图挖掘算法的实现与验证 实验报告

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本实验已在 GitHub 上开源,欢迎查看。

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1. 实验目的

本实验旨在通过实现图的存储、读写、结构挖掘算法和可视化来加深对图算法的理解,并掌握如何在实际工程项目中应用这些算法。同时,通过将Python实现与C++实现进行对比,验证算法的正确性和效率。

2. 实验内容

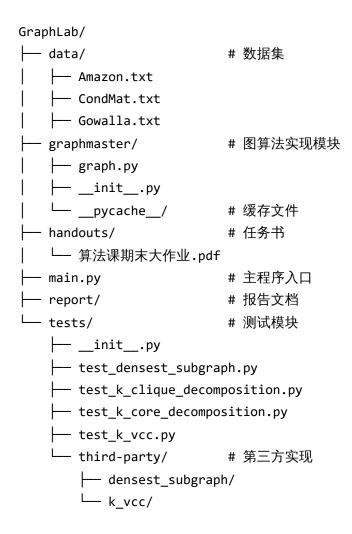
本实验内容包括以下几部分:

- 1. 实现图的存储结构,支持图的创建、节点和边的添加与删除。
- 2. 实现从文件读取图的节点和边信息,并将图数据写入文件。

- 3. 实现多种图结构挖掘算法,包括k-core分解、最密子图、近似最密子图、k-clique分解和k-vcc分解。
- 4. 实现图的可视化,支持节点和边的样式设置以及交互功能。
- 5. 通过详细的测试用例验证算法的正确性,并与C++实现进行对比。

3. 项目结构

项目采用模块化设计,结构如下:



4. 算法实现

图的读写

图的读写是图操作的基础,通过对图的存储结构进行封装,可以方便地实现节点和边的添加、删除、读取和保存。

图的加载

通过读取文件,将文件中的节点和边信息解析并添加到图中。为了保证节点和边的唯一性,使用映射来管理节点。

```
def load(self, file_path):
    with open(file_path, "r") as f:
        lines = f.readlines()
        for i, line in enumerate(lines):
            if not line.startswith("#"):
                 lines = lines[i:]
                 break

        for line in lines:
            numbers = re.findall(r"\d+", line)
            if len(numbers) >= 2:
                 u, v = map(int, numbers[:2])
                 self.add_edge(u, v)
```

图的保存

将图中的节点和边信息保存到文件中,以便后续使用。

```
def save(self, output_path):
    with open(output_path, "w") as f:
        for edge in self.graph.edges():
            u, v = edge
            original_u, original_v = (
                 self.reverse_mapping[u],
                  self.reverse_mapping[v],
            )
            f.write(f"{original_u} {original_v}\n")
```

1. k-core分解

算法说明:

k-core分解是一种用于识别网络中节点的稳健性和紧密性的算法。k-core是一个最大子图,在该子图中,每个节点至少连接有k个其他节点。k-core分解的过程是递归地移除度数小于k的节点,直到图中所有剩余节点的度数都大于等于k。

伪代码:

```
function k_core(graph, k):
    subgraph = graph.copy()
    while true:
        nodes_to_remove = []
        for each node in subgraph:
            if degree(node) < k:
                  nodes_to_remove.append(node)
        if nodes_to_remove is empty:
                  break
        subgraph.remove_nodes(nodes_to_remove)
        return subgraph.nodes()</pre>
```

Python实现:

```
def k_core(self, k):
    subgraph = self.graph.copy()
    while True:
        nodes_to_remove = [node for node, degree in subgraph.degree if degree < k]
        if not nodes_to_remove:
            break
        subgraph.remove_nodes_from(nodes_to_remove)
        k_core_nodes = subgraph.nodes()
    return [self.reverse_mapping[node] for node in k_core_nodes]</pre>
```

2. 最密子图

算法说明:

