Axioms for graph clustering objective functions

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Outline

The motivation

- There is no strict definition of clustering.
- Can we formalize our intuition?
- Previous work is about distance based clustering (hierarchical clustering, K-means, etc.)
- What about graphs?

The setting

Definition (Graph)

A symmetric weighted *graph* is a pair (V, E) of

- a finite set V of *nodes*, and
- a function $E : V \times V \to \mathbb{R}_{\geq 0}$ of *edge weights*,

such that $E(i, j) = E(j, i)$ for all $i, j \in V$.

- Larger weight = stronger connection.
- We allow self loops.

The setting (cont.)

Definition (Clustering)

A *clustering* C of a graph $G = (V, E)$ is a partition of its nodes.

Definition (Clustering function)

A *graph clustering function* f is a function from graphs G to clusterings of G.

Definition (Objective function)

A *graph clustering objective function* Q is a function from graphs G and clusterings of G to $\mathbb{R}$.

- Larger objective value = better.

Outline

The form of axioms

Things that define clusterings

	Form	Notation
1	Clustering function	$f(G) = \text{argmax}_C\, Q(G, C)$
2	Objective function	$Q(G, C)$
3	Objective relation	$Q(G, C) \geq Q(G, D)$ or $C \geq_G D$

Basic axioms

Axiom 1: Scale invariance (first form)

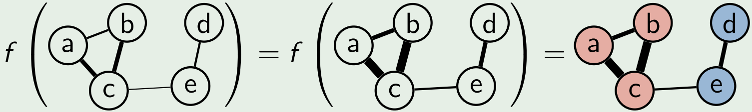
A graph clustering objective function Q is *scale invariant* if

- for all graphs $G = (V, E)$,
- all constants $\alpha > 0$,

$f(G) = f(\alpha G)$.

(where $\alpha G = (V, (i, j) \mapsto \alpha E(i, j))$.)

Example



Basic axioms

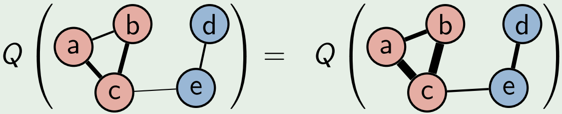
Axiom 1: Scale invariance (second form)

A graph clustering objective function Q is *scale invariant* if

- for all graphs $G = (V, E)$,
- all constants $\alpha > 0$,
- all clusterings C of G,

$Q(G, C) = Q(\alpha G, C)$.
(where $\alpha G = (V, (i, j) \mapsto \alpha E(i, j))$.)

Example



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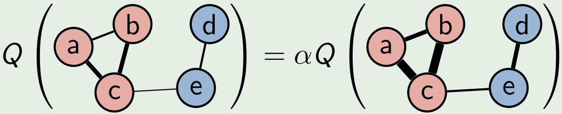
$Q(G, C) = \alpha Q(\alpha G, C)$???
(where $\alpha G = (V, (i,j) \mapsto \alpha E(i,j))$.)

Example



Basic axioms

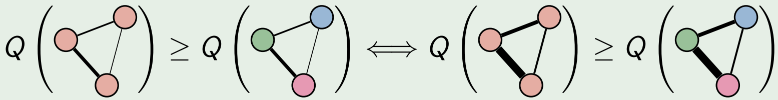
Axiom 1: Scale invariance (third form)

A graph clustering objective function Q is *scale invariant* if

- for all graphs $G = (V, E)$,
- all constants $\alpha > 0$,
- all clusterings C_1, C_2 of G,

$Q(G, C_1) \geq Q(G, C_2)$ if and only if $Q(\alpha G, C_1) \geq Q(\alpha G, C_2)$.
(where $\alpha G = (V, (i, j) \mapsto \alpha E(i, j))$.)

Example



Basic axioms

Axiom 2: permutation invariance

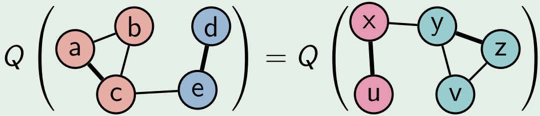
A graph clustering objective function Q is *permutation invariant* if

- for all graphs $G = (V, E)$ and
- all isomorphisms $f : V \to V'$,

it is the case that $Q(G, C) = Q(f(G), f(C))$.

(where f is extended to graphs and clusterings in the obvious way.)

Example



Basic axioms

Axiom 3: Richness

A graph clustering objective function Q is *rich* if

- for all sets V and
- all partitions C^* of V,

there is

- a graph $G = (V, E)$
- such that C^* is the optimal clustering of G.

Intuition:

- No trivial objective functions.
- No fixed number of clusters.

Basic axioms

Definition (Consistent improvement)

Let

- $G = (V, E)$ and $G' = (V, E')$ be graphs, and
- C be a clustering of G and G'.

