19
real1_chains = 6642

real2_triangles = 2784
real2_chains = 151989

real3_triangles = 20197
real3_chains = 550481
```

```
from IPython.display import Markdown

def percentage_error(expected, real):
    return abs(expected - real) / expected * 100 if expected != 0 else 0

Markdown(f"""
### Subgraph Frequencies in Erdős-Rényi \( G(n=500, p) \) Networks

| Subgraph Type        | p = 0.01 (Expected) | p = 0.01 (Real) | Error (%) | p =
|---------------------|--------------------|------------------|-----------|----
| **Triangle**         | {expected_triangles_1:.2f} | {real1_triangles} | {perce
| **Chain (Path-3)**   | {expected_chains_1:.2f}    | {real1_chains}     | {perc

Le's try 1000 nodes for testing if we can obtain lower error values!
""")
```

```
<>:41: SyntaxWarning: invalid escape sequence '\('
<>:41: SyntaxWarning: invalid escape sequence '\('
C:\Users\davib\AppData\Local\Temp\ipykernel_18844\2596487662.py:41: SyntaxWarnin
g: invalid escape sequence '\('
  """)
```

Out[24]:

### Subgraph Frequencies in Erdős–Rényi ( G(n=500, p) ) Networks

| Subgraph Type | p = 0.01 (Expected) | p = 0.01 (Real) | Error (%) | p = 0.05 (Expected) | p = 0.05 (Real) | Error (%) | p = 0.1 (Expected) | p = 0.1 (Real) | Err (% |
|---|---|---|---|---|---|---|---|---|---|
| **Triangle** | 20.71 | 19 | 8.3% | 2588.56 | 2784 | 7.6% | 20708.50 | 20197 | 2.5 |
| **Chain (Path-3)** | 6150.42 | 6642 | 8.0% | 147548.06 | 151989 | 3.0% | 559129.50 | 550481 | 1.5 |

Le's try 1000 nodes for testing if we can obtain lower error values!

n = 1000

In [25]:

```
n = 1000

# Generate the adjency files (Only load the next cell when necessary!!!)
#for p in [0.01, 0.05, 0.1]:
    #generate_erdos_renyi_and_save(1000, p, f"Expected1000_p{p}")

# Calculate the expected frequencies
expected_triangles_1 = expected_triangles(n, 0.01)
expected_chains_1 = expected_chains(n, 0.01)

expected_triangles_2 = expected_triangles(n, 0.05)
expected_chains_2 = expected_chains(n, 0.05)

expected_triangles_3 = expected_triangles(n, 0.1)
expected_chains_3 = expected_chains(n, 0.1)

# Real frequencies (calculated by Gtrie)
real1_triangles = 151
real1_chains = 48076
```

```
real2_triangles = 20717
real2_chains = 1184104

real3_triangles = 164933
real3_chains = 4467024

from IPython.display import Markdown

def percentage_error(expected, real):
    return abs(expected - real) / expected * 100 if expected != 0 else 0

Markdown(f"""
### Subgraph Frequencies in Erdős-Rényi \( G(n=1000, p) \) Networks

| Subgraph Type        | p = 0.01 (Expected) | p = 0.01 (Real) | Error (%) | p =
|---------------------|---------------------|-------------------|-----------|----
| **Triangle**         | {expected_triangles_1:.2f} | {real1_triangles} | {perce
| **Chain (Path-3)**   | {expected_chains_1:.2f}     | {real1_chains}      | {perc
""")
```

```
<>:39: SyntaxWarning: invalid escape sequence '\('
<>:39: SyntaxWarning: invalid escape sequence '\('
C:\Users\davib\AppData\Local\Temp\ipykernel_18844\499219552.py:39: SyntaxWarning:
invalid escape sequence '\('
  """)
```

Out[25]:

### Subgraph Frequencies in Erdős–Rényi ( G(n=1000, p) ) Networks

| Subgraph Type | p = 0.01 (Expected) | p = 0.01 (Real) | Error (%) | p = 0.05 (Expected) | p = 0.05 (Real) | Error (%) | p = 0.1 (Expected) | p = 0.1 (Real) |
|---|---|---|---|---|---|---|---|---|
| **Triangle** | 166.17 | 151 | 9.1% | 20770.88 | 20717 | 0.3% | 166167.00 | 164933 |
| **Chain (Path-3)** | 49351.60 | 48076 | 2.6% | 1183939.88 | 1184104 | 0.0% | 4486509.00 | 4467024 |

### Back to empirical findings: uncovering motifs in bacteria

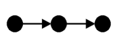
- **QUESTION (c)**

Your task is now to find some network motifs of the transcriptional regulation directed network of the bacteria Escherichia coli. Start by downloading the network as a weighted adjacency list: ecoli.txt (each line is an edge in the format start node end node weight)

This directed network is ready for being fed to gtrieScanner. For example you could run:

```
./gtrieScanner -s 3 -d -m gtrie dir3.gt -g ecoli.txt
```

This would compute the frequency of all possible 13 types of size 3 subgraphs, and it should show you that the most frequent one is the following, appearing 250 times:



Now, if you add the ”-r n” option, it should produce n networks with the same degree sequence and it will you show you how often each subgraph appears on it. For example:

```
./gtrieScanner -s 3 -m gtrie dir3.gt -d -g ecoli.txt -r 500 -raw
```

**Check the results and report on what is the more overrepresented subgraph, including its z-score (Z), frequency on the original network (real), average number of occurrences (avgR) and standard deviation (stdevR)) on the randomized networks**.

The z-score of subgraph i is computed as $Z_i = \frac{(real_i - avgR_i)}{stdevR_i}$ as in (Milo et al. 2004).

Notice how the most frequent subgraph is not the most significant one. Check if your very simplistic analysis is consistent with the known literature (Milo et al. 2002) (Shen-Orr et al. 2002), that is, if the motif you found is also reported (**what is the name given to this motif ?**)

**Answer**:

In [26]:
```python
adj_matrix_1 = np.array([
    [0, 1, 1],
    [0, 0, 1],
    [0, 0, 0]
]) # freq = 130

adj_matrix_2 = np.array([
    [0, 0, 1],
    [1, 0, 0],
    [0, 0, 0]
]) # freq = 250

adj_matrix_3 = np.array([
    [0, 1, 1],
    [0, 0, 0],
    [0, 0, 0]
]) # freq = 168

adj_matrix_4 = np.array([
    [0, 0, 0],
    [1, 0, 0],
    [1, 0, 0]
]) # freq = 126


options2 = {
    "with_labels": False,
    "node_size": 150,
    "node_color": "black",
    "edgecolors": "black",
    "width": 3,
}

adj_matrices = [adj_matrix_1, adj_matrix_2, adj_matrix_3, adj_matrix_4]

# Create output directory if it doesn't exist
```

```
output_dir = "motifs_images_directed"
os.makedirs(output_dir, exist_ok=True)

# Draw all graphs as directed
for i, mat in enumerate(adj_matrices, 1):
    G = nx.from_numpy_array(mat, create_using=nx.DiGraph)  # <-- Make it directe
    plt.figure(figsize=(1.5,1.5))
    plt.title(f"Subgraph {i}", fontsize=8)
    nx.draw(G, pos1, arrows=True, **options2)  # arrows=True to show direction
    plt.axis("off")
    plt.tight_layout()
    filepath = os.path.join(output_dir, f"motif{i}.png")
    plt.savefig(filepath, dpi=200)
    plt.close()


Markdown(f"""
### 🧬 Motif Analysis of *E. coli* Transcriptional Regulatory Network

#### Summary of gtrieScanner Results

We analyzed the directed network using `gtrieScanner` to identify all 3-node sub

`gtrieScanner-s 3-m gtrie dir3.gt-d-g ecoli.txt-r 500-raw`

 After comparing the real network to 500 randomized networks with the same degre


| Subgraph Type (ID) | Structure                                    | Real Freque
|--------------------|----------------------------------------------|------------
| **ID: 011-001-000** | <img src="task7/Task7_NS/motifs_images_directed/motif1.p
| **ID: 001-100-000** | <img src="task7/Task7_NS/motifs_images_directed/motif2.p
| **ID: 011-000-000** | <img src="task7/Task7_NS/motifs_images_directed/motif3.p
| **ID: 000-100-100** | <img src="task7/Task7_NS/motifs_images_directed/motif4.p