最密子图是图中具有最高边密度的子图。为了找到最密子图,可以使用最大流算法。通过构建流网络,并在网络上运行最小割算法来识别密度最大的子图。

伪代码:

```
function densest_subgraph(graph):
   S = "source"
   T = "sink"
   m = number_of_edges(graph)
   n = number_of_nodes(graph)
    function construct_flow_network(g):
        flow_graph = create_directed_graph()
        flow_graph.add_node(S)
        flow_graph.add_node(T)
        for each edge (u, v) in graph:
            flow_graph.add_edge(u, v, capacity=1)
            flow_graph.add_edge(v, u, capacity=1)
        for each node in graph:
            d_i = degree(node)
            flow_graph.add_edge(S, node, capacity=m)
            flow_graph.add_edge(node, T, capacity=m + 2 * g - d_i)
        return flow_graph
    function find_min_cut(flow_graph):
        cut_value, partition = minimum_cut(flow_graph, S, T)
        return partition[0] - {S}, partition[1] - {T}, cut_value
   1, u = 0, m
    xtol = 1 / (n * (n - 1))
   while u - 1 >= xtol:
        g = (u + 1) / 2
        flow_graph = construct_flow_network(g)
        V1, _, _ = find_min_cut(flow_graph)
        if V1 is not empty:
            1 = g
        else:
            u = g
    final_flow_graph = construct_flow_network(1)
   V1, _, _ = find_min_cut(final_flow_graph)
    return V1
```

Python实现:

```
def densest_subgraph(self):
   S = "S"
   T = "T"
   m = self.graph.number_of_edges()
   n = self.graph.number_of_nodes()
   def construct_flow_network(g):
        flow_graph = nx.DiGraph()
        flow_graph.add_node(S)
        flow_graph.add_node(T)
        for u, v in self.graph.edges():
            flow_graph.add_edge(u, v, capacity=1)
            flow_graph.add_edge(v, u, capacity=1)
        for node, d_i in self.graph.degree:
            flow_graph.add_edge(S, node, capacity=m)
            flow_graph.add_edge(node, T, capacity=m + 2 * g - d_i)
        return flow_graph
    def find_min_cut(flow_graph):
        cut_value, partition = nx.minimum_cut(flow_graph, S, T)
        reachable, non_reachable = partition
        return reachable - {S}, non_reachable - {T}, cut_value
    1, u = 0, m
   xtol = 1 / (n * (n - 1))
   while u - 1 >= xtol:
        g = (u + 1) / 2
        flow_graph = construct_flow_network(g)
        V1, _, _ = find_min_cut(flow_graph)
        if len(V1) != 0:
            1 = g
        else:
            u = g
   V1 = find_min_cut(construct_flow_network(1))[0]
    return [self.reverse_mapping[node] for node in V1], Graph.density(
        self.graph.subgraph(V1)
    )
```

3. k-clique分解

算法说明:

k-clique分解用于在图中查找所有包含k个节点的完全子图。使用Bron-Kerbosch算法进行最大团的查找,然后过滤出包含k个节点的子图。

伪代码:

```
function bron_kerbosch(R, P, X, cliques):
    if P and X are both empty:
        cliques.append(R)
        return
    for each vertex in P:
        bron_kerbosch(R union {vertex}, P intersect neighbors(vertex), X intersect neighbors(ver
        P.remove(vertex)
        X.add(vertex)
function find_maximal_cliques(graph):
    cliques = []
    bron_kerbosch(set(), set(graph.nodes()), set(), cliques)
    return cliques
function k_clique_decomposition(graph, k):
    cliques = find_maximal_cliques(graph)
    k_cliques = filter(clique for clique in cliques if size(clique) == k)
    return k_cliques
```

