Experiments with Parameterized Approaches to Hard Graph Problems

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joint work with

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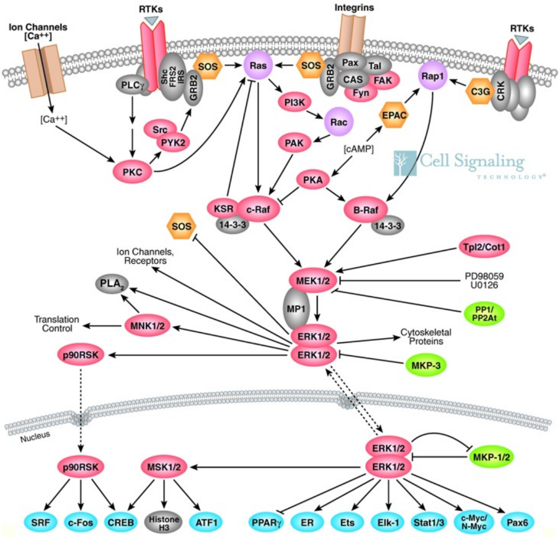
Dagstuhl Seminar N° 07281
Structure Theory and FPT Algorithmics for
Graphs, Digraphs and Hypergraphs

Outline

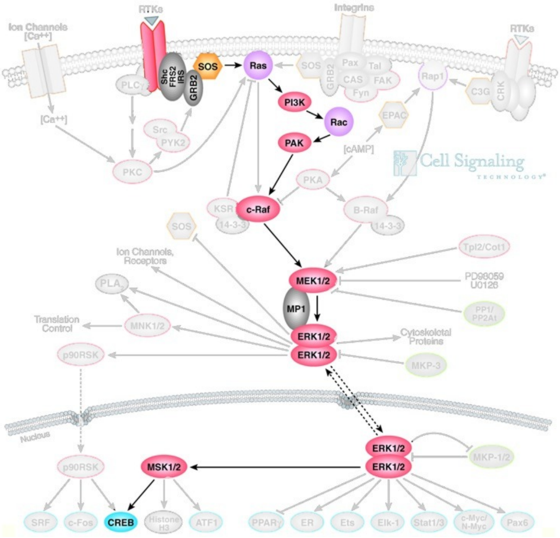
1. Minimum-Weight Path
    - Application: protein interaction networks
    - Color-coding
    - Speedups
2. Minimum-Weight Path experiments
3. Balanced Subgraph
    - Applications
    - Data reduction
    - Iterative compression
4. Balanced Subgraph experiments

Signaling pathways



[www.cellsignal.com]

Signaling pathways



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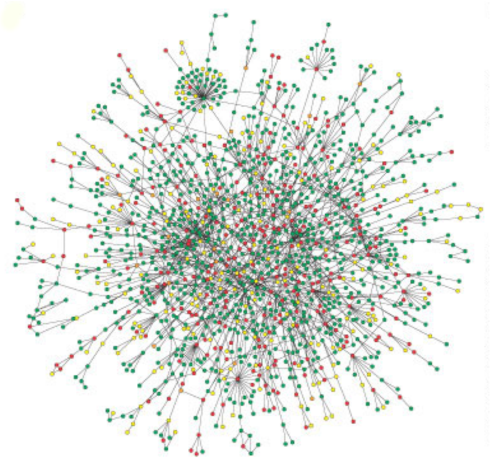
Signaling pathways

Minimum-Weight Path

Input: Graph $G = (V, E)$, weights $w : E \rightarrow \mathbb{R}^+$, integer $k > 0$.
Task: Find a non-overlapping path $v_1, \ldots, v_k$ of length k in G that minimizes $w(v_1, v_2) + \cdots + w(v_{k-1}, v_k)$.

Example: yeast network



4 400 proteins, 14 300 interactions, looking for paths of length 5–15

Minimum-Weight Path

Theorem

MINIMUM-WEIGHT PATH *is NP-hard* [GAREY & JOHNSON 1979].

Idea

Exploit the fact that the paths sought for are rather short ($\approx$ 5–15): parameter k.

Color-coding

Color-coding [Alon, Yuster & Zwick J. ACM 1995]

- randomly color each vertex of the graph with one of k colors
- hope that all vertices in the subgraph searched for obtain different colors (colorful)
- solve the Minimum-Weight Path under this assumption (which is much quicker)
- repeat until it is reasonably certain that the path was colorful at least once

Result: FPT algorithm

Dynamic programming for Minimum-Weight Colorful Path

Idea

Table entry $W[v, C]$ stores the minimum-weight path that ends in v and uses exactly the colors in C.

