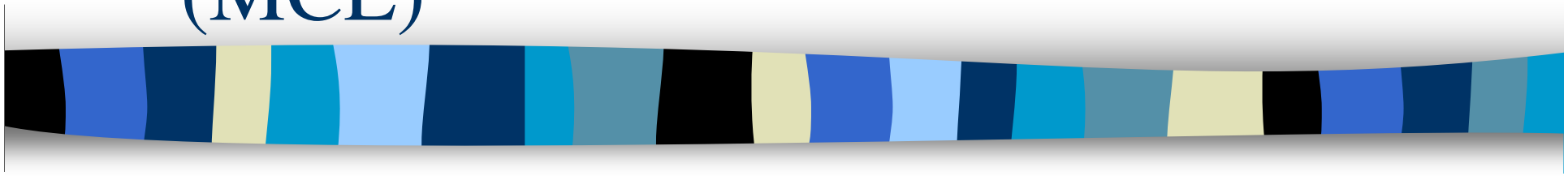
Clustering on Graphs: The Markov Cluster Algorithm (MCL)



CS 595D Presentation

By Kathy Macropol

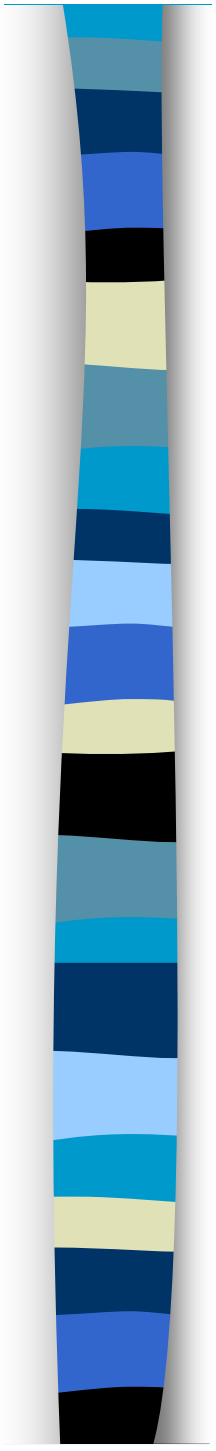
MCL Algorithm

- Based on the PhD thesis by Stijn van Dongen

  Van Dongen, S. (2000) *Graph Clustering by Flow Simulation*. PhD Thesis, University of Utrecht, The Netherlands.

- MCL is a graph clustering algorithm.

- MCL is freely available for download at
  http://www.micans.org/mcl/

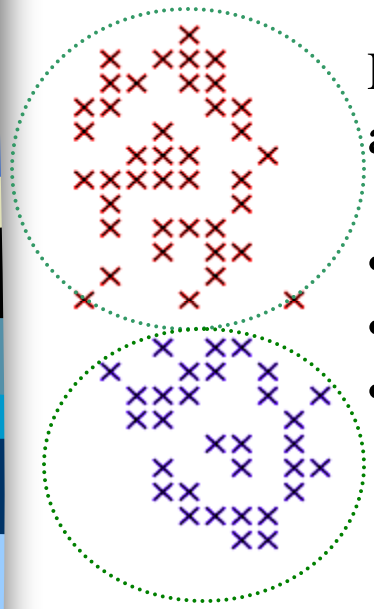


Outline

- Background
  - Clustering
  - Random Walks
  - Markov Chains
- MCL
  - Basis
  - Inflation Operator
  - Algorithm
  - Convergence
- MCL Analysis
  - Comparison to Other Graph Clustering Algorithms
    - RNSC, SPC, MCODE
    - RRW
- Conclusions

Graph Clustering

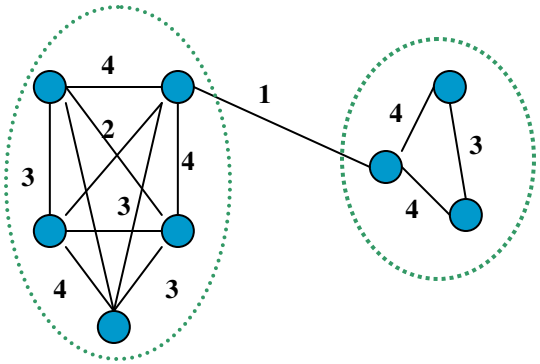
- Clustering – finding natural groupings of items.
- Vector Clustering



Each point has a vector, i.e.

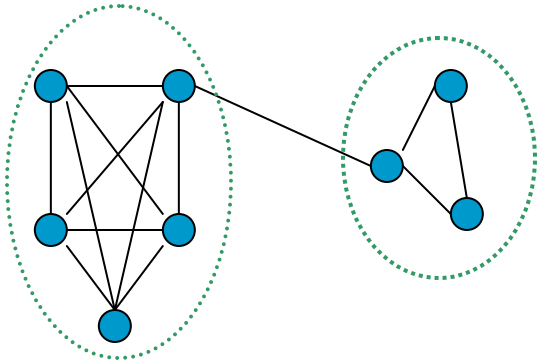
- x coordinate
- y coordinate
- color

Graph Clustering



Each vertex is connected to others by (weighted or unweighted) edges.

Random Walks



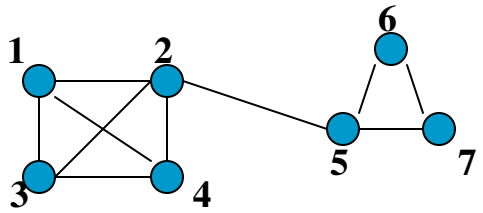
- Considering a graph, there will be many links within a cluster, and fewer links between clusters.
- This means if you were to start at a node, and then randomly travel to a connected node, you're more likely to stay within a cluster than travel between.
- This is what MCL (and several other clustering algorithms) is based on.
  - Other ways to consider graph clustering may include, for example, looking for cliques. This tends to be sensitive to changes in node degree, however.

Random Walks

- By doing random walks upon the graph, it may be possible to discover where the flow tends to gather, and therefore, where clusters are.
- Random Walks on a graph are calculated using “Markov Chains”.

Markov Chains

- To see how this works, an example:



- In one time step, a random walker at node 1 has a 33% chance of going to node 2, 3, & 4, and 0% chance to nodes 5, 6, or 7.
- From node 2, 25% chance for 1, 3, 4, 5 and 0% for 6 and 7.
- Creating a transition matrix gives:

	1	*2*	*3*	*4*	*5*	*6*	*7*
1	0	.25	.33	.33	0	0	0
2	.33	0	.33	.33	.33	0	0
3	.33	.25	0	.33	0	0	0
4	.33	.25	.33	0	0	0	0
5	0	.25	0	0	0	.5	.5
6	0	0	0	0	.33	0	.5
7	0	0	0	0	.33	.5	0

(notice each column sums to one)

Also can be looked at as a probability matrix!