Python实现:

```
def bron_kerbosch(self, r, p, x, cliques):
   if not p and not x:
        cliques.append(r)
        return
   for v in list(p):
        self.bron_kerbosch(
            r | {v},
            p & set(self.graph.neighbors(v)),
            x & set(self.graph.neighbors(v)),
            cliques,
        )
        p.remove(v)
        x.add(v)
def find_maximal_cliques(self):
    cliques = []
    self.bron_kerbosch(set(), set(self.graph.nodes()), set(), cliques)
    return cliques
def k_clique_decomposition(self, k):
    cliques = self.find_maximal_cliques()
    k_cliques = [clique for clique in cliques if len(clique) == k]
    k_{cliques} = [
        [self.reverse_mapping[node] for node in clique] for clique in k_cliques
    return k_cliques
```

4. k-vcc分解

算法说明:

k-vcc分解用于找到图中所有的k-顶点连通分量。k-顶点连通分量是指任意移除k-1个顶点后,图仍然保持连通。使用全局割和重叠分区的思想,通过递归方式找到所有k-vcc。

伪代码:

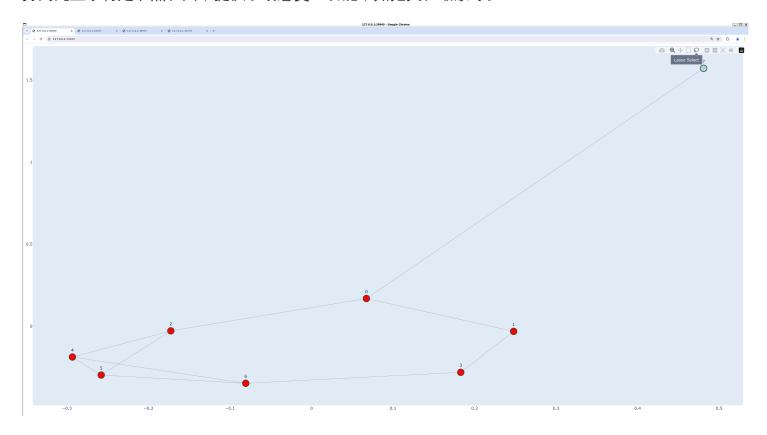
```
function global_cut(graph, k):
    for each pair of nodes (u, v):
        if node_connectivity(u, v) < k:</pre>
            cutset = minimum_node_cut(u, v)
            if size(cutset) < k:</pre>
                return cutset
    return null
function overlap_partition(graph, S):
    subgraphs = []
    graph.remove_nodes(S)
    for each component in connected_components(graph):
        component_with_S = component union S
        subgraph = subgraph_of(graph, component_with_S)
        subgraphs.append(subgraph)
    return subgraphs
function kvcc_enum(graph, k):
    k vccs = []
    G_k_core = k_core_decomposition(graph, k)
    for each component in connected_components(G_k_core):
        cutset = global_cut(subgraph_of(G_k_core, component), k)
        if cutset is null:
            k_vccs.append(subgraph_of(G_k_core, component))
            break
        subgraphs = overlap_partition(subgraph_of(G_k_core, component), cutset)
        for each subgraph in subgraphs:
            k_vccs.extend(kvcc_enum(subgraph, k))
    return k_vccs
function k_vcc(graph, k):
    k_vccs = kvcc_enum(graph, k)
    return k_vccs
```

Python实现:

```
@staticmethod
def global_cut(graph, k):
    for u in graph.nodes():
        for v in graph.nodes():
            if u != v and nx.node_connectivity(graph, u, v) < k:</pre>
                cutset = nx.minimum_node_cut(graph, u, v)
                if len(cutset) < k:</pre>
                    return cutset
    return None
@staticmethod
def overlap_partition(graph, S):
    subgraphs = []
    graph.remove_nodes_from(S)
    for component in nx.connected_components(graph):
        component_with_S = set(component) | S
        subgraph = graph.subgraph(component_with_S).copy()
        subgraphs.append(subgraph)
    return subgraphs
@staticmethod
def kvcc_enum(graph, k):
    k_vccs = []
    G_k_core = nx.k_core(graph, k)
    for component in nx.connected_components(G_k_core):
        cutset = Graph.global_cut(G_k_core.subgraph(component), k)
        if not cutset:
            k_vccs.append(G_k_core)
            break
        subgraphs = Graph.overlap_partition(G_k_core.subgraph(component), cutset)
        for subgraph in subgraphs:
            k_vccs.extend(Graph.kvcc_enum(subgraph, k))
    return k_vccs
def k_vcc(self, k):
    k_vccs = Graph.kvcc_enum(self.graph, k)
    k vccs = [
        [self.reverse_mapping[node] for node in k_vcc.nodes()] for k_vcc in k_vccs
    return k_vccs
```