Then G' *is a C-consistent improvement of G* if

- $E'(i,j) \geq E(i,j)$ for all $i \sim_C j$ and
- $E'(i,j) \leq E(i,j)$ for all $i \not\sim_C j$.

Intuition:

- Consistent improvements make a clustering fit better.

Basic axioms

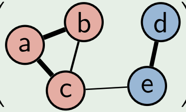
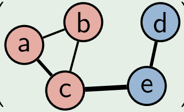
Axiom 4: Monotonicity

A graph clustering objective function Q is *monotonic* if

- for all graphs G,
- all clusterings C of G and
- all C-consistent improvements G' of G

it is the case that $Q(G', C) \geq Q(G, C)$.

Example

Q () $\geq Q$ ()

Local changes

Definition (agreement)

Let

- $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs and
- $V_a \subseteq V_1 \cap V_2$.

The graphs *agree on* V_a if $E_1(i,j) = E_2(i,j)$ for all $i, j \in V_a$.

Definition (agreement on neighborhood)

The graphs also *agree on the neighborhood of* V_a if

$$\begin{aligned} E_1(i,j) &= E_2(i,j) && \text{for all } i \in V_a, j \in V_1 \cap V_2, \text{ and} \\ E_1(i,j) &= 0 && \text{for all } i \in V_a, j \in V_1 \setminus V_2, \text{ and} \\ E_2(i,j) &= 0 && \text{for all } i \in V_a, j \in V_2 \setminus V_1. \end{aligned}$$

What this means:

- For nodes/clusters in V_a, all incident edges are the same.

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Local changes

Axiom 5: Locality

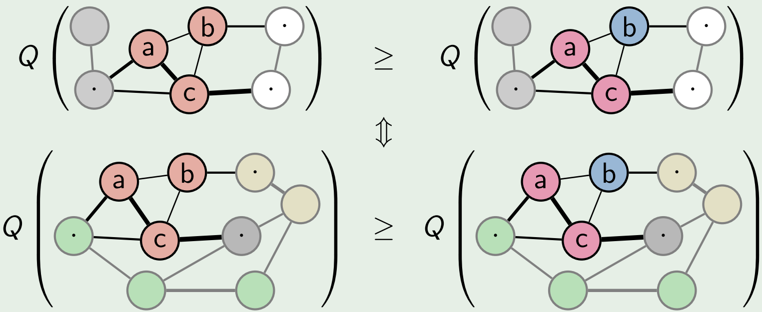
A graph clustering objective function Q is *local* if

- for all graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ that agree on a set V_a and its neighborhood,
- for all clusterings C_1 of $V_1 \setminus V_a$, C_2 of $V_2 \setminus V_a$ and C_a, D_a of V_a.

$$\begin{array}{ll} \text{if} & Q(G_1, C_a \cup C_1) \geq Q(G_1, D_a \cup C_1) \\ \text{then} & Q(G_2, C_a \cup C_2) \geq Q(G_2, D_a \cup C_2). \end{array}$$

Local changes

Example



Local changes

Special cases

- $G_1 = G_2$: change part of a clustering.
  In practice: optimize parts separately (divide and conquer).
- $V_a = \emptyset$: union of two disjoint graphs.

Interlude: Related work

Theorem (Kleinberg 2002)

There is no clustering function that is permutation invariant, scale invariant, monotonic and rich.

Theorem (Ackerman, Ben-David 2008)

There is a clustering quality function that is permutation invariant, scale invariant, monotonic and rich.

Discontinuity is magic

Theorem

There is a graph clustering function that is scale invariant, permutation invariant, monotonic, rich and local.

Connected components

$$f_{\mathrm{coco}}(G) = \text{the connected components of } G$$

$$Q_{\mathrm{coco}}(G, C) = \mathbf{1}[C \text{ are the connected components of } G]$$

Huh!?!?

- Doesn't this contradict Kleinberg's theorem?
- No: edge weight 0 = distance ∞.

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Discontinuity is magic

Why I don't like it

- Adding/removing an edge with tiny weight ϵ changes the graph slightly, but the clustering completely.
- Possibly unstable.
- So don't allow it.

Axiom 6: continuity

An objective function Q is *continuous* if a small change in the graph leads to a small change in the objective value.

Outline

An objective function

Modularity

$$Q_{\text{modularity}}(G, C) = \sum_{c \in C} \left(\frac{w_c}{v_V} - \left(\frac{v_c}{v_V} \right)^2 \right).$$

Where

$$v_c = \sum_{i \in c} \sum_{j \in V} E(i, j) \quad \text{volume of cluster}$$

$$w_c = \sum_{i \in c} \sum_{j \in c} E(i, j) \quad \text{within cluster weight.}$$

Properties

The obvious:

- Modularity is permutation invariant.
- Modularity is scale invariant.
- Modularity is continuous.