Markov Chains

- A simpler example: $\begin{pmatrix} .6 & .2 \\ .4 & .8 \end{pmatrix}$
- Next time step: $t_0 \rightarrow t_1 \rightarrow t_2$

$1 \rightarrow 1 \rightarrow 1 \;+\; 1 \rightarrow 2 \rightarrow 1$

$.6 * .6 + .4 * .2 = .44$

$$\begin{pmatrix} .6 & .2 \\ .4 & .8 \end{pmatrix} \begin{pmatrix} .6 & .2 \\ .4 & .8 \end{pmatrix} = \begin{pmatrix} .44 & .28 \\ .56 & .72 \end{pmatrix} \longrightarrow \begin{pmatrix} .35 & .32 \\ .65 & .68 \end{pmatrix} \longrightarrow \begin{pmatrix} .34 & .33 \\ .66 & .66 \end{pmatrix}$$

$$\xrightarrow{\text{eventually}} \begin{pmatrix} .33 & .33 \\ .66 & .66 \end{pmatrix}$$

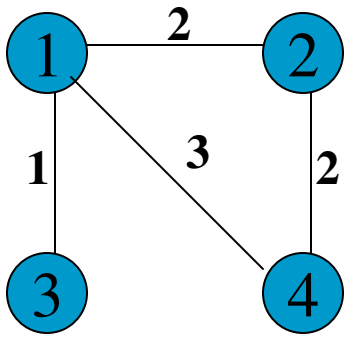
Markov Chain

- Markov Chain:

  A sequence of variables X_1, X_2, X_3, etc (in our case, the probability matrices) where, given the present state, the past and future states are independent.
- Probabilities for the next time step only depend on current probabilities (given the current probability).
- A random walk is an example of a Markov Chain, using the transition probability matrices.

Weighted Graphs

- To turn a weighted graph into a probability (transition) matrix, column normalize.



$$\begin{pmatrix} 0 & 2 & 1 & 3 \\ 2 & 0 & 0 & 2 \\ 1 & 0 & 0 & 0 \\ 3 & 2 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1/2 & 1 & 3/5 \\ 1/3 & 0 & 0 & 2/5 \\ 1/6 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \end{pmatrix}$$

Notice it's no longer symmetric.

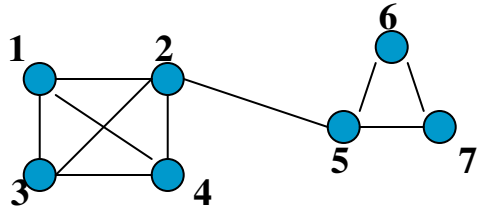
Adding Self Loops

- Small simple path loops can complicate things.
  - There is a strong effect that odd powers of expansion obtain their mass from simple paths of odd length, and likewise for even.
  - Adds a dependence to the transition probabilities on the parity of the simple path lengths.
- The addition of self looping edges on each node resolves this.
  - Adds a small path of length 1, so the mass does not only appear during odd powers of the matrix.

$$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{pmatrix}$$

Markov Chain Cluster Structure

- Example:



$$\begin{pmatrix} 0 & .25 & .33 & .33 & 0 & 0 & 0 \\ .33 & 0 & .33 & .33 & .33 & 0 & 0 \\ .33 & .25 & 0 & .33 & 0 & 0 & 0 \\ .33 & .25 & .33 & 0 & 0 & 0 & 0 \\ 0 & .25 & 0 & 0 & 0 & .5 & .5 \\ 0 & 0 & 0 & 0 & .33 & 0 & .5 \\ 0 & 0 & 0 & 0 & .33 & .5 & 0 \end{pmatrix} \quad \begin{pmatrix} .15 & .15 & .15 & .15 & .15 & .15 & .15 \\ .2 & .2 & .2 & .2 & .2 & .2 & .2 \\ .15 & .15 & .15 & .15 & .15 & .15 & .15 \\ .15 & .15 & .15 & .15 & .15 & .15 & .15 \\ .15 & .15 & .15 & .15 & .15 & .15 & .15 \\ .1 & .1 & .1 & .1 & .1 & .1 & .1 \\ .1 & .1 & .1 & .1 & .1 & .1 & .1 \end{pmatrix}$$

eventually →

Notice that, in the beginning time steps, before the flow really mixes, the cluster structure is pronounced in the matrix!

This is not a coincidence, and MCL uses this, modifying the random walk process to further emphasize the divide between clusters in the matrix.

MCL

- "Flow is easier within dense regions than across sparse boundaries, however, in the long run this effect disappears."
- During the earlier powers of the Markov Chain, the edge weights will be **higher** in links that are *within* clusters, and **lower** *between* the clusters.
- This means there is a correspondence between the distribution of weight over the columns and the clusterings.

MCL

- MCL deliberately boosts this affect by
  - Stopping partway in the Markov Chain
  - Then adjusting the transitions by columns.
    For each vertex, the transition values are changed so that
    - Strong neighbors are further strengthened
    - Less popular neighbors are demoted.
- This adjusting can be done by raising a single column to a non-negative power, and then re-normalizing.
- This operation is named “Inflation”
- (Taking the Markov Chain powers is named “Expansion”)

MCL Inflation

- Example for inflation of 2 (squaring):

$$\begin{pmatrix} 0 \\ 1/2 \\ 0 \\ 1/6 \\ 1/3 \end{pmatrix} \quad \begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \\ 0 \end{pmatrix}$$

Square, and then normalize

$$\begin{pmatrix} 0 \\ 9/14 \\ 0 \\ 1/14 \\ 4/14 \end{pmatrix} \quad \begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \\ 0 \end{pmatrix}$$

MCL Inflation

DEFINITION 3. *Given a matrix* $M \in \mathbb{R}^{k \times l}$, $M \geq 0$, *and a real nonnegative number* r, *the matrix resulting from rescaling each of the columns of* M *with power coefficient* r *is called* $\Gamma_r M$, *and* Γ_r *is called the* ***inflation*** *operator with power coefficient* r. *Formally, the action of* $\Gamma_r : \mathbb{R}^{k \times l} \to \mathbb{R}^{k \times l}$ *is defined by*

$$(\Gamma_r M)_{pq} \quad = \quad (M_{pq})^r \Big/ \sum_{i=1}^{k} (M_{iq})^r$$

If the subscript is omitted, it is understood that the power coefficient equals 2. □

MCL Inflation

- The inflation operator is responsible for both strengthening and weakening of current. (Strengthens strong currents, and weakens already weak currents).
- The inflation parameter, *r*, controls the extent of this strengthening / weakening. (In the end, this influences the granularity of clusters.)

MCL Algorithm

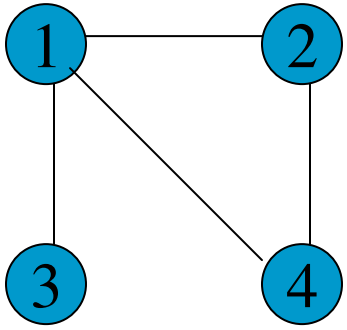
- In MCL, the following two processes are alternated between repeatedly:
  - Expansion (taking the Markov Chain transition matrix powers)
  - Inflation
- The expansion operator is responsible for allowing flow to connect different regions of the graph.
- The inflation operator is responsible for both strengthening and weakening of current.