5. 图的可视化

为了更直观地展示图结构和算法结果,我们实现了图的可视化功能,使用 plotly 库来绘制图形,并支持高亮显示特定节点和团,提供了动态交互功能,如拖拽、缩放等。



在可视化过程中,我们特别关注了四种算法的结果展示,支持高亮显示算法运行结果,并动态交互。

```
def visualize(
   self,
   highlight_nodes=None,
    secondary_highlight_nodes=None,
   highlight_cliques=None,
   node_color="lightblue",
   node_size=20,
   edge_color="gray",
   with_labels=True,
):
    pos = nx.spring_layout(self.graph, k=0.3, iterations=100)
    if highlight_nodes:
        center_x = np.mean([pos[node][0] for node in highlight_nodes])
        center_y = np.mean([pos[node][1] for node in highlight_nodes])
        center = np.array([center_x, center_y])
        contraction_factor = 0.5
        for node in highlight nodes:
            pos[node] = center + contraction_factor * (pos[node] - center)
        expansion factor = 1.5
        for node in set(self.graph.nodes()) - set(highlight_nodes):
            pos[node] = center + expansion_factor * (pos[node] - center)
    edge_x, edge_y = [], []
    for edge in self.graph.edges():
       x0, y0 = pos[edge[0]]
       x1, y1 = pos[edge[1]]
        edge_x += [x0, x1, None]
        edge_y += [y0, y1, None]
    edge_trace = go.Scatter(
       x=edge_x,
        y=edge_y,
        line=dict(width=0.5, color=edge_color),
        hoverinfo="none",
        mode="lines",
    )
    node_x, node_y = zip(*pos.values())
    node_trace = go.Scatter(
        x=node_x,
```

