Approaches to Brain Parcellation using Energy Statistics and Graph Partitioning

Felix Xiao

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Chapter 1

Local Search and Graph Growing Heuristics

We introduce several algorithms for generating brain parcellations. The algorithms in this chapter are all local search heuristics; they begin with N unconnected vertices and iteratively join adjacent ones into components until some stopping criterion is met.

For each algorithm, the resulting parcellation is presented, discussed, and evaluated according to the criteria introduced in the previous chapter.

1.1 Unconstrained Add-Edge

The first and simplest algorithm starts with an empty graph of N vertices and sequentially adds edges between adjacent voxels in order of highest sample distance correlation, until the graph has some prespecified number of connected components K.

We will refer to this algorithm as "Unconstrained Add-Edge". A naive implementation of would re-compute the number of connected components in the graph (using linear-time bread-first or depth-first search) after each addition of an edge, resulting in a costly $O(EN)$ time complexity. A more efficient implementation takes advantage of the fact that each addition of an edge decreases the number of components in the graph by at most 1. Hence the algorithm needs only to compute the number of connected components after adding $k - K$ edges, where k is the current number of connected components of the graph, beginning at N.

```
k := N
i := 1
while k > K
    repeat k - K times
        add the ith highest-weighted edge to the graph
```

```
        i := i + 1
    end
    k := compute number of connected components
end
```

Another implementation uses a binary search-type strategy and is $O((N+E)\log E)$. The idea is to "search" for the last edge to add to the graph by maintaining a range of possible last edges. In each iteration, the algorithm would add to the graph edges 1 to the midpoint of this range, compute the number of connected components, and adjust the range based on whether the number of components is higher or lower than the target K.

```
l := 1
h := E
repeat
    m := (l + h) / 2
    add edges from 1 to m to an empty graph
    k := compute number of connected components
    if k = K
        done
    else if k < K
        h := m
    else if k > K
        l := m
    end
end
```

The Unconstrained Add-Edge algorithm produces severely imbalanced parcellations. In the 100-component graph, there was one component containing over 99.9% of all the vertices in the graph. The following algorithm introduces a modification that address this issue.

1.2 Size-Constrained Add-Edge

The Size-Constrained Add-Edge algorithm works in a similar manner to the Unconstrained version, adding edges to the graph in decreasing order of distance correlation. The Size-Constrained version differs by applying a filter to each edge considered, adding the edge only if at least one of the two following conditions are met:

1. At least one of the two components bridge by the edge is of size less than some prespecified parameter $s_{\min}$.
2. The union of the two components is of size $\leq s_{\max}$.

Letting K denote the target number of components in the graph, the Size-Constrained Add-Edge algorithm can be written as:

```
sort edges in decreasing energy correlation order
k := N, number of components
for e = 1, ..., E
    (i, j) := vertices of edge e
    I := component containing i
    J := component containing j
    if I = J
        continue
    else if (size(I) < s_min or size(J) < s_min)
            or size(I + J) <= s_max
        add e to the graph
        k := k - 1
        if number of components = K
            break
        end
    end
end
```

The naive implementation must use BFS/DFS in each iteration to compute the size of components I and J, and hence must have time complexity $O(EN)$. Fortunately, there is a way to sub-linearly update information on the components of the graph, using the union-find data structure.

1.2.1 Union-Find

The core Union-Find data structure begins with an empty graph of N vertices and supports two operations. union(i, j) adds an edge between vertices i and j. root(i) returns an identifier for the component to which vertex i belongs. All vertices in the same component have the same root. We modified Union-Find to support an additional operation. component_size(i) returns the number of vertices belonging to the component containing i.

Union-Find represents each component as a rooted tree, with vertices in the graph mapping to nodes in the tree. Information about the tree is stored in two arrays of length N, parent and size, which are subject to the following invariants.

1. For each node i, parent[i] = node i's parent on the tree, unless i is a root node. If i is a root node, then parent[i] = i.

2. Nodes i and j are in the same component if and only if they are in the same tree, if and only if they share the same root node.

3. If i is a root node, then size[i] = the size of the component, or the number of nodes in the tree. If i is not a root node, then size[i] can be anything.