As supported by the literature, the most statistically significant motif is the
> *"A transcription factor X regulates a second transcription factor Y, and both
— *Milo et al., 2004*  """)
```

Out[26]:

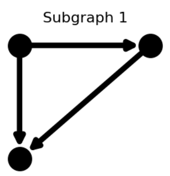
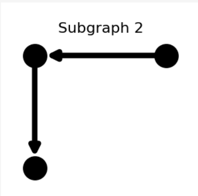
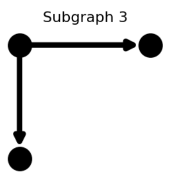
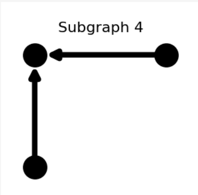
# 🧬 Motif Analysis of *E. coli* Transcriptional Regulatory Network

## Summary of gtrieScanner Results

We analyzed the directed network using `gtrieScanner` to identify all 3-node subgraphs (motifs) with the code bellow:

`gtrieScanner-s 3-m gtrie dir3.gt-d-g ecoli.txt-r 500-raw`

After comparing the real network to 500 randomized networks with the same degree sequence, we obtained the following results:

| Subgraph Type (ID) | Structure | Real Frequency | Random Avg | Std Dev | Z-Score |
|---|---|---|---|---|---|
| **ID: 011-001-000** |  | 130 | 12.05 | 3.22 | **36.63** |
| **ID: 001-100-000** |  | 250 | 345.19 | 13.91 | **-6.84** |
| **ID: 011-000-000** |  | 168 | 278.06 | 7.12 | **-15.46** |
| **ID: 000-100-100** |  | 126 | 237.74 | 5.99 | **-18.66** |

As supported by the literature, the most statistically significant motif is the **Feedforward Loop (FFL)** (see picture of subgraph 1):

> *"A transcription factor X regulates a second transcription factor Y, and both jointly regulate one or more operons $Z_1 \ldots Z_n$. An example of a feedforward loop is the L-arabinose utilization system."*
> *— Milo et al., 2004*

## Characterizing families of networks using motifs

Start by carefully reading the following paper:

Milo et al. "Superfamilies of evolved and designed networks." Science 303.5663 (2004)

The idea here is to perform a very similar analysis, even using some of the same networks!

- **QUESTION (d)**

Download this set of 8 directed networks: networks.zip (inside the zip there is a README.txt explaining what is each network). **Use gtrieScanner to compute motif fingerprints of all networks. You should produce and include in the report the following:**

- Plot(s) showing the (normalized) significance profile (SP) of all 13 directed motifs of size 3 for each network. Try to expose the similarity between groups of networks. It should be clear to which subgraph corresponds each data point (ex: see figure 1 of the paper).
- One heat map of 8 × 8 cells showing the correlation between the SPs of all pairs of networks (ex: see figure 2 of the paper).
- A visual description of the main characteristic motifs of each group of networks (that is, you should draw them). Can you give an interpretation on why are they so significant?

You should use at least 100 random networks for each original network and you can opt to ignore subgraphs that occur only once in the original network (attributing a z-score of zero to them).

For normalizing the z-scores use the suggested formula: $SP_i = \frac{Z_i}{\sqrt{\sum(Z_i^2)}}$

For the heat map you can use any sofware. R and Python have several possible packages, but even Excel or LibreOffice will suffice (use range conditional formatting). You even have some possible online alternatives. If you know about it, you can even use a clustering algorithm to produce a dendrogram showcasing the relationship between the families of networks.

**Answer**:

For completing this task first we ran the following code for each of the 8 networks:

```
gtrieScanner -s 3 -d -m gtrie dir3.gt -g yeast.txt -r 100 -raw
```

After that we extracted the Z scores of all 13 patterns and created a vector with that. An important key to have in mind here is that the motifs are in the same order in the output of `Gtrie` algorithm.

Then we normalize all the vectors and plotted them.

In [27]:
```
# First we Loaded the Z-scores vectors

z_vector_circuit1 = np.array([
```

```
    9.82,    # motif 1
    1.88,    # motif 2
    1.60,    # motif 3
    -2.76,   # motif 4
    0.0,     # motif 5
    0.0,     # motif 6
    0.0,     # motif 7
    0.0,     # motif 8
    0.0,     # motif 9
    0.0,     # motif 10
    0.0,     # motif 11
    0.0,     # motif 12
    0.0      # motif 13
])

z_vector_circuit2 = np.array([
    18.00,    # motif 1
    1.76,    # motif 2
    1.65,    # motif 3
    -6.40,   # motif 4
    0.0,     # motif 5
    0.0,     # motif 6
    0.0,     # motif 7
    0.0,     # motif 8
    0.0,     # motif 9
    0.0,     # motif 10
    0.0,     # motif 11
    0.0,     # motif 12
    0.0      # motif 13
])

z_vector_ecoli = np.array([
    32.94,    # motif 1
    -7.83,    # motif 2
    -16.82,    # motif 3
    -21.81,   # motif 4
    0.0,     # motif 5
    0.0,     # motif 6
    0.0,     # motif 7
    0.0,     # motif 8
    0.0,     # motif 9
    0.0,     # motif 10
    0.0,     # motif 11
    0.0,     # motif 12
    0.0      # motif 13
])

z_vector_english = np.array([
    34.09,   # motif 1
    29.78,   # motif 2
    28.90,   # motif 3
    23.65,   # motif 4
    20.96,   # motif 5
   -14.55,   # motif 6
   -18.66,   # motif 7
   -22.14,   # motif 8
   -24.23,   # motif 9
   -24.55,   # motif 10
   -31.21,   # motif 11
   -33.74,   # motif 12
```