- Each table entry can be calculated in $O(n)$ time
- $n \cdot 2^k$ table entries

$\rightsquigarrow$ Running time per trial: $O(2^k \cdot n^2)$

To obtain error probability ε, one needs $O(-\ln \varepsilon \cdot e^k)$ trials

Theorem ([Alon et al. JACM 1995])

Minimum-Weight Path *can be solved in* $O(-\ln \varepsilon \cdot 5.44^k |G|)$ *time.*

Implementations of color-coding

- Find minimum-weight paths of length 10 in the yeast protein interaction networks within 3 hours ($n = 4\,400$, $k = 10$)
  [Scott et al., RECOMB 2005]
- Pathway queries
  [Shlomi et al., BMC Bioinformatics 2006]
- Protein docking
  [Mayrose et al., Nucleic Acids Research 2007]
- Balanced paths
  [Cappanera & Scutellà, INOC 2007]
- Automated text headline generation
  [Deshpande et al., NAACL HLT 2007]

Increasing the number of colors

Idea

Use $k + x$ colors instead of k colors.

Trial runtime:

$$O(2^k|G|) \to O(2^{k+x}|G|)$$

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Probability P_c for colorful path ($k = 8$, $\varepsilon = 0.001$):

x	0	1	2	3	4	5
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trials	2871	816	378	220	146	106

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Theorem

MINIMUM-WEIGHT PATH *can be solved in* $O(-\ln \varepsilon \cdot 4.32^k|G|)$ *time by choosing* $x = 0.3k$.

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But: Higher memory usage

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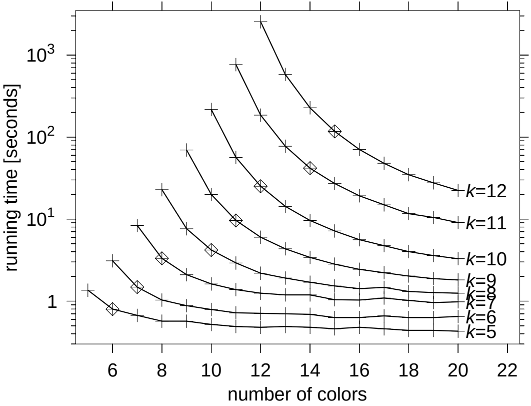

Runtimes for the yeast protein interaction network (highlighted point of each curve marks worst-case optimum)

Exploiting lower bounds

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Use a known solution to prune “hopeless” table entries.

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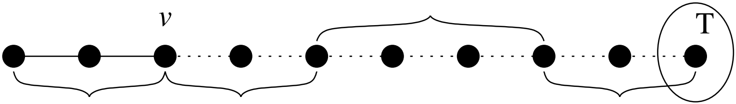
- Discard entries that already have a weight higher than the known solution.
- Discard entries when

$$\text{weight} + (\text{minimum edge weight} \cdot \text{edges left})$$

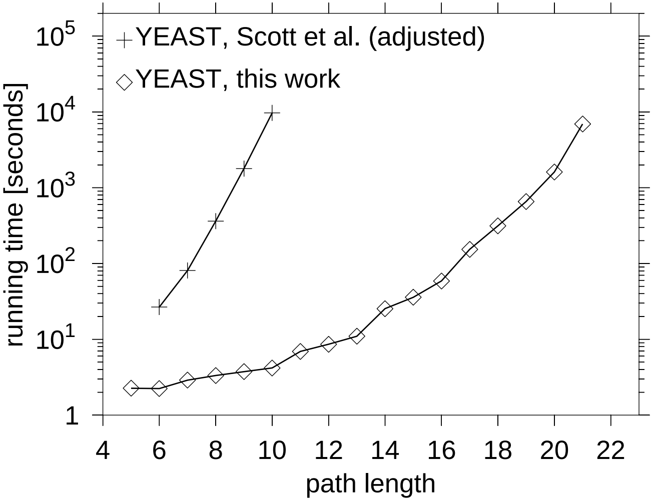
is higher than the weight of the known solution.