A baseline implementation of the three functions is

```
function root(i)
    while parent[i] != i
        i := parent[i]
    end
    return i
end

function union(i, j)
    parent[root(j)] := root(i)
end

function component_size(i)
    return size[root(i)]
end
```

In addition to the baseline code above, there are two important optimizations:

1. Weighted union maintains information of the sizes of each component so that the root of the smaller component always becomes a child of the larger component's root.

2. Path compression flattens the tree with each call to root. Specifically, when root is called on node i, each node traversed from i to the root has its parent set to be the root.

With these two optimizations, the time complexity of root, union, and component_size was proven in (Hopcroft 1973) to be at least as good as $O(\log^* N)$ where $\log^*$ is the iterated logarithm, defined as the number of times the natural log must be applied to N so that it becomes less than or equal to 1.

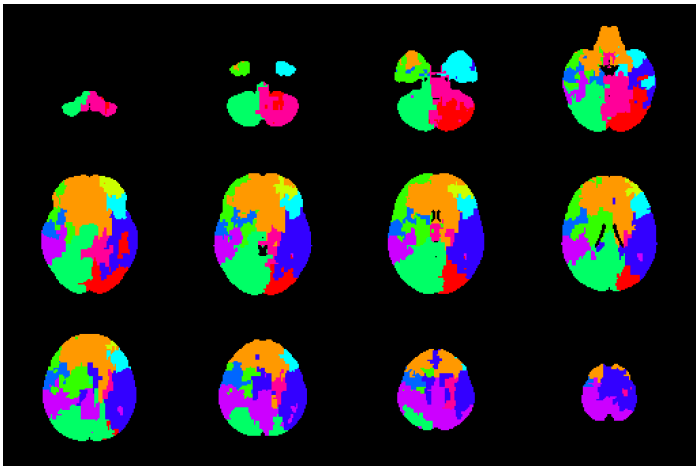
1.2.2 Results of Size-Constrained Add-Edge Parcellation

We ran Size-Constrained Add-Edge on the distance correlation graph and on a copy of the graph with randomized edge weights. We used parcellation criteria discussed in chapter 3 to evaluate the quality of the two resulting parcellations on the fMRI data used to generate the distance correlation graph. The results of the in-sample evaluation are shown in the table below:

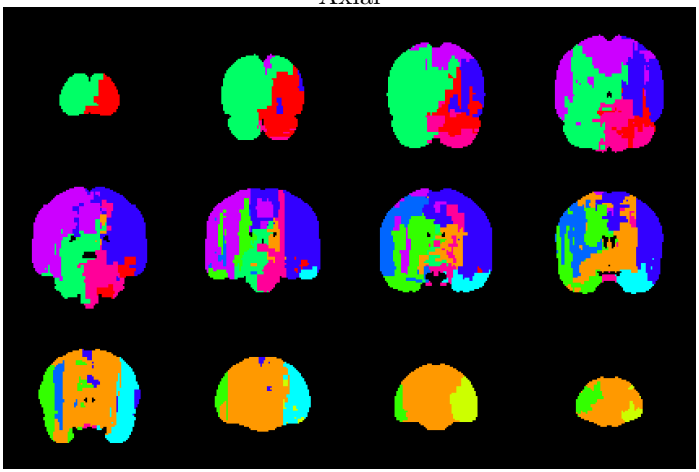
$s_{\min}$	$s_{\max}$	Within	Adjacent	Between	Boundary
1000	15000	0.314	0.726	0.296	0.521
1000	10000	0.313	0.719	0.306	0.517
1000	7500	0.328	0.721	0.313	0.514
1000	5000	0.320	0.727	0.303	0.516
1500	10000	0.318	0.711	0.315	0.518
750	10000	0.313	0.721	0.302	0.521
500	10000	0.318	0.718	0.307	0.521
	Random	0.304	0.705	0.295	0.719

The criterion that has seen the most significant improvement compared with the random graph parcellation is the Boundary-Score, with a decrease from 0.719 in the random graph parcellation to the range of 0.514 - 0.521. The Within- and Adjacent-Scores saw smaller but still noticeable improvements, and Between-Score saw no improvement from the random baseline.