MCL Algorithm

1. Input is an un-directed graph, power parameter *e,* and inflation parameter *r*.
2. Create the associated matrix
3. Add self loops to each node (optional)
4. Normalize the matrix
5. Expand by taking the e^{th} power of the matrix
6. Inflate by taking inflation of the resulting matrix with parameter *r*
7. Repeat steps 5 and 6 until a steady state is reached (convergence).
8. Interpret resulting matrix to discover clusters.

MCL Algorithm

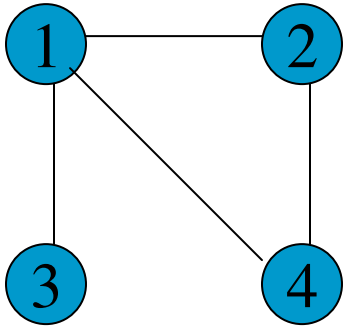
1. Input is an un-directed graph, power parameter *e*, and inflation parameter *r*.
2. Create the associated matrix
3. Add self loops to each node (optional)
4. Normalize the matrix
5. Expand by taking the e^{th} power of the matrix
6. Inflate by taking inflation of the resulting matrix with parameter *r*
7. Repeat steps 5 and 6 until a steady state is reached (convergence).
8. Interpret resulting matrix to discover clusters.



Power of 2
Inflation of 2

MCL Algorithm

1. Input is an un-directed graph, power parameter *e*, and inflation parameter *r*.
2. Create the associated matrix
3. Add self loops to each node (optional)
4. Normalize the matrix
5. Expand by taking the e^{th} power of the matrix
6. Inflate by taking inflation of the resulting matrix with parameter *r*
7. Repeat steps 5 and 6 until a steady state is reached (convergence).
8. Interpret resulting matrix to discover clusters.

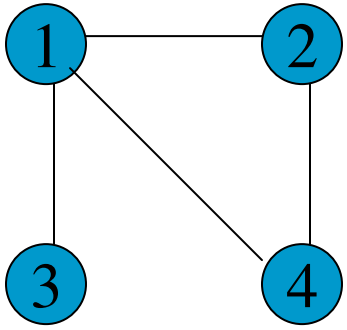


Power of 2
Inflation of 2

$$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

MCL Algorithm

1. Input is an un-directed graph, power parameter *e*, and inflation parameter *r*.
2. Create the associated matrix
3. Add self loops to each node (optional)
4. Normalize the matrix
5. Expand by taking the e^{th} power of the matrix
6. Inflate by taking inflation of the resulting matrix with parameter *r*
7. Repeat steps 5 and 6 until a steady state is reached (convergence).
8. Interpret resulting matrix to discover clusters.



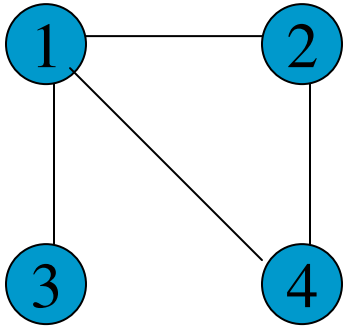
Power of 2
Inflation of 2

$$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{pmatrix}$$

MCL Algorithm

1. Input is an un-directed graph, power parameter *e*, and inflation parameter *r*.
2. Create the associated matrix
3. Add self loops to each node (optional)
4. Normalize the matrix
5. Expand by taking the e^{th} power of the matrix
6. Inflate by taking inflation of the resulting matrix with parameter *r*
7. Repeat steps 5 and 6 until a steady state is reached (convergence).
8. Interpret resulting matrix to discover clusters.



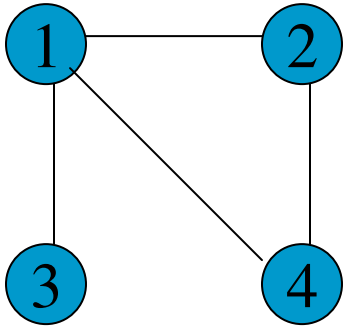
Power of 2
Inflation of 2

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1/4 & 1/3 & 1/2 & 1/3 \\ 1/4 & 1/3 & 0 & 1/3 \\ 1/4 & 0 & 1/2 & 0 \\ 1/4 & 1/3 & 0 & 1/3 \end{pmatrix}$$

MCL Algorithm

1. Input is an un-directed graph, power parameter *e*, and inflation parameter *r*.
2. Create the associated matrix
3. Add self loops to each node (optional)
4. Normalize the matrix
5. Expand by taking the e^{th} power of the matrix
6. Inflate by taking inflation of the resulting matrix with parameter *r*
7. Repeat steps 5 and 6 until a steady state is reached (convergence).
8. Interpret resulting matrix to discover clusters.



Power of 2
Inflation of 2

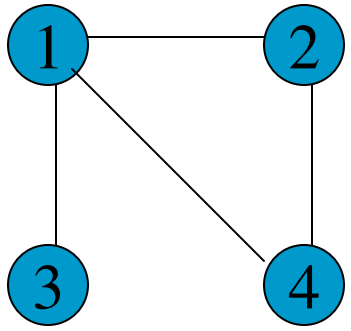
$$\begin{pmatrix} ¼ & 1/3 & ½ & 1/3 \\ ¼ & 1/3 & 0 & 1/3 \\ ¼ & 0 & ½ & 0 \\ ¼ & 1/3 & 0 & 1/3 \end{pmatrix} \quad \begin{pmatrix} ¼ & 1/3 & ½ & 1/3 \\ ¼ & 1/3 & 0 & 1/3 \\ ¼ & 0 & ½ & 0 \\ ¼ & 1/3 & 0 & 1/3 \end{pmatrix}$$

=

$$\begin{pmatrix} .35 & .31 & .38 & .31 \\ .23 & .31 & .13 & .31 \\ .19 & .08 & .38 & .08 \\ .23 & .31 & .13 & .31 \end{pmatrix}$$

MCL Algorithm

1. Input is an un-directed graph, power parameter *e*, and inflation parameter *r*.
2. Create the associated matrix
3. Add self loops to each node (optional)
4. Normalize the matrix
5. Expand by taking the e^{th} power of the matrix
6. Inflate by taking inflation of the resulting matrix with parameter *r*
7. Repeat steps 5 and 6 until a steady state is reached (convergence).
8. Interpret resulting matrix to discover clusters.



