

Fixed-Parameter and Integer Programming Approaches for Clustering Problems

Falk Hüffner

joint work with

Sharon Bruckner¹ Christian Komusiewicz²
Adrian Liebrau³ Rolf Niedermeier² Sven Thiel³
Johannes Uhlmann²

¹Institut für Mathematik, Freie Universität Berlin

²Institut für Softwaretechnik und Theoretische Informatik, TU Berlin

³Institut für Informatik, Friedrich-Schiller-Universität Jena

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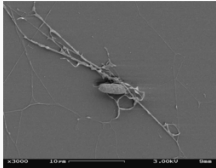
Labyrinthulomycetes

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The **Labyrinthulomycetes** (ICBN) or **Labyrinthula**^[1] (ICZN), or **Slime nets** are a class of protists that produce a network of filaments or tubes,^[2] which serve as tracks for the cells to glide along and absorb nutrients for them. There are two main groups, the labyrinthulids and thraustochytrids. They are mostly marine, commonly found as parasites on alga and seagrass or as decomposers on dead plant material. They also include some parasites of marine invertebrates.

Although they are outside the cells, the filaments are surrounded by a membrane. They are formed and connected with the cytoplasm by a unique organelle called a sagenogen or bothrosome. The cells are uninucleate and typically ovoid, and move back and forth along the amorphous network at speeds varying from 5-150 μm per minute. Among the labyrinthulids the cells are enclosed within the tubes, and among the thraustochytrids they are attached to their sides.

Slime nets



The cell with the network of filaments *Aplanochytrium* sp.

Scientific classification

Domain: Eukaryota
Kingdom: Chromalveolata
Phylum: Heterokontophyta
Class: **Labyrinthulomycetes** DICK, 2001 or

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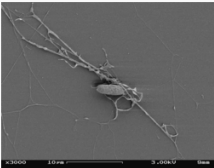
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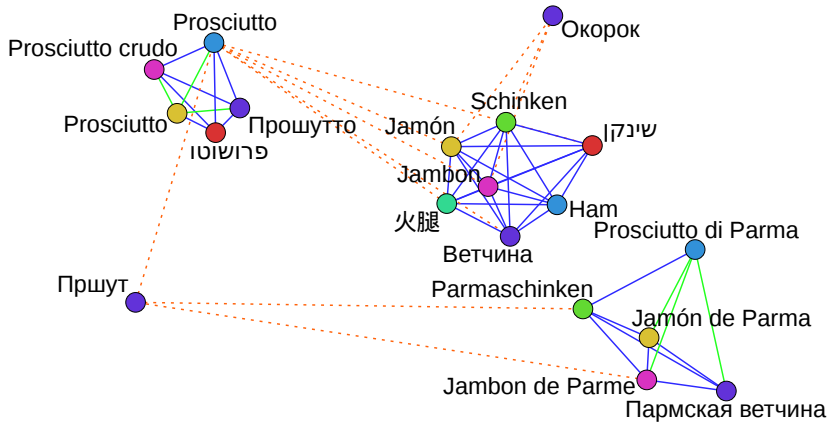
Netzschleimpilze

Die **Netzschleimpilze** oder **Schleimnetze** (Labyrinthulomycetes) bilden ein **Taxon** innerhalb der **Stramenopilen** und sind somit näher mit **Braunalgen**, **Goldalgen**

attached to their sides.

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Model

COLORFUL COMPONENTS

Instance: An undirected graph $G = (V, E)$ and a coloring of the vertices $\chi : V \rightarrow \{1, \dots, c\}$.

Task: Delete a minimum number of edges such that all connected components are *colorful*, that is, they do not contain two vertices of the same color.

Complexity of Colorful Components

- COLORFUL COMPONENTS with two colors can be solved in $O(\sqrt{nm})$ time by matching techniques.

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- COLORFUL COMPONENTS can be approximated by a factor of $4\ln(c + 1)$.

Fixed-parameter algorithm

Observation

COLORFUL COMPONENTS can be seen as the problem of destroying by edge deletions all **bad paths**, that is, simple paths between equally colored vertices.

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Theorem

COLORFUL COMPONENTS can be solved in $O(c^k \cdot m)$ time, where k is the number of edge deletions.



Limits of fixed-parameter algorithms

Exponential Time Hypothesis (ETH)

3-SAT cannot be solved within a running time of $2^{o(n)}$ or $2^{o(m)}$.

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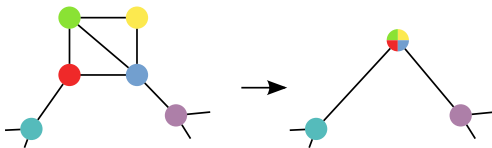
Theorem

COLORFUL COMPONENTS with three colors cannot be solved in $2^{o(k)} \cdot n^{O(1)}$ unless the ETH is false.