```
    -35.17    # motif 13
])

z_vector_french = np.array([
    26.48,    # motif 1
    22.87,    # motif 2
    19.89,    # motif 3
    15.14,    # motif 4
    4.85,     # motif 5
   -9.23,     # motif 6
  -12.98,     # motif 7
  -19.35,     # motif 8
  -23.15,     # motif 9
  -26.22,     # motif 10
  -27.53,     # motif 11
  -27.73,     # motif 12
  -42.95      # motif 13
])

z_vector_highschool = np.array([
    186.95,    # motif 1
    42.97,     # motif 2
    15.37,     # motif 3
    14.24,     # motif 4
    11.75,     # motif 5
    5.45,      # motif 6
    3.86,      # motif 7
    3.05,      # motif 8
   -5.29,      # motif 9
   -5.66,      # motif 10
  -14.80,      # motif 11
  -16.13,      # motif 12
  -17.94       # motif 13
])

z_vector_residence = np.array([
    907.12,    # motif 1
    164.64,    # motif 2
    145.86,    # motif 3
    31.01,     # motif 4
    18.22,     # motif 5
    17.31,     # motif 6
    16.86,     # motif 7
    3.14,      # motif 8
   -17.91,     # motif 9
   -25.81,     # motif 10
   -46.94,     # motif 11
   -49.09,     # motif 12
   -51.75      # motif 13
])

z_vector_yeast = np.array([
    0.0,      # motif 1: 010-100-110 → inf
    0.0,      # motif 2: 011-100-010 → inf
    13.98,    # motif 3: 011-001-000
    2.91,     # motif 4: 011-100-000
   -9.79,     # motif 5: 001-100-000
  -10.13,     # motif 6: 011-000-000
  -14.44,     # motif 7: 000-100-100
   0.0,       # motif 8: 001-100-010 → nan
```

```
    0.0,      # motif 9: 010-100-100 → nan
    0.0,      # motif 10: 011-100-100 → nan
    0.0,      # motif 11: 011-101-000 → nan
    0.0,      # motif 12: 011-101-100 → nan
    0.0       # motif 13: 011-101-110 → nan
])

def normalize_Z(vector):
    vector = np.array(vector)
    norm = np.linalg.norm(vector)  # sqrt(sum of squares)
    return vector / norm if norm != 0 else vector

z_vector_circuit1_norm = normalize_Z(z_vector_circuit1)
z_vector_circuit2_norm = normalize_Z(z_vector_circuit2)
z_vector_ecoli_norm = normalize_Z(z_vector_ecoli)
z_vector_english_norm = normalize_Z(z_vector_english)
z_vector_french_norm = normalize_Z(z_vector_french)
z_vector_highschool_norm = normalize_Z(z_vector_highschool)
z_vector_residence_norm = normalize_Z(z_vector_residence)
z_vector_yeast_norm = normalize_Z(z_vector_yeast)
```

In [28]:

```
# Define your 13 directed 3-node motif adjacency matrices
adj_matrices = [
    np.array([[0, 1, 0], [1, 0, 0], [1, 1, 0]]),
    np.array([[0, 1, 1], [1, 0, 0], [0, 1, 0]]),
    np.array([[0, 1, 1], [0, 0, 1], [0, 0, 0]]),
    np.array([[0, 1, 1], [1, 0, 0], [0, 0, 0]]),
    np.array([[0, 0, 1], [1, 0, 0], [0, 0, 0]]),
    np.array([[0, 1, 1], [0, 0, 0], [0, 0, 0]]),
    np.array([[0, 0, 0], [1, 0, 0], [1, 0, 0]]),
    np.array([[0, 0, 1], [1, 0, 0], [0, 1, 0]]),
    np.array([[0, 1, 0], [1, 0, 0], [1, 0, 0]]),
    np.array([[0, 1, 1], [1, 0, 0], [1, 0, 0]]),
    np.array([[0, 1, 1], [1, 0, 1], [0, 0, 0]]),
    np.array([[0, 1, 1], [1, 0, 1], [1, 0, 0]]),
    np.array([[0, 1, 1], [1, 0, 1], [1, 1, 0]])
]

# Drawing options
options2 = {
    "with_labels": False,
    "node_size": 100,
    "node_color": "black",
    "edgecolors": "black",
    "width": 2.5,
}