Power of 2
Inflation of 2

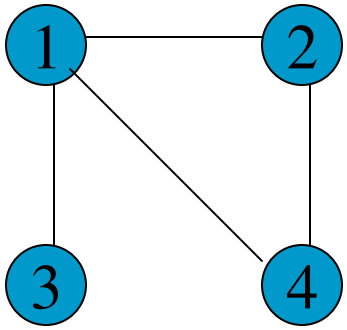
$$\begin{pmatrix} .35 & .31 & .38 & .31 \\ .23 & .31 & .13 & .31 \\ .19 & .08 & .38 & .08 \\ .23 & .31 & .13 & .31 \end{pmatrix}$$

$$\begin{pmatrix} .13 & .09 & .14 & .09 \\ .05 & .09 & .02 & .09 \\ .04 & .01 & .14 & .01 \\ .05 & .09 & .02 & .09 \end{pmatrix}$$

$$\begin{pmatrix} .47 & .33 & .45 & .33 \\ .20 & .33 & .05 & .33 \\ .13 & .02 & .45 & .02 \\ .20 & .33 & .05 & .33 \end{pmatrix}$$

MCL Algorithm

1. Input is an un-directed graph, power parameter *e*, and inflation parameter *r*.
2. Create the associated matrix
3. Add self loops to each node (optional)
4. Normalize the matrix
5. Expand by taking the e^{th} power of the matrix
6. Inflate by taking inflation of the resulting matrix with parameter *r*
7. Repeat steps 5 and 6 until a steady state is reached (convergence).
8. Interpret resulting matrix to discover clusters.



Power of 2
Inflation of 2

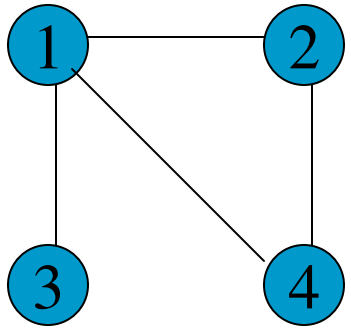
.70	.33	.49	.33
.12	.33	.01	.33
.05	.02	.49	--
.12	.33	.01	.33

.94	.33	.50	.33
.03	.33	--	.33
.01	--	.50	--
.13	.33	--	.33

1	.33	.50	.33
--	.33	--	.33
--	--	.50	--
--	.33	--	.33

MCL Algorithm

1. Input is an un-directed graph, power parameter *e*, and inflation parameter *r*.
2. Create the associated matrix
3. Add self loops to each node (optional)
4. Normalize the matrix
5. Expand by taking the e^{th} power of the matrix
6. Inflate by taking inflation of the resulting matrix with parameter *r*
7. Repeat steps 5 and 6 until a steady state is reached (convergence).
8. Interpret resulting matrix to discover clusters.



Power of 2
Inflation of 2

Expand on in just a minute.

MCL Algorithm Convergence

- Not obvious that result will converge. Convergence is not proven in the thesis, however it is shown experimentally that it often does occur.
- In practice, the algorithm converges nearly always to a "doubly idempotent" matrix:
    1. It's at steady state.
    2. Every value in a single column has the same number (homogeneous).

$$
\begin{pmatrix}
1.000 & -- & -- & -- & -- & 1.000 & 1.000 & -- & -- & 1.000 & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & 1.000 & 1.000 & -- & 1.000 & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & 0.500 & -- & -- & -- & 0.500 & 0.500 & -- & 0.500 & 0.500 \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & 0.500 & -- & -- & -- & 0.500 & 0.500 & -- & 0.500 & 0.500 \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & --
\end{pmatrix}
$$

M_{mcl}^{∞}

MCL Algorithm Convergence

- It *is* proven that when the matrix is in the neighborhood of being doubly idempotent, it converges quadratically.
- However, the final steady state may sometimes be cyclic and consist of a repeating series of matrices.
  - In certain cases, the expansion and inflation act as inverses of each other. However, a slight change of parameters and the equilibrium is broken.
  - Without self loops, it's possible on bipartite graphs because of odd path lengths. Adding self loops and slightly changing parameters fixes most of the problems.
  - Other graphs that may have periodic behavior are described, but will most likely be "a curiosity lacking cluster structure anyhow".

MCL Algorithm Convergence

$$
\begin{pmatrix}
0.200 & 0.250 & -- & -- & -- & 0.333 & 0.250 & -- & -- & 0.250 & -- & -- \\
0.200 & 0.250 & 0.250 & -- & 0.200 & -- & -- & -- & -- & -- & -- & -- \\
-- & 0.250 & 0.250 & 0.200 & 0.200 & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & 0.250 & 0.200 & -- & -- & -- & 0.200 & 0.200 & -- & 0.200 & -- \\
-- & 0.250 & 0.250 & -- & 0.200 & -- & 0.250 & 0.200 & -- & -- & -- & -- \\
0.200 & -- & -- & -- & -- & 0.333 & -- & -- & -- & 0.250 & -- & -- \\
0.200 & -- & -- & -- & 0.200 & -- & 0.250 & -- & -- & 0.250 & -- & -- \\
-- & -- & -- & 0.200 & 0.200 & -- & -- & 0.200 & 0.200 & -- & 0.200 & -- \\
-- & -- & -- & 0.200 & -- & -- & -- & 0.200 & 0.200 & -- & 0.200 & 0.333 \\
0.200 & -- & -- & -- & -- & 0.333 & 0.250 & -- & -- & 0.250 & -- & -- \\
-- & -- & -- & 0.200 & -- & -- & -- & 0.200 & 0.200 & -- & 0.200 & 0.333 \\
-- & -- & -- & -- & -- & -- & -- & -- & 0.200 & -- & 0.200 & 0.333
\end{pmatrix}
$$

M

$$
\begin{pmatrix}
0.380 & 0.087 & 0.027 & -- & 0.077 & 0.295 & 0.201 & -- & -- & 0.320 & -- & -- \\
0.047 & 0.347 & 0.210 & 0.017 & 0.150 & 0.019 & 0.066 & 0.012 & -- & 0.012 & -- & -- \\
0.014 & 0.210 & 0.347 & 0.056 & 0.150 & -- & 0.016 & 0.046 & 0.009 & -- & 0.009 & -- \\
-- & 0.027 & 0.087 & 0.302 & 0.062 & -- & -- & 0.184 & 0.143 & -- & 0.143 & 0.083 \\
0.058 & 0.210 & 0.210 & 0.056 & 0.406 & -- & 0.083 & 0.046 & 0.009 & 0.019 & 0.009 & -- \\
0.142 & 0.017 & -- & -- & -- & 0.295 & 0.083 & -- & -- & 0.184 & -- & -- \\
0.113 & 0.069 & 0.017 & -- & 0.062 & 0.097 & 0.333 & 0.012 & -- & 0.147 & -- & -- \\
-- & 0.017 & 0.069 & 0.175 & 0.049 & -- & 0.016 & 0.287 & 0.143 & -- & 0.143 & 0.083 \\
-- & -- & 0.017 & 0.175 & 0.012 & -- & -- & 0.184 & 0.288 & -- & 0.288 & 0.278 \\
0.246 & 0.017 & -- & -- & 0.019 & 0.295 & 0.201 & -- & -- & 0.320 & -- & -- \\
-- & -- & 0.017 & 0.175 & 0.012 & -- & -- & 0.184 & 0.288 & -- & 0.288 & 0.278 \\
-- & -- & -- & 0.044 & -- & -- & -- & 0.046 & 0.120 & -- & 0.120 & 0.278
\end{pmatrix}
$$

