Partitioning into Colorful Components by Minimum Edge Deletions

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Multiple Sequence Alignment

T_1 A_2 C_3 G_4 T_5 A_6

T_1 A_2 G_3 T_4 A_5

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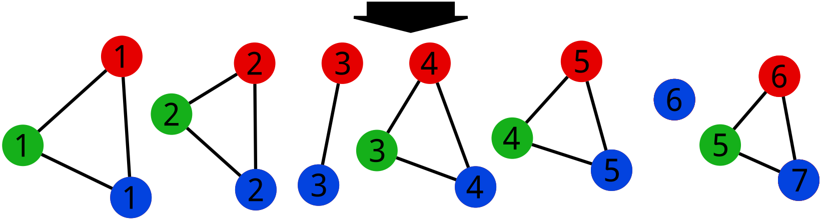

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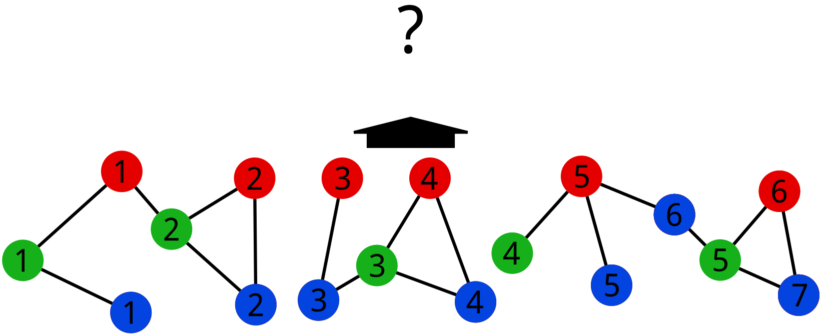
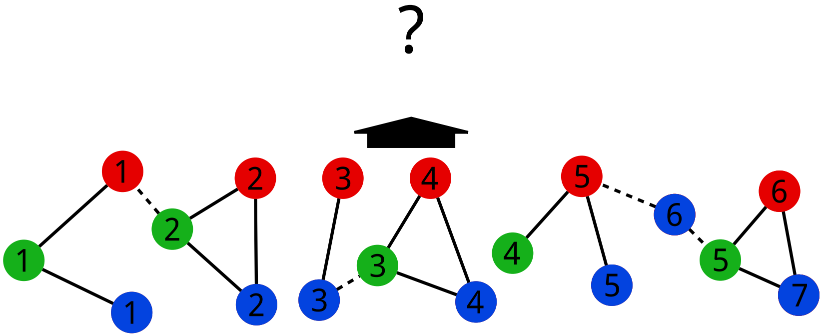


Idea

Use alignment graph constructed by local alignment to reconstruct global alignment.

Multiple Sequence Alignment



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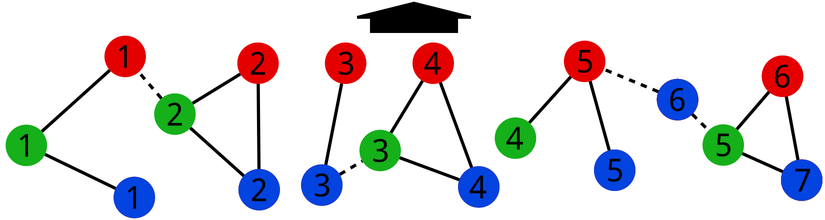

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Colorful Components

Part of a Multiple Sequence Alignment pipeline suggested by Corel, Pitschi & Morgenstern (Bioinformatics 2010).

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COLORFUL COMPONENTS

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

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Other application: Wikipedia interlanguage links

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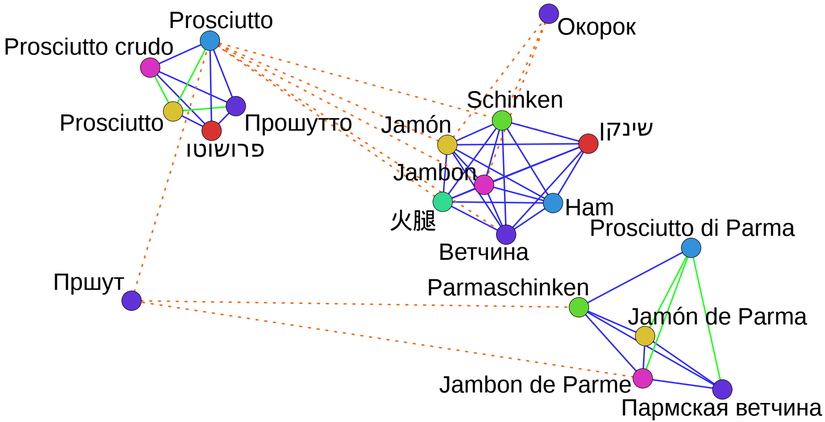
Wikipedia interlanguage link graph example