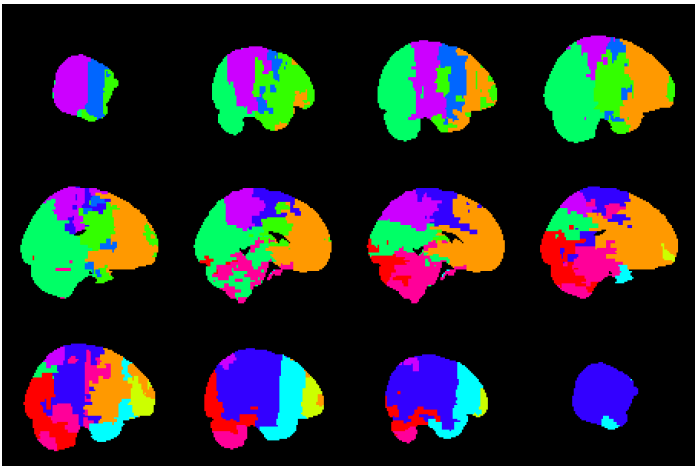
We display the parcellation obtained from setting parameters $s_{\min} = 1000$ and $s_{\max} = 7500$ below. While the sizes of the parcels are much more balanced than the result of the Unconstrained Add-Edge, there are still noticeable differences in parcel size.



Axial



Coronal



Sagittal

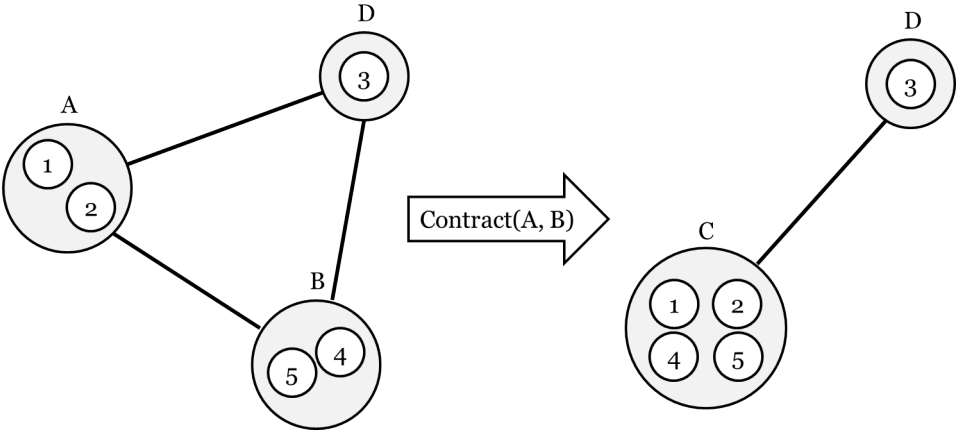
1.3 The Contractible Graph Data Structure and Edge-Contraction Algorithm

We propose a new data structure called the *Contractible Graph* (CG) for brain parcellation. The rationale behind the CG is a heuristic procedure for partitioning a graph into somewhat balanced components so as to minimize the Boundary-Score (**??**) or maximize the Adjacency-Score (**??**).

The CG is a mapping of the vertices of the original graph to the vertices of a new graph. The vertices of the CG are called *components* and between any two components there exists exactly one weighted edge, henceforth called a *link*. The weight of a link $w(A, B)$ between two components A and B in the CG equals the average weight of all edges in the original graph between vertices mapped to A and vertices mapped to B. If no such edges exist, the weight of the link is 0. Formally,

$$E(A, B) = \{(i, j) \in E : i \in A, j \in B\}$$

$$w(A, B) = \begin{cases} \frac{1}{|E(A,B)|} \sum_{(i,j)\in E(A,B)} w_{ij} & \text{if } |E(A, B)| > 0 \\ 0 & \text{otherwise} \end{cases}$$



The *size* of a component is the number of vertices it contains. A *contraction* of a link (A, B) in a CG replaces components A and B with a new component (call it C) containing all vertices mapped to A or B, as illustrated in the figure above. Component C has one link to every other component in the CG, whose weights are the mean of the weights of the corresponding vertex edges, or 0 if no edge exists. Thus the contraction operation maintains the link-invariant property of CG. This leads to the Edge-Contraction algorithm, which begins with the original graph with all vertices as singleton components and contracts edges in a certain order until the graph has only k components in all.