$\Gamma_2 M^2$,

MCL Algorithm Convergence

$$
\begin{pmatrix}
0.448 & 0.080 & 0.023 & -- & 0.068 & 0.426 & 0.359 & -- & -- & 0.432 & -- & -- \\
0.018 & 0.285 & 0.228 & 0.007 & 0.176 & 0.006 & 0.033 & 0.005 & -- & 0.007 & -- & -- \\
0.005 & 0.223 & 0.290 & 0.022 & 0.173 & -- & 0.010 & 0.017 & 0.003 & 0.001 & 0.003 & 0.001 \\
-- & 0.018 & 0.059 & 0.222 & 0.040 & -- & 0.001 & 0.187 & 0.139 & -- & 0.139 & 0.099 \\
0.027 & 0.312 & 0.314 & 0.028 & 0.439 & 0.005 & 0.054 & 0.022 & 0.003 & 0.010 & 0.003 & 0.001 \\
0.116 & 0.007 & 0.001 & -- & 0.004 & 0.157 & 0.085 & -- & -- & 0.131 & -- & -- \\
0.096 & 0.040 & 0.013 & -- & 0.037 & 0.083 & 0.197 & 0.001 & -- & 0.104 & -- & -- \\
-- & 0.012 & 0.042 & 0.172 & 0.029 & -- & 0.002 & 0.198 & 0.133 & -- & 0.133 & 0.096 \\
-- & 0.001 & 0.015 & 0.256 & 0.009 & -- & -- & 0.266 & 0.326 & -- & 0.326 & 0.346 \\
0.290 & 0.021 & 0.002 & -- & 0.017 & 0.323 & 0.260 & -- & -- & 0.316 & -- & -- \\
-- & 0.001 & 0.015 & 0.256 & 0.009 & -- & -- & 0.266 & 0.326 & -- & 0.326 & 0.346 \\
-- & -- & 0.001 & 0.037 & 0.001 & -- & -- & 0.039 & 0.069 & -- & 0.069 & 0.112
\end{pmatrix}
$$

$\Gamma_2(\Gamma_2 M^2 \cdot \Gamma_2 M^2)$

$$
\begin{pmatrix}
0.807 & 0.040 & 0.015 & -- & 0.034 & 0.807 & 0.807 & -- & -- & 0.807 & -- & -- \\
-- & 0.090 & 0.092 & -- & 0.088 & -- & -- & -- & -- & -- & -- & -- \\
-- & 0.085 & 0.088 & -- & 0.084 & -- & -- & -- & -- & -- & -- & -- \\
-- & 0.001 & 0.001 & 0.032 & 0.001 & -- & -- & 0.032 & 0.031 & -- & 0.031 & 0.031 \\
-- & 0.777 & 0.798 & -- & 0.786 & -- & 0.001 & -- & -- & -- & -- & -- \\
0.005 & -- & -- & -- & -- & 0.005 & 0.005 & -- & -- & 0.005 & -- & -- \\
0.003 & 0.001 & -- & -- & 0.001 & 0.003 & 0.003 & -- & -- & 0.003 & -- & -- \\
-- & -- & 0.001 & 0.024 & -- & -- & -- & 0.024 & 0.024 & -- & 0.024 & 0.024 \\
-- & -- & 0.002 & 0.472 & 0.001 & -- & -- & 0.472 & 0.472 & -- & 0.472 & 0.472 \\
0.185 & 0.005 & 0.001 & -- & 0.004 & 0.185 & 0.184 & -- & -- & 0.185 & -- & -- \\
-- & -- & 0.002 & 0.472 & 0.001 & -- & -- & 0.472 & 0.472 & -- & 0.472 & 0.472 \\
-- & -- & -- & 0.001 & -- & -- & -- & 0.001 & 0.001 & -- & 0.001 & --
\end{pmatrix}
$$

$(\Gamma_2 \circ Squaring)$ iterated four times on M

MCL Algorithm Convergence

$$M_{mcl}^{\infty} = \begin{pmatrix}
1.000 & -- & -- & -- & -- & 1.000 & 1.000 & -- & -- & 1.000 & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & 1.000 & 1.000 & -- & 1.000 & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & 0.500 & -- & -- & -- & 0.500 & 0.500 & -- & 0.500 & 0.500 \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & 0.500 & -- & -- & -- & 0.500 & 0.500 & -- & 0.500 & 0.500 \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & --
\end{pmatrix}$$

MCL Animated

MCL Interpreting Clusters

- To interpret clusters, the vertices are split into two types. **Attractors**, which attract other vertices, and vertices that are *being* attracted by the attractors.
- Attractors have at least one positive flow value within their corresponding row (in the steady state matrix).
- Each attractor is attracting the vertices which have positive values within its row.

$$
\begin{pmatrix}
1.000 & -- & -- & -- & -- & 1.000 & 1.000 & -- & -- & 1.000 & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & 1.000 & 1.000 & -- & 1.000 & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & 0.500 & -- & -- & -- & 0.500 & 0.500 & -- & 0.500 & 0.500 \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\
-- & -- & -- & 0.500 & -- & -- & -- & 0.500 & 0.500 & -- & 0.500 & 0.500 \\
-- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & --
\end{pmatrix}
$$

M_{mcl}^{∞}

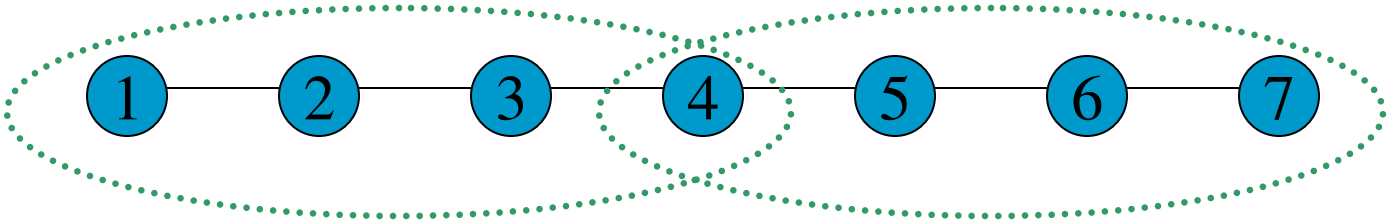
MCL Interpreting Clusters

$$M_{mcl}^{\infty} = \begin{pmatrix} 1.000 & -- & -- & -- & -- & 1.000 & 1.000 & -- & -- & 1.000 & -- & -- \\ -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\ -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\ -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\ -- & 1.000 & 1.000 & -- & 1.000 & -- & -- & -- & -- & -- & -- & -- \\ -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\ -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\ -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\ -- & -- & -- & 0.500 & -- & -- & -- & 0.500 & 0.500 & -- & 0.500 & 0.500 \\ -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \\ -- & -- & -- & 0.500 & -- & -- & -- & 0.500 & 0.500 & -- & 0.500 & 0.500 \\ -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- & -- \end{pmatrix}$$

