

# Chapter 1

## Modularity and Neural Networks

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### 1.1 Introduction

Community detection is useful unsupervised way to understand more information about a graph. One way to do community detection is by maximizing a global property of the graph known as modularity. Maximizing modularity has been used in a wide variety of applications with some success in not only biological networks, but other social networks and beyond for community detection [9] [11]. Specifically, modularity maximization techniques have been shown to out perform other community detection algorithms [11].

A lot is known about the human brain, but seemingly nothing is known about it. To study the human brain scientists typically look at different, more simple examples of connections between neurons, also known as *connectomes*. Mapping and knowing the functionality of connectomes is a hard problem because someone has to look at when a stimulus is received, what neurons fire when and where. Since these are structures of neurons, it seems like a good assumption that these neurons would form topologically dense communities in order to send information where it needs to go.

### 1.2 The Problem as a Graph

Individual neurons can be thought of as nodes, and each neuron has two types of connectors, either gap junctions or chemical synapses.[12] Chemical synapses as seen in Figure 1.1, can have 1, 2, or 3 directed outputs to another neuron, while similarly, gap junctions can have multiple outputs, but these outputs are undirected as the electrical flow can technically flow either way [12].

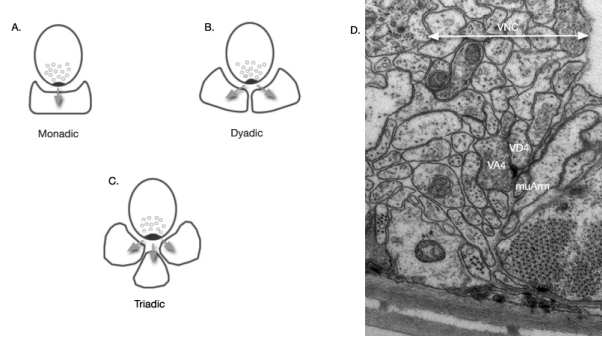


Figure 1.1: A view of the neurons and their chemical synapses [3]

### 1.3 Some Realistic Data Sets

The *c. elegans* is a transparent roundworm that has had all of its neurons mapped along with all of the connections. There are a total of 279 neurons, and between them there are around 6393 chemical synapses and 890 electrical gap junctions[3]. Each neuron has an attribute of whether the neuron itself is either a motor, sensory, or inter neuron (or a combination of), and the distribution of those are roughly equal across neurons [3].

The worm data is the only complete data, but there does exist partial data for other animals including partial data from flies, cats, macaques, mice, rats, and humans. Bigger datasets to be used in the enhanced implementation. This will include these partial datasets like the connectome of a mouse retina, which is 1123 neurons and 577350 connections between neurons [7].

### 1.4 Louvain-A Key Graph Kernel

Modularity,  $Q$ , is a measure of how dense a community is compared to how dense a community is expected to be. This is defined as the following [4]

$$Q = \frac{1}{2m} \sum_{i,j} [A_{ij} - \frac{k_i k_j}{2m}] \delta(c_i, c_j)$$

where  $2m$  is the weight of all edges,  $A_{ij}$  is the weight between  $i$  and  $j$ ,  $k_i$  and  $k_j$  are the total weights attached to each  $i$  and  $j$ , and  $c_i$  and  $c_j$  are the communities. The goal is to find which combinations of nodes when grouped into certain communities, which combination maximizes modularity.

#### 1.4.1 Undirected Louvain

Since the goal is to maximize modularity, the approach of the Louvain algorithm is greedy optimization. To do this, the algorithm first starts with every node in its own community [4]. Next, each node is put into a neighboring community and the change in modularity is calculated by

$$\Delta Q = [\frac{\sum_{in} + k_{i,in}}{2m} - (\frac{\sum_{tot} + k_i}{2m})^2] - [\frac{\sum_{in}}{2m} - (\frac{\sum_{tot}}{2m})^2 - (\frac{k+i}{2m})^2]$$

where  $\sum_{in}$  are the total weights inside community  $C$ ,  $\sum_{tot}$  is the sum of edges of the links incident to nodes in  $C$ ,  $k_i$  are the sum of incident links of node  $i$ , and  $k_{i,in}$  is the sum of weights from  $i$  in  $C$  with  $m$  being the total sum of weights in the network [4].