Algorithm 1 Edge-Contraction

Input: Undirected positive-weighted graph G and target component number k
Create a CG from G so that every vertex maps to a unique component
repeat
  $\mathcal{S} \leftarrow$ smallest component(s) in the CG
  $(A, B) \leftarrow \underset{A \in \mathcal{S}}{\operatorname{argmax}}\, w(A, B)$
  Contract (A, B)
until CG has k components
Output: Components of CG

Why does Edge-Contraction work better than the previous algorithms? The Edge-Contraction algorithm attempts to address two problems of the Size-Constrained Add-Edge algorithm: poor Adjacent-Score relative to randomized graph and unbalanced parcels. We hypothesized that one reason for a relatively low Adjacent-Score might be the following scenario: when a vertex is added to a component, it might have multiple edges to that component. One edge might have a very high weight; this is the one that is officially "added". However, the other edges with far lower weights are implicitly added as well, lowering the average edge weights within the component.

The Edge-Contraction algorithm handles this issue by maintaining that there

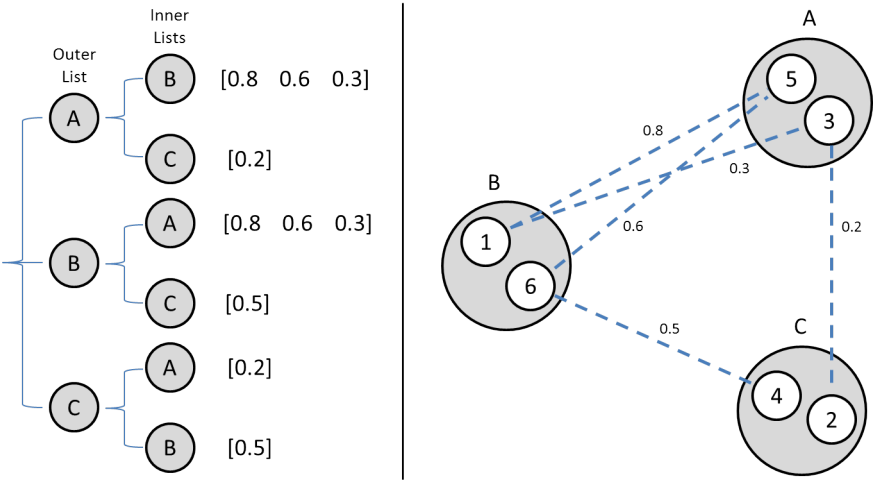
can be at most one edge between any two components A and B, and further that the weight on such an edge is the mean of the weights on all edges that connect a vertex in A with a vertex in B.

1.3.1 Implementation using Multi-Edge Adjacency List and Priority Queue

The adjacency list is the most common implementation choice for sparse graphs and it lists, for each node in the graph, the nodes connected to it by an edge and the weight of that edge.

In a Contractible Graph, the weight of the link between two components A and B depends on all edges between vertices in A and vertices in B. Therefore our implementation of the CG data structure uses an extended variant of the adjacency list that allows for multiple edges between two nodes.

The Multi-Edge Adjacency List associates every *pair* of components connected by a non-zero link to the set of edges that comprise that link. In **R**, this is achieved by a list of lists.



Implementing the contraction of components B and C into a new component D on this list of lists requires the following steps:

1. Compute $\mathcal{X}$, the set of all components that either B or C is linked to.
2. Create a new element in the outer list, D, and associate it with an empty inner list.
3. For each component $X \in \mathcal{X}$,
   - Find $E(X)$, the weights of the set of all edges connecting X to B and X to C.
   - Delete elements B and C from the inner list of X. Add a new element D and map it to $E(X)$.

- In the inner list of D, add a new element X and map it to $E(X)$.

4. Delete B and C from the outer list.

Incidentally, we note that it is also possible to implement the average edge property of the CG without the Multi-Edge Adjacency List, by recording for each pair of components, the *sum* of edge weights and the number of edges rather than a set of all original edge weights. This allows for a more space and time efficient implementation, but this simplification was unfortunately overlooked in the first implementation of Edge-Contract.

Having described the contraction step, we will next discuss how to efficiently locate the link to be contracted. In computer science, a *Priority Queue* data type is a set of ordered (in the sense that for any two objects one has greater or equal priority to the other) objects that supports the following operations:

- *add(obj)*: Adds an object to the set.
- *remove_minimum()*: Removes and returns an object with the smallest priority in the set.

Using the heap data structure, the above two operations both run in $O(\log n)$ time.