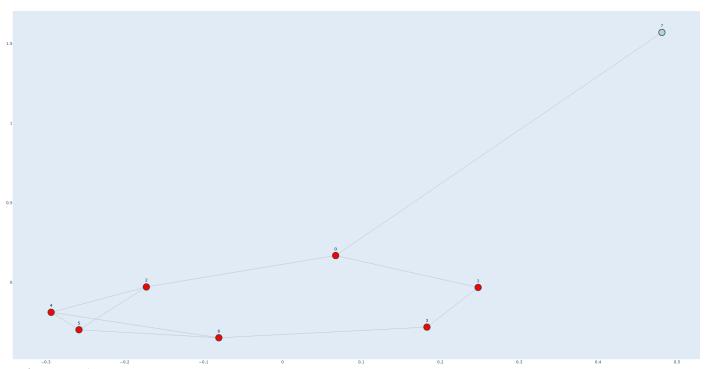
```
y=node_y,
    mode="markers+text" if with_labels else "markers",
    marker=dict(size=node_size, color=node_color, line_width=2),
    text=list(self.graph.nodes()) if with_labels else None,
    hoverinfo="text" if with_labels else "none",
    textposition="top center" if with_labels else None,
)
fig = go.Figure(
    data=[edge_trace, node_trace],
    layout=go.Layout(
        showlegend=False,
        hovermode="closest",
        margin=dict(b=0, l=0, r=0, t=0),
        xaxis=dict(showgrid=False, zeroline=False),
        yaxis=dict(showgrid=False, zeroline=False),
    ),
)
if highlight_nodes:
    highlight_x, highlight_y = zip(*[pos[node] for node in highlight_nodes])
    highlight_trace = go.Scatter(
        x=highlight_x,
        y=highlight_y,
        mode="markers+text" if with_labels else "markers",
        marker=dict(size=node_size, color="red", line_width=2),
        text=highlight_nodes if with_labels else None,
        hoverinfo="text" if with_labels else "none",
        textposition="top center" if with_labels else None,
    fig.add_trace(highlight_trace)
if secondary_highlight_nodes:
    secondary_highlight_x, secondary_highlight_y = zip(
        *[pos[node] for node in secondary_highlight_nodes]
    )
    secondary_highlight_trace = go.Scatter(
        x=secondary_highlight_x,
        y=secondary_highlight_y,
        mode="markers+text" if with_labels else "markers",
        marker=dict(size=node_size, color="green", line_width=2),
        text=secondary_highlight_nodes if with_labels else None,
        hoverinfo="text" if with_labels else "none",
```

```
textposition="top center" if with_labels else None,
    )
    fig.add_trace(secondary_highlight_trace)
colors = itertools.cycle(
    ["orange", "purple", "cyan", "magenta", "yellow", "green", "blue", "red"]
)
if highlight_cliques:
   for clique in highlight_cliques:
        color = next(colors)
        clique_x, clique_y = zip(*[pos[node] for node in clique])
        clique_trace = go.Scatter(
            x=clique_x,
           y=clique_y,
            mode="markers+text" if with_labels else "markers",
            marker=dict(size=node_size, color=color, line_width=2),
            text=clique if with_labels else None,
            hoverinfo="text" if with_labels else "none",
            textposition="top center" if with_labels else None,
        fig.add_trace(clique_trace)
fig.show()
```

为了展示四种算法的结果,我们在 tiny.txt 图上运行了这四种算法,并将结果可视化。 原数据与输出结果保存在report/tiny_data文件夹中。

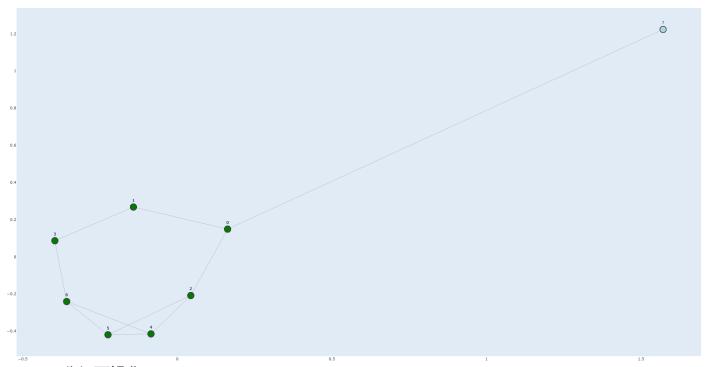
• k-core分解可视化:

```
python main.py data/tiny.txt k_core --k 2 --visualize --with-labels
```



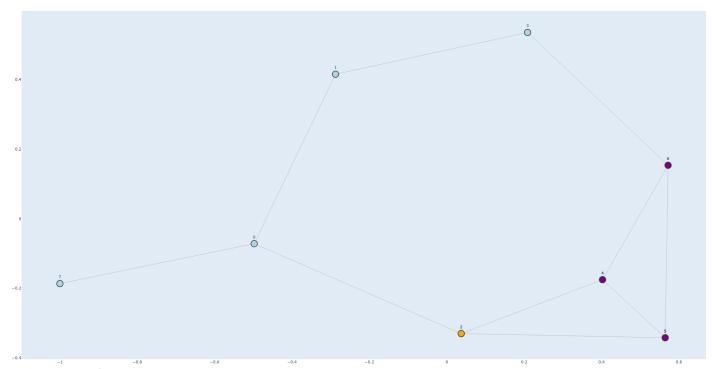
• 最密子图可视化:

python main.py data/tiny.txt densest_subgraph --k 3 --visualize --with-labels



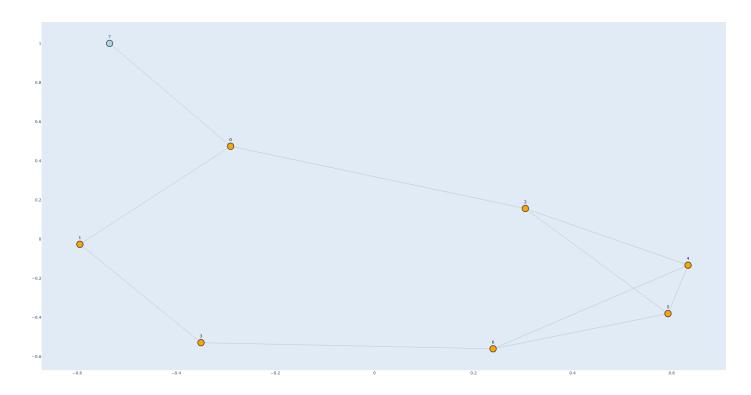
• k-clique分解可视化:

python main.py data/tiny.txt k_clique_decomposition --k 2 --visualize



• k-vcc分解可视化:

python main.py data/tiny.txt k_vcc --k 2 --visualize --with-labels



6. 测试与验证

为了确保实现的算法正确性,我们通过详细的单元测试用例对其进行验证。四种算法均在不同类型的随机图上进行了测试,包括Erdos-Renyi图、尺度无关图、小世界图和稀疏图,然后与 NetworkX 库的实现、或第三方 C++ 实现进行对比。

可以看到,所有算法在这些图上的表现都符合预期,能够正确找到对应的结构。这充分保证了我们实现的算法的正确性。



值得一提的是,我们还略加修改了 panjd/KVCC 的 C++ 实现(见 $tests/third-party/k_vcc),作为我们的测试对照。经过测试,我们的 Python 实现能通过对 <math>KVCC$ 的验证,且与 C++ 实现的结果一致,进一步证明了我们实现的正确性。