## Louvain

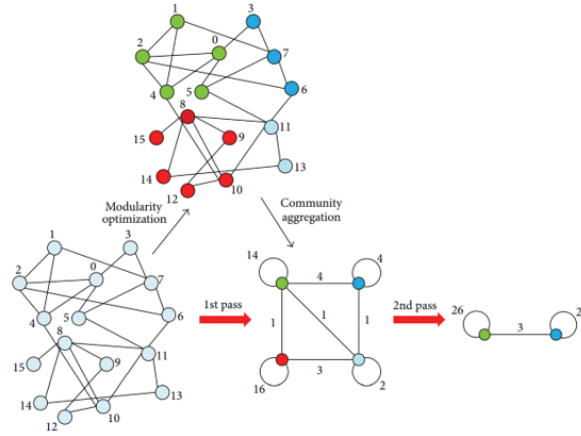


Figure 1.2: Example of the Louvain Algorithm [8]

The other half of the algorithm takes the previous phase, and turns each community into its own node with a self loop with the weight of all the edges of all the nodes inside the community. When this finishes, the process goes back to the first half, and the process is repeated until modularity no longer increases between iterations. This process is shown visually in figure 1.2.

### 1.4.2 Resolution Limit

One of the problems with maximizing modularity is that there is a problem known as the "resolution limit". Since the formula for modularity is a global property and uses the strength within a community compared to the strength between communities, in some networks the strength between real communities may be so close to the strength between communities that modularity may be optimized if a strong link between two communities is joined into one community [6].

A solution proposed to solve this problem is to introduce a time-scale parameter  $t$  to help stabilize modularity giving the formula [10]

$$Q_{NL}(t) = (1 - t) + \frac{1}{2m} \sum_{i,j} [A_{ij}t - \frac{k_i k_j}{2m}] \delta(c_i, c_j)$$

### 1.4.3 Directed Louvain

Although modularity is usually defined for unweighted graphs, in directed graphs it can be defined as

$$Q_d = \frac{1}{m} \sum_{i,j} [A_{ij} - \frac{d_i^{in} d_j^{out}}{m}] \delta(c_i, c_j)$$

where the only difference is that  $m$  is now the weight of all the arcs (directed edges), and  $d^{in}$  stands for the in degree of  $i$  while  $d_j^{out}$  stands for the out degree of  $j$  [5].

Similarly, change in modularity can be defined as

$$\Delta_{Q_d} = \frac{d_i^C}{m} - \left[ \frac{d_i^{out} \sum_{tot}^{in} + d_i^{in} \sum_{in}^{out}}{m^2} \right]$$

where  $\sum_{tot}^{in}$  is the sum of all in-going arcs into community  $C$ , and  $\sum_{tot}^{out}$  are all the out-going arcs out of community  $C$  [5].

#### 1.4.4 Psuodcode

The psuodcode of the algorithm appears to run with time complexity  $O(n \log n)$ , because at every step nodes are guaranteed to join a community, meaning the number of communities will decrease every time giving it a  $\log n$  appearance. Though it can be argued that the time complexity is actually closer  $O(n^2)$  because if only 1 node joins a community at a time, then the algorithm has to run  $n$  times for  $n$  number of nodes. The psuodcode is as follows [9]