Precalculated lower bounds

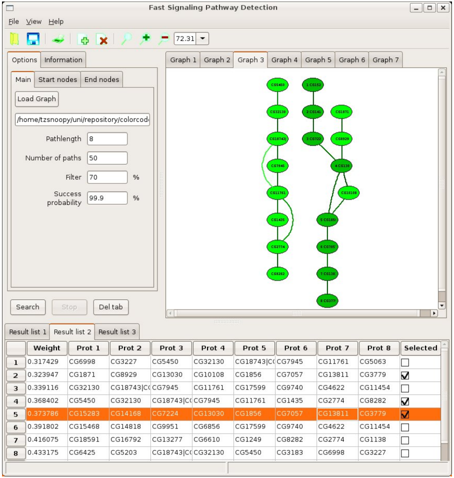
For each vertex u and a range of lengths $1 \leq i \leq d$, determine the minimum weight of a path of i edges that starts at u.



Yeast network



Graphical user interface: FASPAD



Free software, available at
http://theinf1.informatik.uni-jena.de/faspad/

Conclusion & Outlook

Color-coding, with some algorithm engineering, is a practical method for finding signaling pathways in protein interaction networks.

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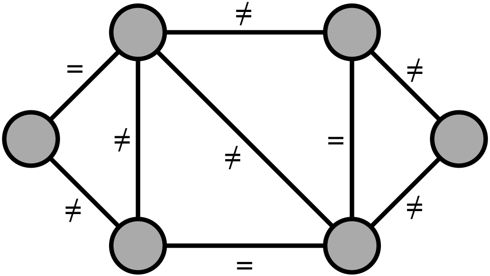
Future work:

- Pathway queries
- Richer motifs (cycles, trees, . . .)
- "Divide-and-color" [Kneis et al., WG 2007; Chen et al., SODA 2007]: Improvement from 4.32^k to 4^k. But: "$\Omega(4^k)$"

Balanced graphs

Definition

A graph with edges labeled by $=$ or $\neq$ (signed graph) is balanced if the vertices can be colored with two colors such that the relation on each edge holds.



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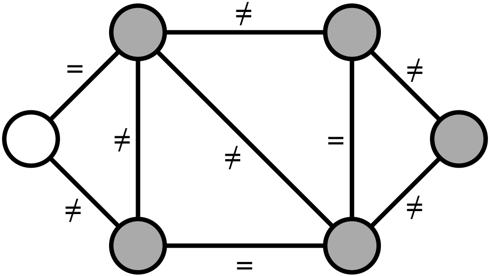

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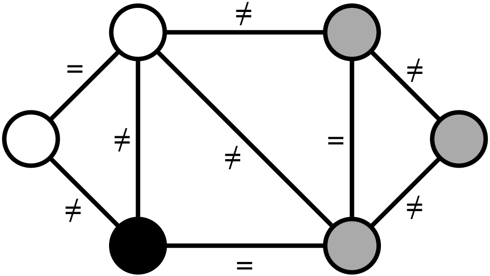

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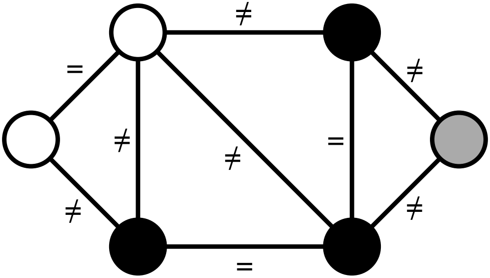

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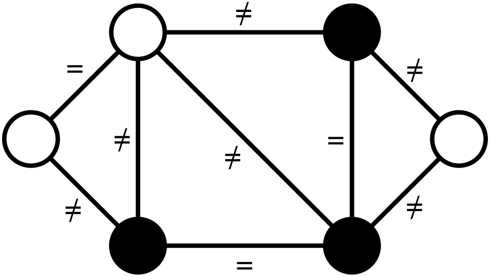

Characterization of balance

Special case

Bipartite graphs are balanced graphs that contain only $\neq$-edges.

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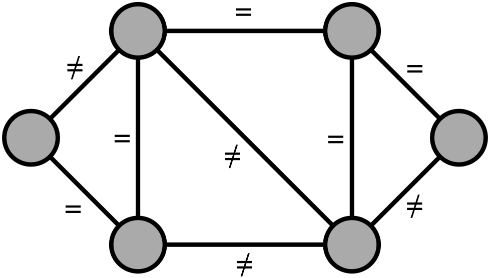
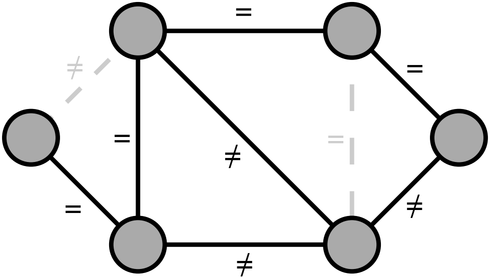
Theorem (Kőnig 1936)

A signed graph is balanced iff it contains no cycle with an odd number of $\neq$-edges.