Data reduction

Data reduction

Let $V' \subseteq V$ be a colorful subgraph. If the cut between V' and $V \setminus V'$ is at least as large as the connectivity of V' , then merge V' into a single vertex.



Method 1: Implicit Hitting Set

HITTING SET

Instance: A ground set U and a set of *circuits* S_1, \dots, S_n with $S_i \subseteq U$ for $1 \leq i \leq n$.

Task: Find a minimum-size *hitting set*, that is, a set $H \subseteq U$ with $H \cap S_i \neq \emptyset$ for all $1 \leq i \leq n$.

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We can reduce COLORFUL COMPONENTS to HITTING SET: The ground set U is the set of edges, and the circuits to be hit are the paths between identically-colored vertices.

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Problem

Exponentially many circuits!

Method 1: Implicit Hitting Set

In an *implicit hitting set* problem, the circuits have an implicit description, and a polynomial-time oracle is available that, given a putative hitting set H , either confirms that H is a hitting set or produces a circuit that is not hit by H .

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Several approaches to solving implicit hitting set problems are known, which use an ILP solver as a black box for the HITTING SET subproblems.

Method 2: Row generation

Idea

Instead of using the ILP solver as a black box, we can use *row generation* ("*lazy constraints*") to add constraints inside the solver.

Method 3: Clique Partitioning ILP formulation

- 0/1 variables for each vertex pair indicates whether it is contained in a cluster
- Constraints ensure consistency

Cutting Planes

Definition

A *cutting plane* is a valid constraint that cuts off fractional solutions.

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Tree cut

Let $T = (V_T, E_T)$ be a subgraph of G that is a tree such that all leaves L of the tree have color c , but no inner vertex has. Then

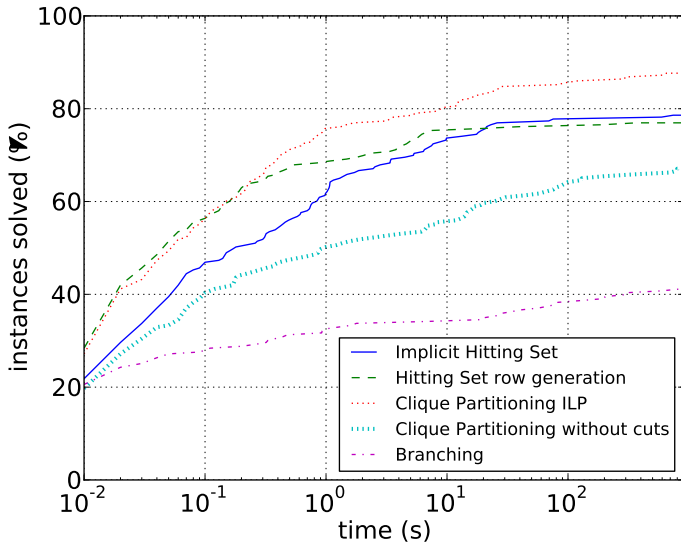
$$\sum_{e \in E_T} d_e \geq |L| - 1$$

is a valid inequality.

Wikipedia interlanguage links

- 30 most popular languages
- 11,977,500 vertices, 46,695,719 edges
- 2,698,241 connected components, of which 2,472,481 are already colorful
- largest connected component has 1,828 vertices and 14,403 edges
- solved optimally by data reduction + CLIQUE PARTITIONING algorithm in about 80 minutes
- 618,660 edges deleted, 434,849 inserted.

Random graph model



Greedy Heuristics (random instances)

| | optimal | average error | max. error |
|-------------|---------|---------------|------------|
| move-based | 25.8 % | 4.9 % | 38.7 % |
| merge-based | 58.2 % | 0.9 % | 12.5 % |

Clustering

Graph-based clustering

Find a partition of the vertices of a graph into clusters such that

- Vertices within a cluster have many connections;
- Vertices in different clusters have few connections.

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Definition ([Hartuv & Shamir '00])

A graph with n vertices is called *highly connected* if more than $n/2$ edges need to be deleted to make it disconnected.

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A graph with n vertices is called *highly connected* if more than $n/2$ edges need to be deleted to make it disconnected.

Lemma ([Chartrand '66])

A graph with n vertices is highly connected iff each vertex has degree more than $n/2$.

Clustering algorithm

Min-cut algorithm [Hartuv & Shamir '00]

If the graph is highly connected, terminate; otherwise, delete the edges of a minimum cut and recurse on the two sides.