Each component on the CG will be associated with an element of the priority queue. The priority of component A is defined as

$$|A| - \max\ w(A)$$

where $w(A)$ is the set of weights of links between A and any other component. Since our graph edge weights are all between 0 and 1, the smallest priority element in the queue is the first to undergo contraction in our algorithm, provided the max link weight is up-to-date.

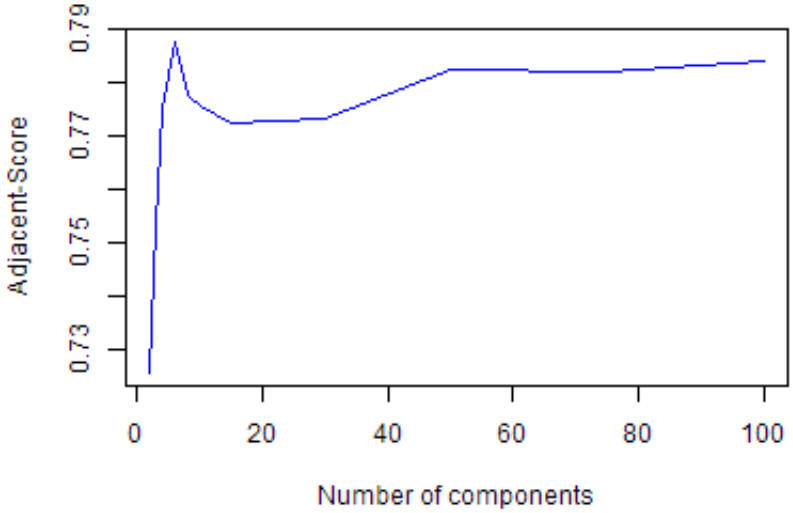
If components A and B are contracted, and there is a component C with positive links to both A and B, then the $C - A$ and $C - B$ links will be replaced by a $C - (AB)$ link with a different weight. If either $C - A$ or $C - B$ links happened to be the maximum-weighted links of C, then C's position on the priority queue may no longer be accurate, and its true position may be further down the queue.

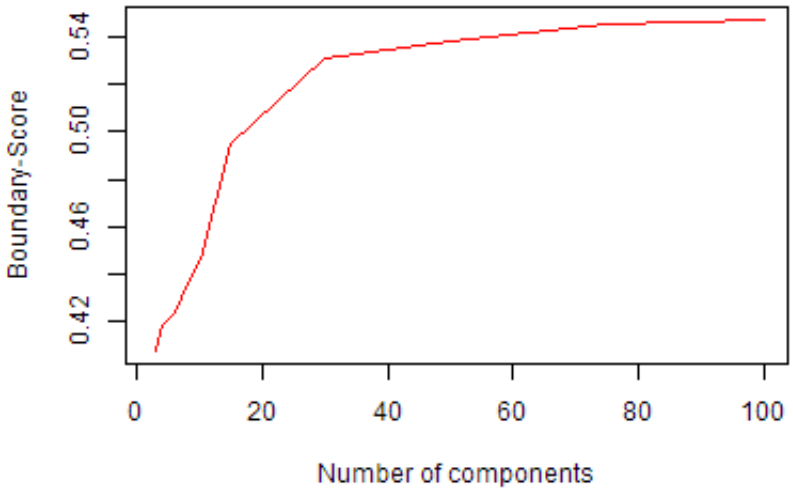
To address this issue, the max weight link of the minimum priority component must be re-computed when the element is removed from the queue. If the component's actual priority is not the minimum, then it is re-inserted into the queue with updated priority. Additionally, the minimum priority component may no longer exist in the CG due to contraction with another component. In this case it is simply discarded.

Without using an efficient priority queue, the linear searching method of finding the next link to contract results in a $O\big(n(n-k)\big)$ time algorithm. Using the priority queue the time complexity of Edge-Contraction is $O\big((n-k)(m+\log n)\big)$, where m is the average number of positve links a component has.

1.3.2 Optimal Number of Components

The Edge-Contraction algorithm has the benefit of requiring only one parameter, the target component number. We assessed the validity of EC parcellations with varying numbers of components. The plots below show how the Adjacent-Score and Boundary-Score varied according to the number of components in the EC algorithm. The peak in the Adjacent-Score occurred at 6 components.


Adjacent-Score
0.73
0.75
0.77
0.79
0
20
40
60
80
100
Number of components


Boundary-Score
0.42
0.46
0.50
0.54
0
20
40
60
80
100
Number of components

Bibliography