# Fixed position layout
pos1 = {
    0: (0, 1), 1: (1, 1),
    2: (0.5, 0)
}

# Output folder
output_dir = "motifs_pngs_3"
os.makedirs(output_dir, exist_ok=True)

# Draw and export as PNG
for i, mat in enumerate(adj_matrices, 1):
    G = nx.from_numpy_array(mat, create_using=nx.DiGraph)
```

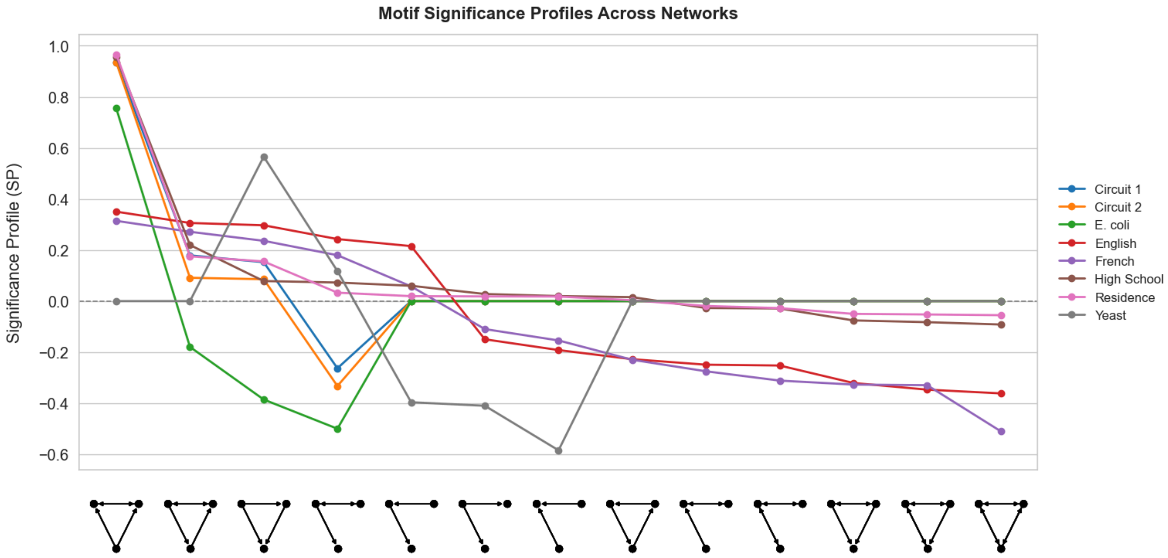
```
    plt.figure(figsize=(1, 1))
    #plt.title(f"Motif {i}", fontsize=8)
    nx.draw(G, pos=pos1, arrows=True, **options2)
    plt.axis("off")
    #plt.tight_layout()
    filepath = os.path.join(output_dir, f"motif{i}.png")
    plt.savefig(filepath, format='png', dpi=200)
    plt.close()
```

In [29]:

```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.image as mpimg
from matplotlib.offsetbox import OffsetImage, AnnotationBbox
from matplotlib import gridspec
import seaborn as sns

sns.set(style="whitegrid", context="notebook", font_scale=1.3)

# SP matrix (replace with your normalized vectors)
sp_matrix = np.array([
    z_vector_circuit1_norm,
    z_vector_circuit2_norm,
    z_vector_ecoli_norm,
    z_vector_english_norm,
    z_vector_french_norm,
    z_vector_highschool_norm,
    z_vector_residence_norm,
    z_vector_yeast_norm
])

network_labels = [
    "Circuit 1", "Circuit 2", "E. coli", "English",
    "French", "High School", "Residence", "Yeast"
]

motif_image_paths = [f"motifs_pngs_3/motif{i+1}.png" for i in range(13)]

# Create figure with two subplots: top for SP, bottom for motif images
fig = plt.figure(figsize=(16, 9))
gs = gridspec.GridSpec(2, 1, height_ratios=[5, 1], hspace=0.05)

# --- Top subplot: SP plot ---
ax0 = plt.subplot(gs[0])
palette = sns.color_palette("tab10", n_colors=len(sp_matrix))

for i, sp in enumerate(sp_matrix):
    ax0.plot(range(13), sp, marker='o', label=network_labels[i],
             linewidth=2.0, markersize=6, color=palette[i], zorder=3)

ax0.axhline(0, color='gray', linestyle='--', linewidth=1.2, zorder=1)

ax0.set_xlim(-0.5, 12.5)
ax0.set_xticks([])  # No ticks because we'll use images
ax0.set_ylabel("Significance Profile (SP)", labelpad=15)
ax0.set_title("Motif Significance Profiles Across Networks", fontsize=16, weight
ax0.legend(loc='center left', bbox_to_anchor=(1.01, 0.5), frameon=False, fontsiz