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Applications

- Clustering cDNA fingerprints;
- Finding complexes in protein–protein interaction (PPI) data;
- Grouping protein sequences hierarchically into superfamily and family clusters;
- Finding families of regulatory RNA structures.

Maximizing Edge Coverage

HIGHLY CONNECTED DELETION

Instance: An undirected graph.

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Lemma

The min-cut algorithm can delete $\Omega(k^2)$ edges, where k is the optimal solution size.

Complexity

Theorem

HIGHLY CONNECTED DELETION is NP-hard even on 4-regular graphs.

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Theorem

If the Exponential Time Hypothesis (ETH) is true, then HIGHLY CONNECTED DELETION cannot be solved in subexponential time (that is, $2^{o(k)} \cdot n^{O(1)}$ or $2^{o(n)} \cdot n^{O(1)}$ time).

Data reduction

Lemma

In a highly connected graph, if two vertices are connected by an edge, they have at least one common neighbor; otherwise, they have at least three common neighbors.

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In a highly connected graph, if two vertices are connected by an edge, they have at least one common neighbor; otherwise, they have at least three common neighbors.

Reduction rule

If there are two vertices that are connected by an edge but have no common neighbors, then delete the edge.

Data reduction

Reduction rule

If G contains a vertex set S such that

- $|S| \geq 4$,
- $G[S]$ is highly connected, and
- $|D(S)| \leq 0.3 \cdot \sqrt{|S|}$,

then remove S from G . Here, $D(S)$ is the size of the edge cut between S and the rest of the graph.

Data reduction

Reduction rule

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Theorem

HIGHLY CONNECTED DELETION admits a problem kernel with at most $10 \cdot k^{1.5}$ vertices, which can be computed in $O(n^2 \cdot mk \log n)$ time.

Fixed-parameter algorithm

Using a combination of kernelization and dynamic programming, we obtain:

Theorem

HIGHLY CONNECTED DELETION can be solved in $O(3^{4k} \cdot k^2 + n^2 mk \cdot \log n)$ time.

Column generation

Idea

Use a 0/1-variable to indicate that a particular cluster is in the solution, and successively add only those variables (“columns”) that are “needed”, that is, their introduction improves the objective.

PPI networks: data reduction

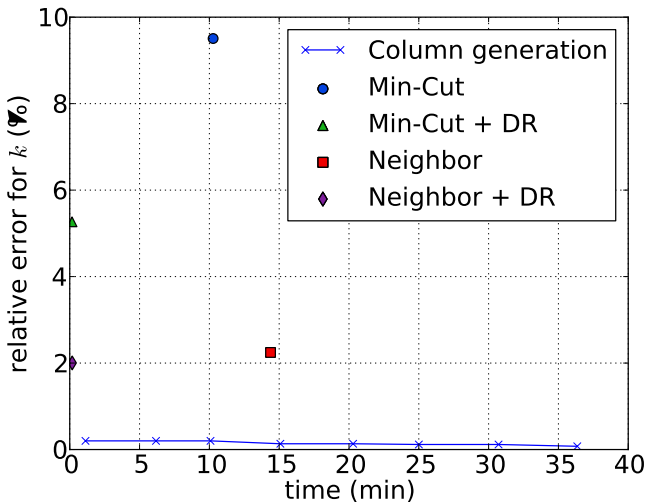
| | n | m | Δk | Δk [%] | n' | m' |
|--------------------------|------|-------|------------|----------------|------|------|
| <i>C. elegans</i> phys. | 157 | 153 | 100 | 92.6 | 11 | 38 |
| <i>C. elegans</i> all | 3613 | 6828 | 5204 | 80.1 | 373 | 1562 |
| <i>M. musculus</i> phys. | 4146 | 7097 | 5659 | 85.3 | 426 | 1339 |
| <i>M. musculus</i> all | 5252 | 9640 | 7609 | 84.8 | 595 | 1893 |
| <i>A. thaliana</i> phys. | 1872 | 2828 | 2057 | 83.1 | 187 | 619 |
| <i>A. thaliana</i> all | 5704 | 12627 | 8797 | 79.5 | 866 | 3323 |

n' , m' : size of largest connected component after data reduction

PPI networks: Column generation

- Using column generation, an solve optimally e. g. PPI network of *A. thaliana* with 5 704 vertices and 12 627 edges, in a few hours ($k = 12096$ edges deleted)
- Cannot solve network of *S. pombe* with 3 735 vertices and 51 620 edges

Heuristics (A. thaliana network)



FPT and ILP

Observations

- FPT algorithms give useful running time bounds and are often fast in practice
- ILP approaches are often even faster in practice, but do not have useful running time bounds
- Combining kernelization and ILPs works quite well