测试用例: test_kvcc.py

```
import os
import unittest
import subprocess
from graphmaster.graph import Graph
import networkx as nx
from itertools import combinations
def run_cpp_program(graph_file, k, executable, cwd, output_file):
    result = subprocess.run(
        os.path.join(cwd, executable),
            "-g",
            graph_file,
            "-k",
            str(k),
            "-o",
            output_file,
        ],
        capture_output=True,
        text=True,
        check=True,
        cwd=cwd,
    )
    return result.stdout
def parse_cpp_output(output_file):
    with open(output_file, "r") as f:
        lines = f.readlines()
    kvccs = []
    current kvcc = []
    for line in lines:
        if line.startswith("Node num"):
            if current_kvcc:
                kvccs.append(current_kvcc)
                current_kvcc = []
        else:
            try:
                nodes = list(map(int, line.split()))
```

```
if nodes:
                    current_kvcc.extend(nodes)
            except ValueError:
                continue # Ignore lines that can't be parsed
    if current_kvcc:
        kvccs.append(current_kvcc)
    return kvccs
class TestKVCC(unittest.TestCase):
   @classmethod
    def setUpClass(cls):
        cls.cwd = os.path.join(os.path.dirname(__file__), "third-party", "k_vcc")
        cls.executable = os.path.join(cls.cwd, "kvcc_baseline")
        cls.output_file = os.path.join(cls.cwd, "kvcc_output.txt")
        try:
            result = subprocess.run(
                ["make"],
                check=True,
                stderr=subprocess.PIPE,
                stdout=subprocess.PIPE,
                cwd=cls.cwd,
        except subprocess.CalledProcessError as e:
            print("Compilation failed:")
            print(e.stderr.decode())
            raise
    @classmethod
    def tearDownClass(cls):
        try:
            subprocess.run(
                ["make", "clean"],
                check=True,
                stderr=subprocess.PIPE,
                stdout=subprocess.PIPE,
                cwd=cls.cwd,
        except subprocess.CalledProcessError as e:
            print("Clean up failed:")
            print(e.stderr.decode())
```

```
raise
    if os.path.exists(cls.output_file):
        os.remove(cls.output_file)
def setUp(self):
   self.num_nodes = 20
    self.edge_prob = 0.05
    self.k = 3
    self.graphs = {
        "erdos_renyi": nx.erdos_renyi_graph(self.num_nodes, self.edge_prob),
        "scale_free": nx.barabasi_albert_graph(self.num_nodes, 3),
        "small_world": nx.watts_strogatz_graph(self.num_nodes, 4, 0.1),
        "sparse": nx.gnm random graph(self.num nodes, 15),
    }
    self.graph instances = {
        name: self.create_graph_instance(g) for name, g in self.graphs.items()
    }
def create_graph_instance(self, nx_graph):
   g = Graph()
   for u, v in nx_graph.edges():
        g.add_edge(u, v)
    return g
def save_graph_to_file(self, graph, filename):
   with open(filename, "w") as f:
        f.write(f"{graph.number_of_nodes()} {graph.number_of_edges()}\n")
        for u, v in graph.edges():
            f.write(f"{u + 1} {v + 1}\n")
def verify_kvcc(self, k_vcc, k):
    for subset in combinations(k_vcc.nodes, k - 1):
        subgraph = k_vcc.copy()
        subgraph.remove_nodes_from(subset)
        if not nx.is_connected(subgraph):
            return False
    return True
def verify_maximality(self, graph, k_vcc, k):
   nodes = set(k_vcc)
    for node in graph.nodes:
        if node not in nodes:
            new_nodes = nodes | {node}
```

```
subgraph = graph.subgraph(new_nodes).copy()
                if self.verify_kvcc(subgraph, k):
                    return False
        return True
    def verify_kvcc_results(self, graph, k_vccs, k):
        for k_vcc in k_vccs:
            if not self.verify_kvcc(graph.subgraph(k_vcc), k):
                return False
            if not self.verify_maximality(graph, k_vcc, k):
                return False
        return True
   def test_kvcc(self):
        for graph_name, graph in self.graphs.items():
            with self.subTest(graph=graph_name):
                graph_wrapper = self.create_graph_instance(graph)
                python_kvccs = graph_wrapper.k_vcc(self.k)
                self.assertTrue(self.verify_kvcc_results(graph, python_kvccs, self.k))
                graph_file = os.path.join(self.cwd, f"{graph_name}.txt")
                self.save_graph_to_file(graph, graph_file)
                run_cpp_program(
                    graph_file, self.k, self.executable, self.cwd, self.output_file
                )
                cpp_kvccs = parse_cpp_output(self.output_file)
                cpp_kvccs = [
                    [node - 1 for node in kvcc] for kvcc in cpp_kvccs
                ]
                for python_kvcc in python_kvccs:
                    self.assertIn(sorted(python_kvcc), sorted(cpp_kvccs))
                os.remove(graph_file)
if __name__ == "__main__":
   unittest.main()
```

7. 总结与展望

通过本次实验,我们成功实现了多个图挖掘算法,并通过详细的测试验证了它们的正确性。项目采用模块化设计,具备良好的扩展性和可维护性。在未来的工作中,我们可以进一步优化算法的性能,探索更多图挖掘算法,并将其应用于实际的图数据分析中。

本实验不仅加深了我们对图算法的理解,也提升了我们在实际工程项目中应用这些算法的能力。通过与C++实现的对比,我们对算法的正确性和效率有了更深刻的认识,为未来的研究和应用奠定了坚实的基础。通过 plotly 库的可视化功能,我们能够直观地展示算法的运行结果,增强了算法结果的解释性和易用性。