# --- Bottom subplot: Motif images ---
ax1 = plt.subplot(gs[1])
ax1.axis("off")  # Hide axis completely
```

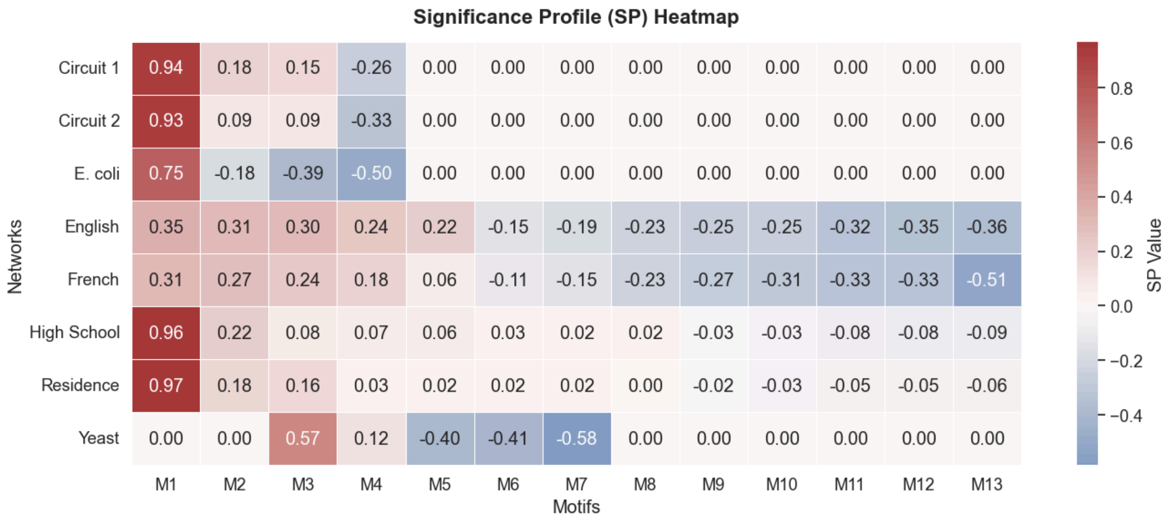
```
for x, img_path in enumerate(motif_image_paths):
    try:
        img = mpimg.imread(img_path)
        imagebox = OffsetImage(img, zoom=0.25)
        ab = AnnotationBbox(imagebox, (x, 0.5), frameon=False, box_alignment=(0.
        ax1.add_artist(ab)
    except FileNotFoundError:
        print(f"Image not found: {img_path}")

ax1.set_xlim(-0.5, 12.5)
ax1.set_ylim(0, 1)

plt.tight_layout()
plt.show()
```

```
C:\Users\davib\AppData\Local\Temp\ipykernel_18844\2132356139.py:65: UserWarning:
This figure includes Axes that are not compatible with tight_layout, so results m
ight be incorrect.
  plt.tight_layout()
```



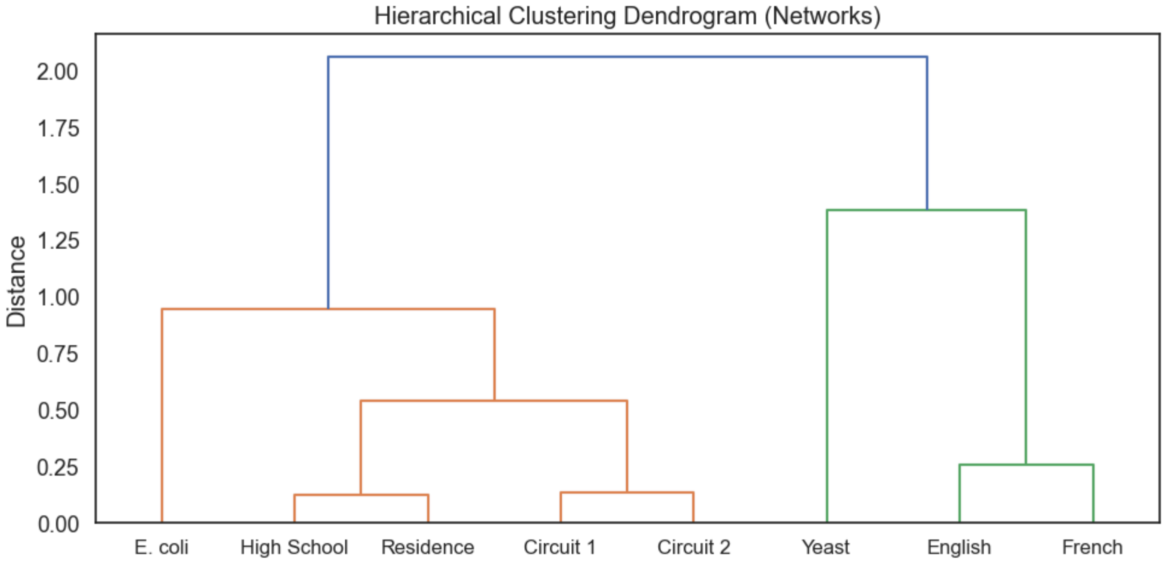

In [30]:
```
# SP matrix: shape (8 networks, 13 motifs)
sp_matrix = np.array([
    z_vector_circuit1_norm,
    z_vector_circuit2_norm,
    z_vector_ecoli_norm,
    z_vector_english_norm,
    z_vector_french_norm,
    z_vector_highschool_norm,
    z_vector_residence_norm,
    z_vector_yeast_norm
])

network_labels = [
    "Circuit 1", "Circuit 2", "E. coli", "English",
    "French", "High School", "Residence", "Yeast"
]

motif_labels = [f"M{i+1}" for i in range(13)]

plt.figure(figsize=(14, 6))
sns.set(style="white", context="notebook", font_scale=1.2)
```