- Attractors and the elements they attract are swept together into the same cluster.
- In this case, {1, 6, 7, 10}, {2, 3, 5}, {4, 8, 9, 11, 12}

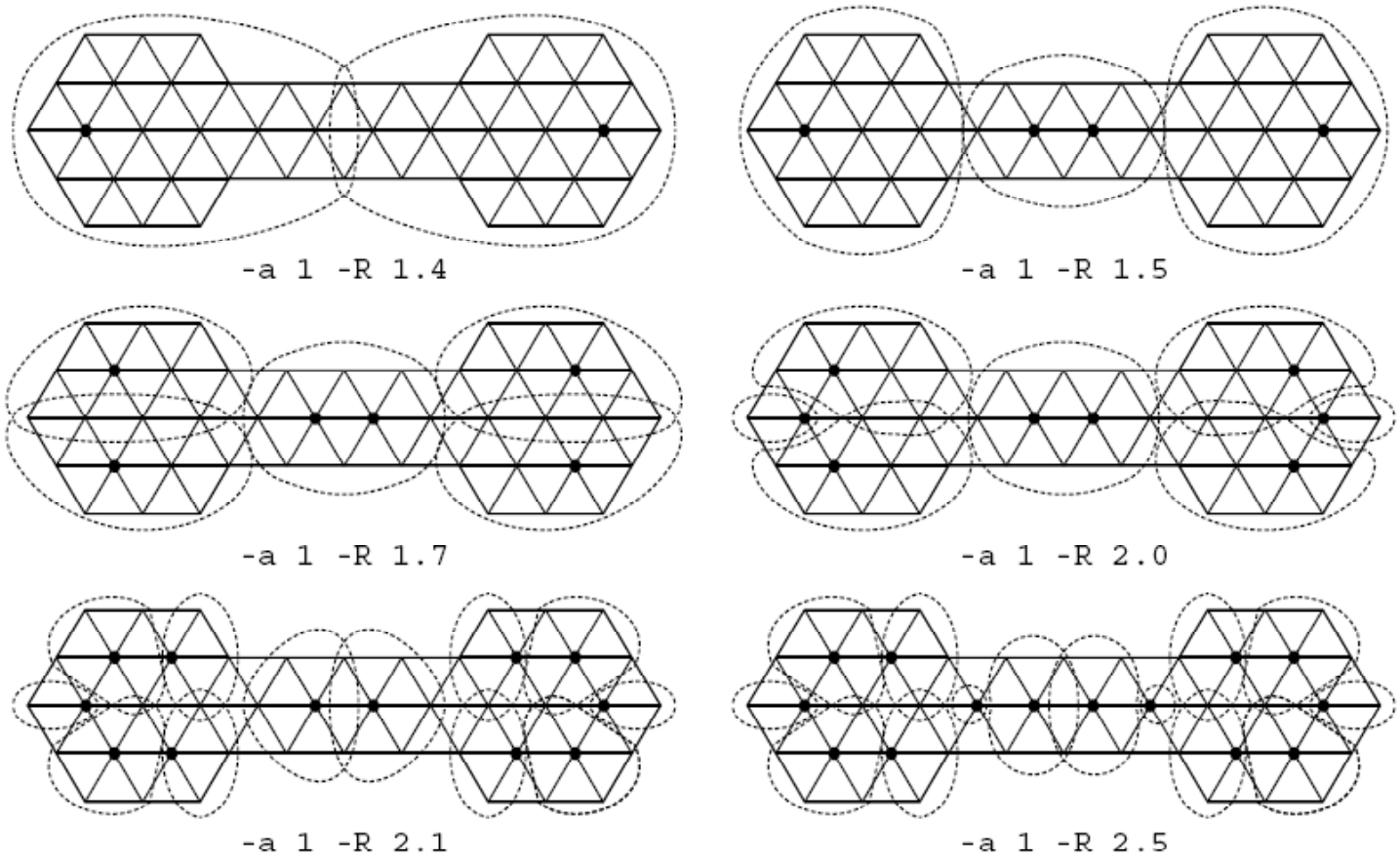
MCL Interpreting Clusters

- In general, overlapping clusters (where one node is contained in multiple clusters) are only found in very special cases of graph symmetry:
  - Only when a vertex is attracted *exactly* equally by more than one cluster
  - This occurs only when both clusters are isomorphic



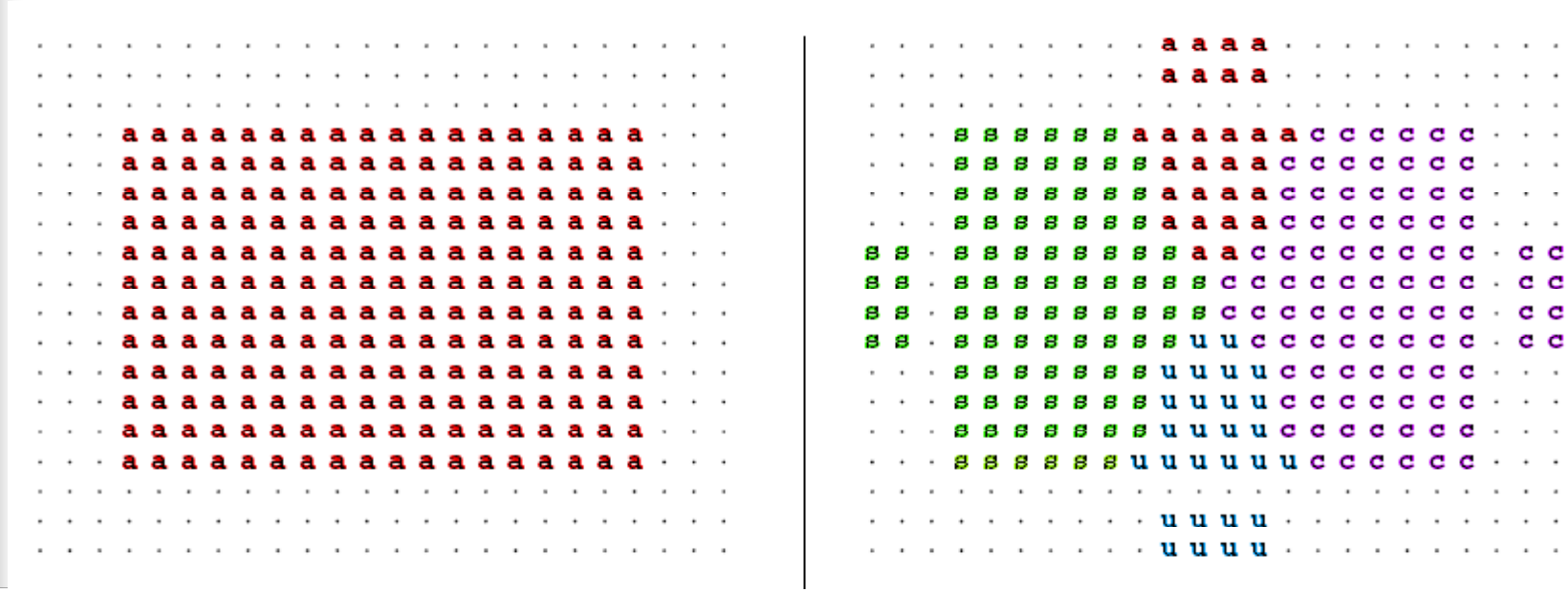
MCL Clusters

- The inflation parameter affects cluster granularity
  (a is the weight for added self loops)