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#### Algorithm 1 Louvain

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```

1:  $V$ : a set of vertices
2:  $E$ : a set of edges
3:  $W$ : a set of weights of edges, initialized to 1
4:  $G \leftarrow (V, E, W)$ 
5: repeat
6:    $C \leftarrow \{\{v_i\} | v_i \in G(V)\}$ 
7:   Calculate current modularity  $Q_{cur}$ 
8:    $Q_{new} \leftarrow Q_{cur}$ 
9:    $Q_{old} \leftarrow Q_{new}$ 
10:  repeat
11:    for  $v_i \in V$  do
12:       $Q_{new} \leftarrow Q_{cur}$ 
13:      remove  $v_i$  from its current community
14:       $N_{v_i} \leftarrow \{c_k | v_i \in G(V), v_j \in c_k, e_{ij} \in G(E)\}$ 
15:      find  $c_x \in N_{v_i}$  that has  $max \Delta Q_{\{v_i\}, c_x} > 0$ 
16:      Calculate new modularity  $Q_{new}$ 
17:    until no membership change or  $Q_{new} = Q_{cur}$ 
18:     $V' \leftarrow \{c_i | c_i \in C\}$ 
19:     $E' \leftarrow \{e_{ij} | \forall e_{ij} \text{ if } v_i \in C_i, v_j \in C_j, \text{ and } C_i \neq C_j\}$ 
20:     $W' \leftarrow \{w_{ij} | \sum w_{ij}, \forall e_{ij} \text{ if } v_i \in C_i \text{ and } v_j \in C_j\}$ 
21:  until  $Q_{new} = Q_{old}$ 

```

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## 1.5 Prior and Related Work

This is space to add in discussion of **prior work** - work on the same problem or kernel that your paper assumes, and **related work** - work on the same application but using different approach or kernel, or a different but similar application..

## 1.6 A Sequential Algorithm

The initial sequential algorithm can be simply generated by following the psuodcode in section 1.4. The implementation in the next section uses dendograms [2] for processing and NetworkX uses hash tables [1] for the storage of graphs, although this isn't the most efficient, it is simple and easy to implement.

## 1.7 A Reference Sequential Implementation

For my implementation, I used NetworkX (python), as there already existed a library that implemented Louvain [2], but this library did not support directed graphs, so I had to change the definition of modularity from the original

```

inc = dict([])
deg = dict([])
links = graph.size(weight=weight)
if links == 0:
    raise ValueError("A graph without link has an undefined modularity")

for node in graph:
    com = partition[node]
    deg[com] = deg.get(com, 0.) + graph.degree(node, weight=weight)
    for neighbor, datas in graph[node].items():
        edge_weight = datas.get(weight, 1)
        if partition[neighbor] == com:
            if neighbor == node:
                inc[com] = inc.get(com, 0.) + float(edge_weight)
            else:
                inc[com] = inc.get(com, 0.) + float(edge_weight) / 2.

res = 0.
for com in set(partition.values()):
    res += (inc.get(com, 0.) / links) - \
        (deg.get(com, 0.) / (2. * links)) ** 2
return res

```

to the now directed version of modularity.

```

inc = dict([])
deg = dict([])
links = graph.size(weight=weight)
if links == 0:
    raise ValueError("A graph without link has an undefined modularity")

for node in graph:
    com = partition[node]
    deg[com] = deg.get(com, 0.) + graph.out_degree(node, weight=weight)
    deg2[com] = deg.get(com, 0.) + graph.in_degree(node, weight=weight)
    for neighbor, datas in graph[node].items():
        edge_weight = datas.get(weight, 1)
        if partition[neighbor] == com:
            if neighbor == node:
                inc[com] = inc.get(com, 0.) + float(edge_weight)
            else:
                inc[com] = inc.get(com, 0.) + float(edge_weight) / 2.

```