```
ax = sns.heatmap(sp_matrix, cmap="vlag", center=0, linewidths=0.5,
                 xticklabels=motif_labels, yticklabels=network_labels,
                 annot=True, fmt=".2f", cbar_kws={'label': 'SP Value'})

ax.set_title("Significance Profile (SP) Heatmap", fontsize=16, weight='bold', pa
plt.xlabel("Motifs")
plt.ylabel("Networks")
plt.tight_layout()
plt.show()
```




In [31]:

```
from scipy.cluster.hierarchy import dendrogram, linkage
from scipy.spatial.distance import pdist

# Assuming sp_matrix and network_labels are already defined
# sp_matrix shape: (8 networks, 13 motifs)
# Rows = networks

# Perform hierarchical clustering
linked = linkage(sp_matrix, method='ward')  # or 'average', 'complete'

# Plot the dendrogram
plt.figure(figsize=(10, 5))
dendrogram(linked,
           labels=network_labels,
           orientation='top',
           distance_sort='ascending',
           show_leaf_counts=True)

plt.title("Hierarchical Clustering Dendrogram (Networks)")
plt.ylabel("Distance")
plt.tight_layout()
plt.show()
```




- **QUESTION (e)**

**Your task is to find the "family" of the three "unknown" networks** given in unknown.zip You should justify your answer by computing and plotting their motif significance profiles and by adding them to the previous heatmap. Each network will clearly belong to one of the groups discovered on the previous question.

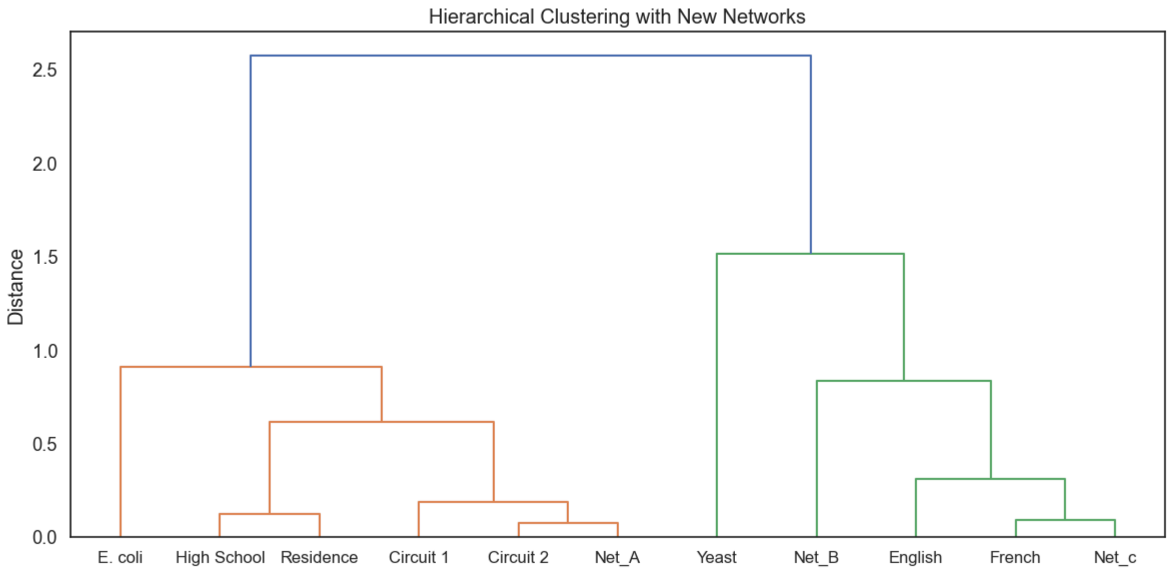
**Answer**:

In [32]:
```
z_vector_netA = np.array([
    43.93,    # motif 1
    1.99,     # motif 2
    1.50,     # motif 3
    -15.18,   # motif 4
    0.0,      # motif 5
    0.0,      # motif 6
    0.0,      # motif 7
    0.0,      # motif 8
    0.0,      # motif 9
    0.0,      # motif 10
    0.0,      # motif 11
    0.0,      # motif 12
    0.0       # motif 13
])