Balanced Subgraph



Balanced Subgraph



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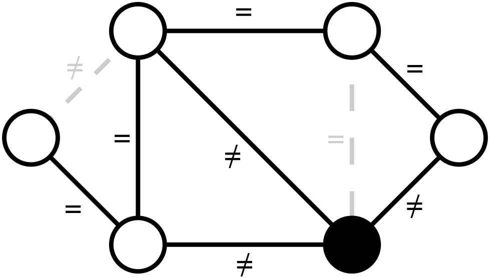

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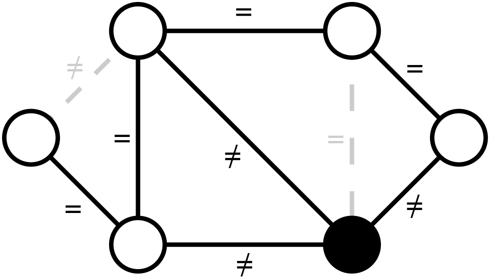


Definition (Balanced Subgraph)

Input: A graph with edges labeled by $=$ or $\neq$.
Task: Find a minimum set of edges to delete such that the graph becomes balanced.

Balanced Subgraph: known results

- Balanced Subgraph is NP-hard, since it is a generalization of Max-Cut (Max-Cut is the special case where all edges are $\neq$)
- A solution that keeps at least 87.8 % of the edges can be found in polynomial time [DasGupta et al., WEA 2006]
- A solution that deletes at most c times the edges that need to be deleted can probably not be found in polynomial time [Khot, STOC 2002]

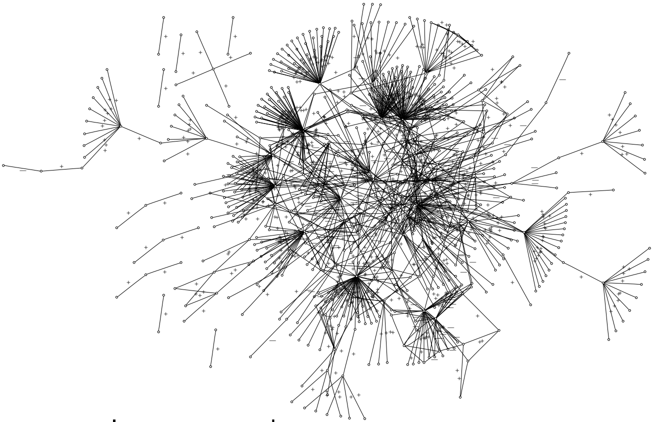
Applications of Balanced Subgraph

- "Monotone subsystems" in gene regulatory networks
  [DasGupta et al., WEA 2006]
- Balance in social networks
  [Harary, Mich. Math. J. 1953]
- Portfolio risk analysis
  [Harary et al., IMA J. Manag. Math. 2002]
- Minimum energy state of magnetic materials (spin glasses)
  [Kasteleyn, J. Math. Phys. 1963]
- Stability of fullerenes
  [Došlić & Vikičević, Discr. Appl. Math. 2007]
- Integrated circuit design
  [Chiang et al., IEEE Trans. CAD of IC & Sys. 2007]

Graph structure

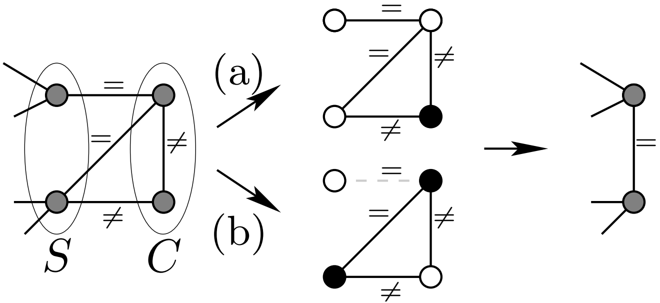
Idea

Exploit the structure of the relevant networks



Yeast gene regulatory network

Vertex cut-based data reduction



Data reduction scheme

Data reduction scheme

- Find cut S that cuts off small component C
- For each of the (up to symmetry) $2^{|S|-1}$ colorings of S, determine the size of an optimal solution for $G[S \cup C]$
- Replace in G the subgraph $G[S \cup C]$ by an equivalent smaller gadget

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Subsumes all 8 data reduction rules given by [Wernicke, 2003] for Edge Bipartization

Filling in the data reduction scheme

- Need to restrict both $|S|$ and $|C|$: we use $|S| \leq 4$ and $|C| \leq 32$

Filling in the data reduction scheme

- Need to restrict both $|S|$ and $|C|$: we use $|S| \leq 4$ and $|C| \leq 32$
- How to construct gadgets that behave equivalently to $S \cup C$?