MCL Clusters

- For clusters with large diameter, MCL has problems
- Distributing flow across cluster needs long expansion and low inflation (otherwise the cluster will split).
- Takes many iterations and causes MCL to be sensitive to small perturbations in the graph.
  - The addition of small diameter clusters disturbs the clustering, since the low inflation parameter will cause them to disproportionately ‘inflate’ surrounding probabilities.



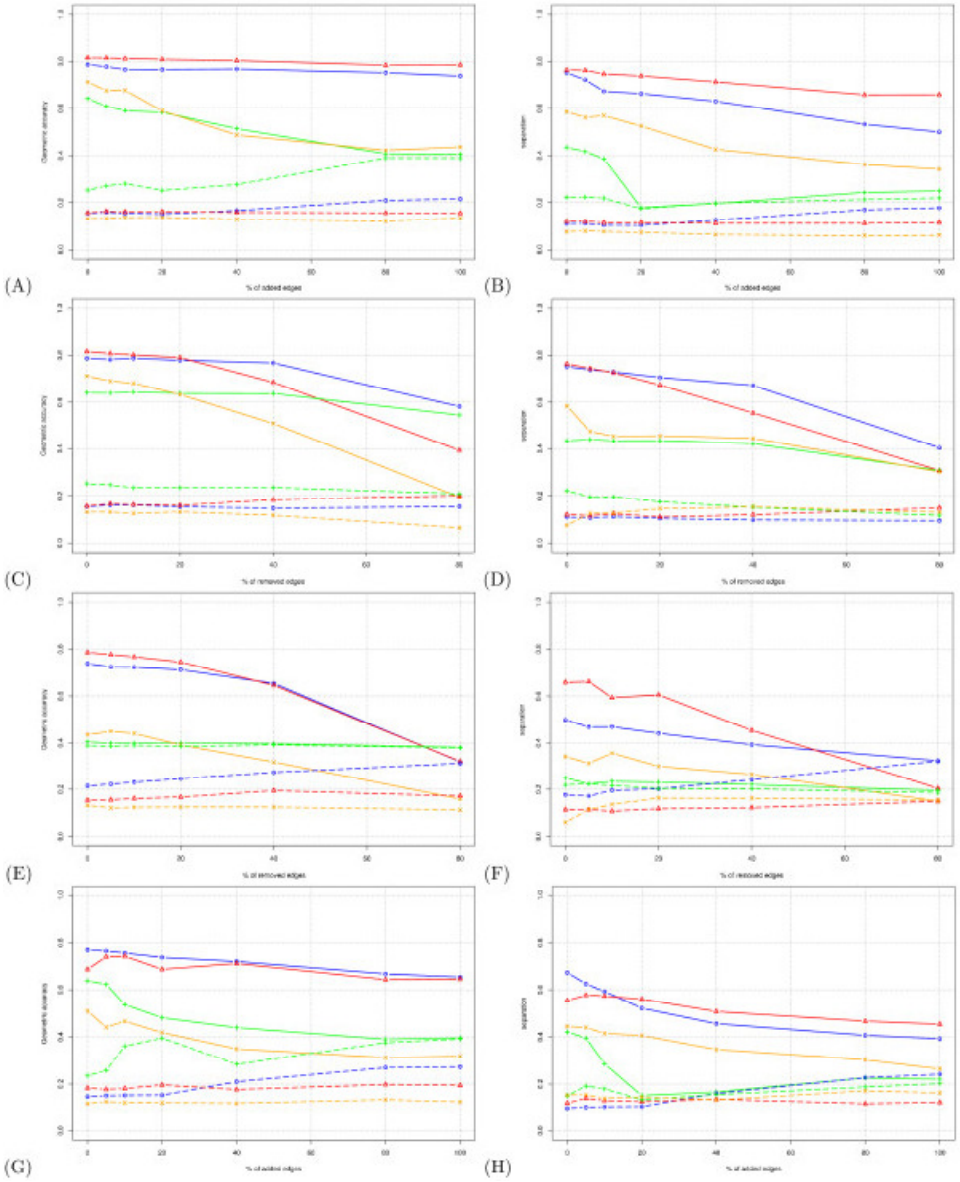
Analysis of MCL

- $O(N^3)$, where N is the number of vertices.
  - N^3 cost of one matrix multiplication on two matrices of dimension N.
  - Inflation can be done in $O(N^2)$ time
  - The number of steps to converge is not proven, but experimentally shown to be ~10 to 100 steps, and mostly consist of sparse matrices after the first few steps.
- Speed may be improved through pruning.
  - Inspect matrix and set small values directly to zero (assume they would have reached there eventually anyways).
  - Works well when the diameter of the clusters is small. (Non-homogeneous distributions of weight)

Analysis of MCL

- **In 2006, MCL fared well in a paper comparing it to three other clustering techniques**
  - **Brohee S, van Helden J (2006) Evaluation of clustering algorithms for protein–protein interaction networks. *BMC Bioinformatics* 7: 488**
  - **MCL vs. Restricted Neighborhood Search Clustering (RNSC) vs. Super Paramagnetic Clustering (SPC) vs. Molecular Complex Detection (MCODE)**