z_vector_netB = np.array([
    0,     # motif 1
    6.50,     # motif 2
    4.77,     # motif 3
    2.92,    # motif 4
    2.49,      # motif 5
    1.68,      # motif 6
    1.14,      # motif 7
    0.95,      # motif 8
    -1.55,      # motif 9
    -2.00,      # motif 10
    -4.03,      # motif 11
    -4.83,      # motif 12
    -4.83       # motif 13
```

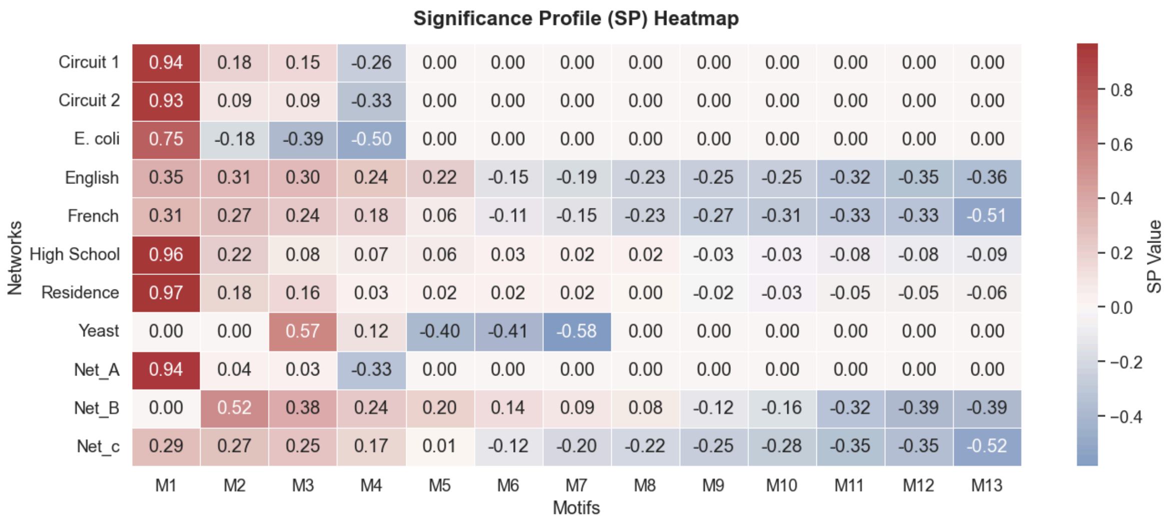
```
])

z_vector_netC = np.array([
    9.23,    # motif 1
    8.53,    # motif 2
    8.05,    # motif 3
    5.56,   # motif 4
    0.41,     # motif 5
    -3.84,     # motif 6
    -6.31,     # motif 7
    -7.00,     # motif 8
    -7.89,     # motif 9
    -8.93,     # motif 10
    -11.05,     # motif 11
    -11.24,     # motif 12
    -16.45      # motif 13
])

z_vector_netA_norm = normalize_Z(z_vector_netA)
z_vector_netB_norm = normalize_Z(z_vector_netB)
z_vector_netC_norm = normalize_Z(z_vector_netC)
```

In [33]:

```
new_sp_matrix = np.array([
    z_vector_netA_norm,
    z_vector_netB_norm,
    z_vector_netC_norm
])

# Stack them vertically
combined_matrix = np.vstack([sp_matrix, new_sp_matrix])

# Perform hierarchical clustering
linked_all = linkage(combined_matrix, method='ward')

# Combined labels (original + new)
combined_labels = network_labels + ["Net_A", "Net_B", "Net_c"]

# Plot dendrogram
plt.figure(figsize=(12, 6))
dendrogram(linked_all,
           labels=combined_labels,
           orientation='top',
           distance_sort='ascending',
           show_leaf_counts=True)
plt.title("Hierarchical Clustering with New Networks")
plt.ylabel("Distance")
plt.tight_layout()
plt.show()
```




In [34]:
```
plt.figure(figsize=(14, 6))
sns.set(style="white", context="notebook", font_scale=1.2)

ax = sns.heatmap(combined_matrix, cmap="vlag", center=0, linewidths=0.5,
                 xticklabels=motif_labels, yticklabels=combined_labels,
                 annot=True, fmt=".2f", cbar_kws={'label': 'SP Value'})

ax.set_title("Significance Profile (SP) Heatmap", fontsize=16, weight='bold', pa
plt.xlabel("Motifs")
plt.ylabel("Networks")
plt.tight_layout()
plt.show()
```




As shown above, the unknown networks belong to different clusters:

- `Net_A` shows similar patterns to *circuit1 and circuit2*, suggesting it may be a circuit network.
- `Net_B` shows simmilar patterns to *english or yeast*, indicating it could be either a language or a biological network.
- `Net_C` shows simmilar patterns to *english and french* so it could be a language network.