```

res = 0.
for com in set(partition.values()):
    res += (inc.get(com, 0.) / links) - \
           (deg.get(com, 0.) * deg2.get(com, 0.) / (links))
return res

```

The main thing that was changed that it now uses both in and out degrees, instead of just total degree and dividing by 2.

## 1.8 Sequential Scaling Results

Since the worm database was small enough, this was able to run on my computer in under a second. The parameter that was varied was  $t$ , the resolution value, explained in 1.4.2. My thought process was that because there were less communities generated, and the algorithm starts at every node being in its own community, that would imply that it would take longer to converge to fewer communities and that a resolution of 1 would take the longest. This is ignoring the intuition of what the time-scaling is doing though, as  $t \rightarrow 0$ , the communities are more fine-grained and more nodes are less likely to switch communities at each time step, making the algorithm closer to worst case [10].

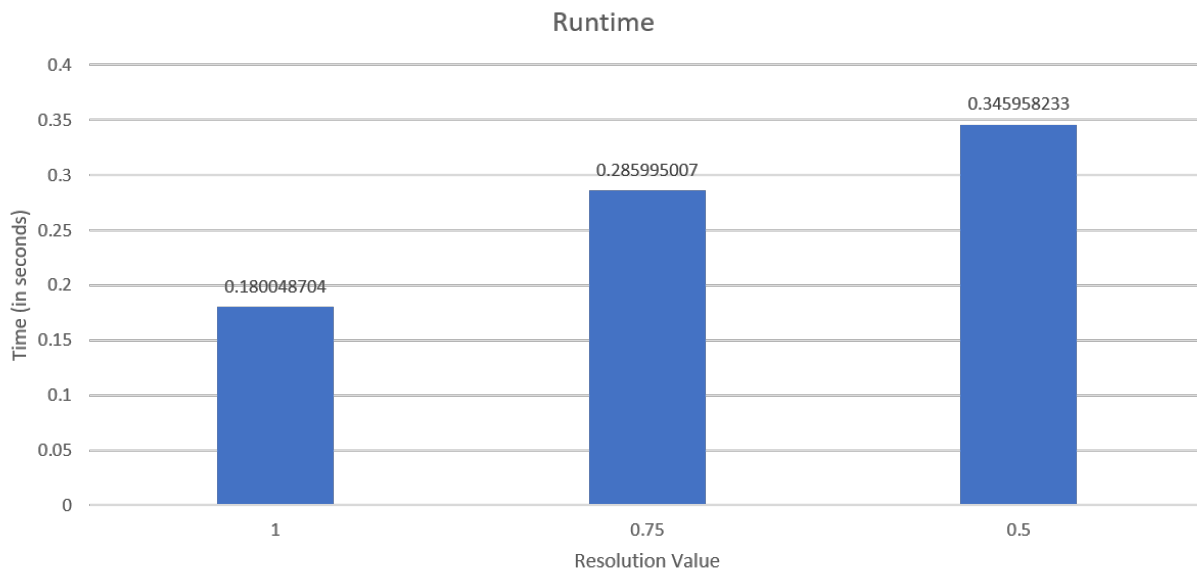


Figure 1.3: Runtime as resolution value decreases

## 1.9 An Enhanced Algorithm

Discuss here the outlines of an enhanced algorithm. This could be a parallel code, a code with some significant heuristics, or a code written in a non-traditional programming paradigm. Pseudocode is fine. Discuss what you think is the computational complexity.

## **1.10 A Reference Enhanced Implementation**

Discuss here an implementation of the enhanced algorithm. Include what language/paradigm you used for the code.

## **1.11 Enhanced Scaling Results**

Discuss here results from the enhanced algorithm. Include software and hardware configuration, where the input graph data sets came from, and how input data set characteristics were varied. Ideally plots of performance vs BOTH problem size changes AND hardware resources are desired. Did the performance as a function of size vary as you predicted?

## **1.12 Conclusion**

Summarize your paper. Discuss possible future work and/or other options that may make sense.

## **1.13 Response to Reviews**

The paper before did not include enough detail in the first few sections, so more was added in terms of motivation, along with some sprinkles of more intuition of ideas, along with a new subsection of a topic I forgot to touch on, resolution limits, and adding to the discussion of time complexity. I also fixed some graphical glitches where the pseudocode wasn't in the pseudocode section.

# Bibliography

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