The less obvious:

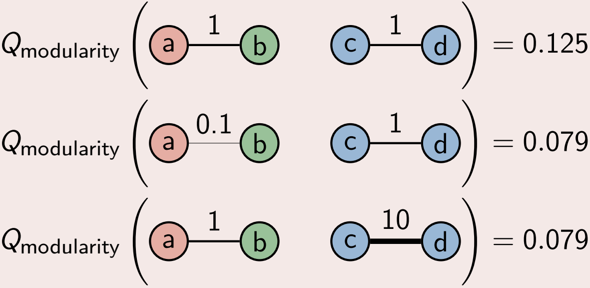
- Modularity is rich.

The bad:

- Modularity is *not* local.
- Modularity is *not* monotonic.

What goes wrong?

Modularity is not monotonic.



□

Outline

Fixed Scale modularity

Idea 1

Fix the scale

$$Q_{M\text{-fixed}}(G, C) = \sum_{c \in C} \left(\frac{w_c}{M} - \left(\frac{v_c}{M} \right)^2 \right)$$

Is it monotonic?

Take $v_c = w_c + b_c$ (within + between)

$$\frac{\partial Q_{M\text{-fixed}}(G, C)}{\partial w_c} = \frac{1}{M} - \frac{2w_c + 2b_c}{M^2}.$$

This is negative when $2v_c > M$

$\Rightarrow$ not monotonic

Fixed Scale modularity

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This is negative when $2v_c > M$

$\Rightarrow$ **not monotonic**

Adaptive Scale Modularity

Idea 2

Add some v_c to the denominator

$$Q_{M,\gamma}(G,C) = \sum_{c \in C} \left(\frac{w_c}{M + \gamma v_c} - \left(\frac{v_c}{M + \gamma v_c} \right)^2 \right).$$

Theorem

Adaptive scale modularity is monotonic for all $M \geq 0$ and $\gamma \geq 2$.

Theorem

Adaptive scale modularity is rich for all $M \geq 0$ and $\gamma \geq 1$.

Theorem

Adaptive scale modularity is scale invariant for $M = 0$.

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Adaptive Scale Modularity

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Theorem

Adaptive scale modularity is monotonic for all $M \geq 0$ and $\gamma \geq 2$.

Theorem

Adaptive scale modularity is rich for all $M \geq 0$ and $\gamma \geq 1$.

Theorem

Adaptive scale modularity is scale invariant for $M = 0$.

Adaptive Scale Modularity: related objectives

- When $\gamma = 0$, we get fixed scale modularity. Equivalent to other modularity variants.
- When $\gamma = 0$ and $M = v_V$, we get modularity.
- When $M = 0$ we get

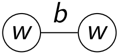
$$Q_{0,\gamma}(G, C) \propto \sum_{c \in C} \left(\frac{w_c}{v_c} - \frac{1}{\gamma} \right),$$

  i.e. normalized cut.
- When $M \to \infty$ we get

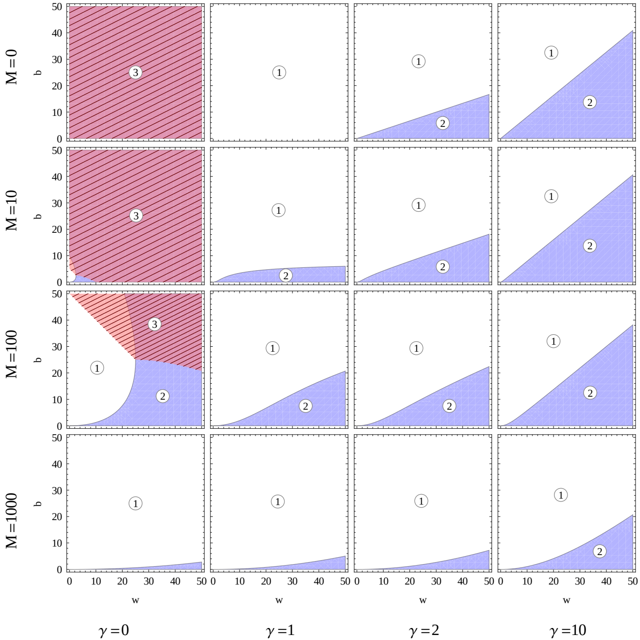
$$Q_{\infty,\gamma}(G, C) \propto \sum_{c \in C} w_c,$$

  i.e. unnormalized cut.

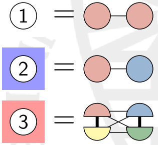
Adaptive Scale Modularity: behavior

Take a simple graph: 

- Two cliques each with w within weight
- Connected by edges with total weight b.
- Total volume $2w + 2b$.
- What is the behavior of adaptive scale modularity?



Legend:



Outline

Summary

- 6 axioms for graph clustering objectives.
- Graph setting allows for locality.
- Modularity is not monotonic.
- Non-monotonicity leads to splitting of cliques.
- Adaptive scale modularity satisfies all axioms (when $M = 0$).
- Generalizes both modularity and normalized cut.

Thank you for your attention.

Axioms for graph clustering objective functions

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