Analysis of MCL



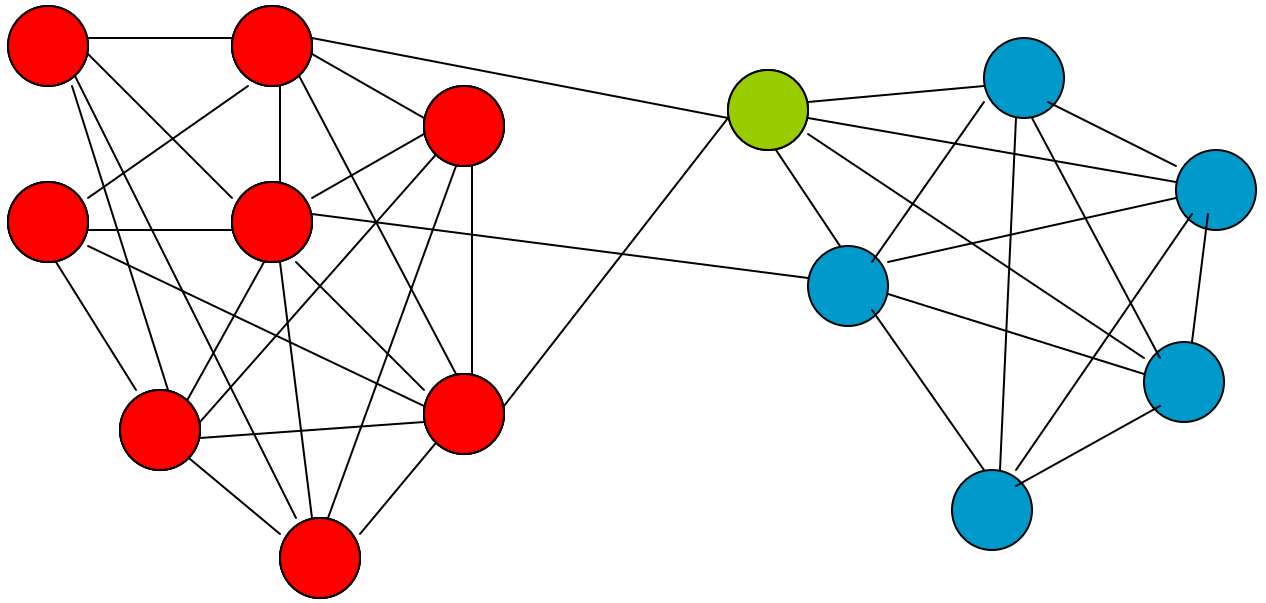
Each curve represents the value of accuracy (left panels) or separation (right panels).

(A-B) edge addition to the test graph. **(C-D)** edges removal from the test graph. **(E-F)** Edge removal from an altered graph with 100% of randomly added edges. **(G-H)** Edge addition to an altered test graph with 40% of randomly removed edges.

Color code: *blue* : MCL, *red* : RNSC, *orange* : MCODE, *green* : SPC. Dotted lines show the results obtained by permuting the clusters (negative control).

MCL Compared to RRW

- Comparison to Repeated Random Walks (RRW)
  - RRW is another Graph Clustering Method.



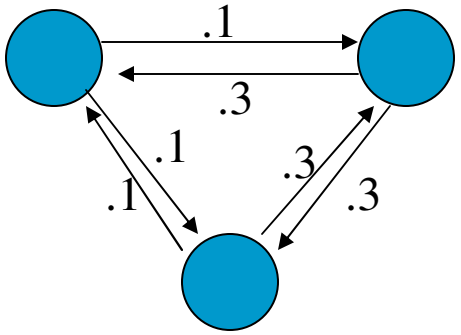
- Every cluster (including intermediate clusters) is stored.
- Clusters that overlap more than a threshold are later compared, and lower ranking clusters removed.

MCL Compared to RRW

- RRW Cluster p-value approximation:

$$\text{p-value} = 1 - (\text{score} \cdot \sqrt{n})$$

where *n* is the number of vertices in the cluster, and *score* is the average random walk distance between nodes in the cluster.



$$\text{score} = \frac{(.1+.3+.1+.1+.3+.3)}{6} = .2$$

$$\text{p-value} = 1 - (.2 * \sqrt{3}) = 0.653$$

MCL Compared to RRW

- MCL, RRW, and a naïve nearest neighbor approach were run on a biological protein network for yeast (WI-PHI[1]), as well as "noisy" versions of the network (edges added and deleted).
- Proteins with the same biological function should be clustered together
- The resulting clusters were compared to known protein groupings.

[1]Kiemer L, Costa S, Ueffing M, Cesareni G: **WI-PHI: A weighted yeast interactome enriched for direct physical interactions**. *Proteomics* 2007, **7**:932–943.

MCL Compared to RRW

Table 1: Results for the WI-PHI network

% in same MIPS category	RRW	MCL	Naïve
90+%	55%	17%	7.8%
80+%	69%	30%	19%
70+%	74%	42%	31%
60+%	84%	57%	44%
50+%	92%	77%	70%
25+%	100%	99%	98%

Table 2: Results for the FP40 network

% in same MIPS category	RRW	MCL	Naïve
90+%	56%	20%	6.3%
80+%	71%	34%	17%
70+%	78%	50%	26%
60+%	83%	63%	37%
50+%	92%	82%	63%
25+%	98%	99%	96%

Table 3: Results for the FN40 network

% in same MIPS category	RRW	MCL	Naïve
90+%	55%	10%	7.7%
80+%	67%	23%	19%
70+%	73%	32%	26%
60+%	80%	49%	44%
50+%	89%	79%	63%
25+%	99%	98%	95%

Table 4: Results for the Rewire40 network

% in same MIPS category	RRW	MCL	Naïve
90+%	33%	17%	4.8%
80+%	54%	32%	13%
70+%	58%	46%	21%
60+%	65%	65%	33%
50+%	76%	81%	57%
25+%	95%	98%	93%

Table 6: Precision, Recall, and Accuracy on preselected MIPS clusters

Network	Precision RRW / MCL / Naïve	Recall RRW / MCL / Naïve	Accuracy RRW / MCL / Naïve
WI-PHI	.771 / .512 / .363	.672 / .832 / .791	.720 / .657 / .535
FP40	.791 / .538 / .362	.689 / .768 / .795	.738 / .643 / .537
FN40	.533 / .423 / .326	.536 / .670 / .699	.534 / .532 / .477
Rewire40	.654 / .480 / .370	.520 / .565 / .706	.583 / .520 / .511

Average cluster size: RRW = 6, MCL = 12, Naïve = 9

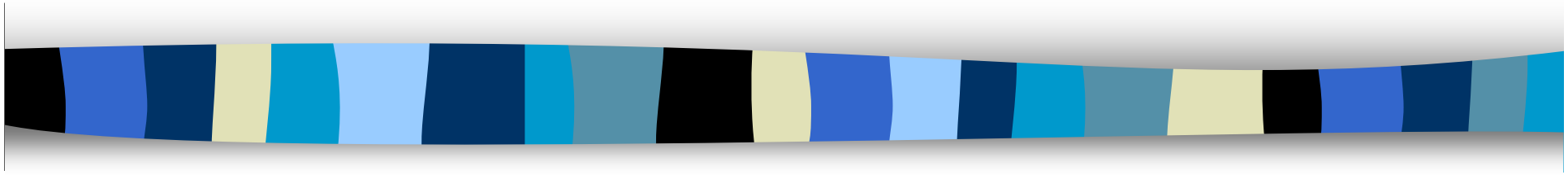
Analysis of MCL

- Scales well with increasing graph size.
- Works with both weighted and unweighted graphs.
- Produces good clustering results.
- Robust against noise in graph data

- Number of clusters not specified ahead of time, but can adjust cluster granularity with parameters.

- Cannot find overlapping clusters (in general)
- Not suitable for clusters with large diameter.

Thank You!



Any Questions?