Gadget construction

Idea

Use atomic gadgets and describe their effect by cost vectors.

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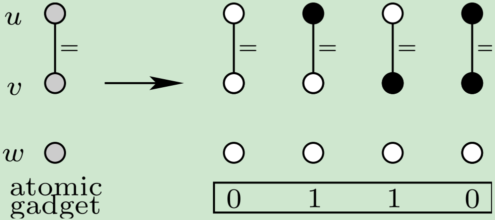
Use atomic gadgets and describe their effect by cost vectors.

Example



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With 10 atomic gadgets, we can emulate the behavior of any component behind a 3-vertex cut.

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All cuts with $|S| = 2$ *and* $|C| \geq 1$ *and and all cuts with* $|S| = 3$ *and* $|C| \geq 2$ *are subject to data reduction.*

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- 4-cuts: 2948 atomic gadgets

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Given a set S of n vectors of length l with nonnegative integer components and a target vector t of length l, find a sub-(multi)-set of vectors from S that sums to t.

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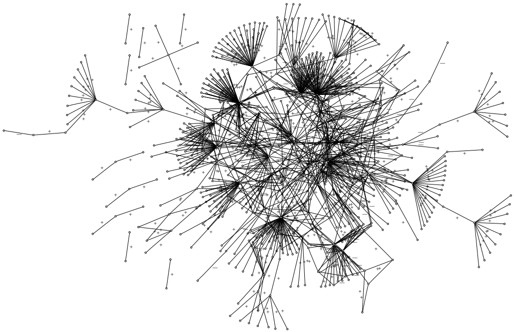
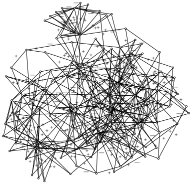
- “Equality-constrained multidimensional knapsack”
- In our implementation: simple branch & bound
- Sometimes this is a bottleneck!

Reduction. . . and then?

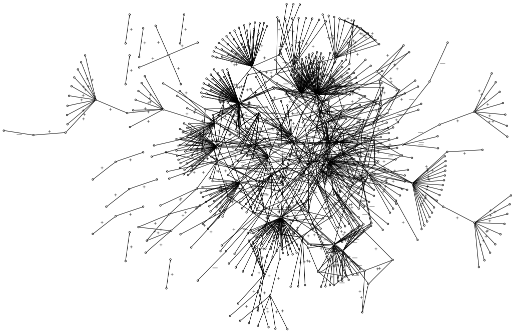


$n = 690,\ m = 1082$



$n = 144,\ m = 405$

Reduction… and then?



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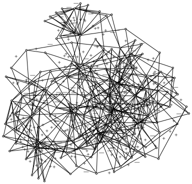

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After data reduction, a hard "core" remains.

Fixed-parameter tractability

Theorem

BALANCED SUBGRAPH *can be solved in* $O(2^k \cdot m^2)$ *time by a reduction to* EDGE BIPARTIZATION *and using an algorithm based on iterative compression* [GUO et al., JCSS 2006].

Fixed-parameter tractability

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BALANCED SUBGRAPH can be solved in $O(2^k \cdot m^2)$ time by a reduction to EDGE BIPARTIZATION and using an algorithm based on iterative compression [Guo et al., JCSS 2006].

A heuristic speedup trick can give large speedups over this worst-case running time.

Experimental results

			Approximation			Exact alg.	
Data set	n	m	$k \geq$	$k \leq$	t [min]	k	t [min]
EGFR	330	855	196	219	7	210	108
Yeast	690	1082	0	43	77	41	1
Macr.	678	1582	218	383	44	374	1

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- Yeast is not solvable without reducing 4-cuts
- A real-world network with 688 vertices and 2208 edges could not be solved

Outlook

- Kernel for Balanced Subgraph?
- Directed case of Balanced Subgraph (delete minimum number of edges to remove all unbalanced cycles): FPT?
    - Problem: Characterization by two-coloring does not work
- The data reduction scheme is applicable to all graph problems where a coloring or a subset of the vertices is sought. For example:
    - Vertex Cover
    - Dominating Set
    - 3-Coloring
    - Feedback Vertex Set

  but: need small cuts (e. g., small-world networks)

References

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