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Complexity of Colorful Components

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- COLORFUL COMPONENTS is NP-hard on trees.
- COLORFUL COMPONENTS on trees with c colors can be solved in $2^c \cdot n^{O(1)}$ time.

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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.

Improved fixed-parameter algorithm

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Colorful Components can be solved in $O((c-1)^k \cdot m)$ time, where k is the number of edge deletions.

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Proof.

If there is a degree-3 or higher vertex v, find a bad path with at most $(c-1)$ edges by BFS from v. Otherwise, the instance is easy. □

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Limits of fixed-parameter algorithms

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Exponential Time Hypothesis (ETH)

For all $x \geqslant 3$, x-SAT, which asks whether a Boolean input formula in conjunctive normal form with n variables and m clauses and at most x variables per clause is satisfiable, 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.

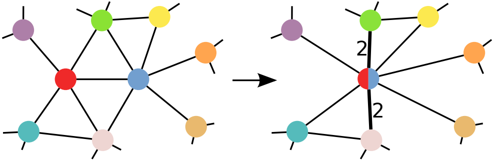
Weighted version

Problem

If we know that two vertices must belong to the same colorful component, we want to be able to simplify the instance by merging them.

Idea

Introduce color *sets* per vertex and edge weights.



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Uses of the merge operation

Edge branching

Can branch into two cases: delete an edge, or merge its endpoints.

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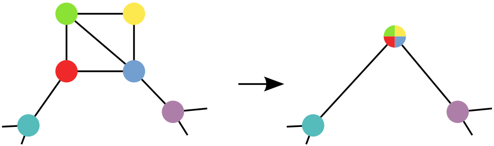
Data reduction

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.



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Merge-based heuristic

Idea

Repeatedly merge the two vertices "most likely" to be in the same component, while immediately deleting edges connecting vertices with intersecting color sets.

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We always merge the endpoints of the edge that maximizes cut cost minus merge cost.

- *merge cost*: weight of the edges that would need to be deleted when merging
- *cut cost*:

$$3w(\{u,v\}) + \sum_{w \in V | \{\{u,w\},\{v,w\}\} \subseteq E} \min\{w(\{u,w\}), w(\{v,w\})\}$$

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Data

- We generated one COLORFUL COMPONENTS instance for each multiple alignment instance from the BAliBASE 3.0 benchmark.
- We restricted the experiments to the 135 of instances that have at most 10 colors.

Data reduction: Largest connected component

(1) originally
(2) after data reduction in the COLORFUL COMPONENTS formulation
(3) after data reduction in the weighted formulation

	(1)			(2)			(3)		
	n	*m*	*c*	*n*	*m*	*c*	*n*	*m*	*c*
average	504	921	6.2	407	697	4.7	354	607	5.3
median	149	232	6	46	90	5	42	58	5

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Branching algorithms: running time

	< 1 s	1 s to 10 min	> 10 min
bad-path branching	61	6	68
merging branching	70	9	56

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Note

In ongoing research, we are able to solve several more instances to optimality with integer linear programming (ILP) based approaches.

Heuristics: relative error

	min.	max.	avg.	med.
min-cut heuristic [1]	0 % (1)	70.0 %	29.2 %	27.8 %
merging heuristic	0 % (76)	12.7 %	0.6 %	0 %

[1] Corel, Pitschi & Morgenstern (Bioinformatics 2010)

Sequence alignment quality

DIALIGN with several methods for solving the COLORFUL COMPONENTS subproblem:

	TC score
min-cut heuristic	53.6 %
merge heuristic	55.1 %
exact algorithm	56.6 %

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DIALIGN with the min-cut heuristic is about 10 percentage points worse than current state-of-the-art multiple alignment methods. Hence, an improvement of 3 percentage points is a sizable step towards closing the gap between DIALIGN and these methods.

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Outlook

- ILP-based solutions
- Application to network alignment
- Relaxation of the colorfulness constraint

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Acknowledgments

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