Minimum-Weight Path experiments

Balanced Subgraph

Balanced Subgraph experiments

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

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Minimum-Weight Path	Minimum-Weight Path experiments	Balanced Subgraph	Balanced Subgraph experiments
Outline			

- Application: protein interaction networks
- Color-coding
- Speedups

2 Minimum-Weight Path experiments

3 Balanced Subgraph

- Applications
- Data reduction
- Iterative compression

4 Balanced Subgraph experiments

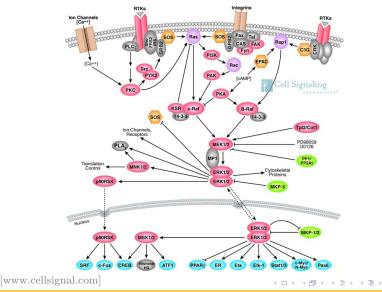
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Signaling pathways



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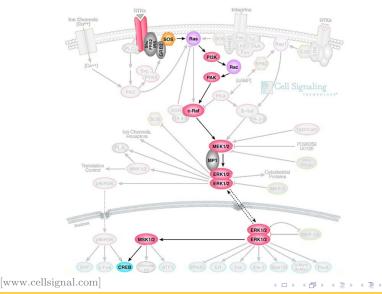
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Signaling pathways



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Signaling pathways

MINIMUM-WEIGHT PATH

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

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Example: yeast network



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

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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.

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Minimum-Weight Path experiments

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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

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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

→ 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.

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Implementations of color-coding

- Find minimum-weight paths of length 10 in the yeast protein interaction networks within 3 hours (n = 4400, 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]

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Minimum-Weight Path experiments

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Increasing the number of colors

Idea

Use k + x colors instead of k colors.

Trial runtime:

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

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

Probability P_c for colorful path (k = 8, c = 0.001):

x	0	1	2	3	4	5
P _c	0.0024	0.0084	0.0181	0.0310	0.0464	0.0636
trials	2871	816	378	220	146	106

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Minimum-Weight Path experiments

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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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Increasing the number of colors

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Theorem

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But: Higher memory usage

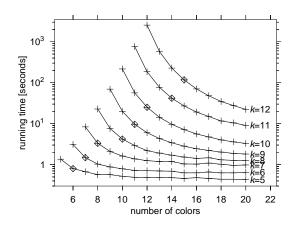
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Increasing the number of colors



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

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Exploiting lower bounds

Idea

Use a known solution to prune "hopeless" table entries.

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

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Minimum-Weight Path experiments

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Exploiting lower bounds

Idea

Use a known solution to prune "hopeless" table entries.

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

weight + (minimum edge weight · edges left)

is higher than the weight of the known solution.

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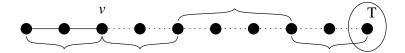
Minimum-Weight Path experiments

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Precalculated lower bounds

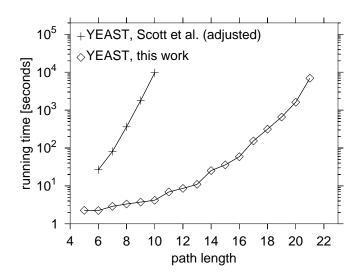
For each vertex u and a range of lengths $1 \le i \le d$, determine the minimum weight of a path of i edges that starts at u.



Experiments with Parameterized Approaches to Hard Graph Problems

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Minimum-Weight Path	Minimum-Weight Path experiments	Balanced Subgraph	Balanced Subgraph experiments
Yeast netwo	rk		



Minimum-Weight Path experiments

Balanced Subgraph

Balanced Subgraph experiments

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

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Experiments with Parameterized Approaches to Hard Graph Problems

Minimum-Weight Path experiments

Balanced Subgraph

Balanced Subgraph experiments 000

Conclusion & Outlook

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

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Minimum-Weight Path experiments

Balanced Subgraph

Balanced Subgraph experiments

Conclusion & Outlook

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

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: " $\Omega(4^k)$ "

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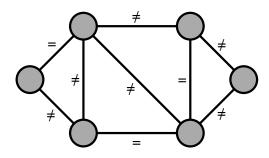
Minimum-Weight Path experiments

Balanced Subgraph

Balanced Subgraph experiments

Balanced graphs

Definition



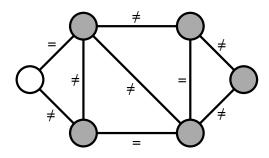
Minimum-Weight Path experiments

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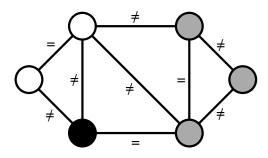
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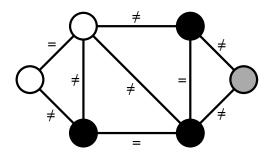
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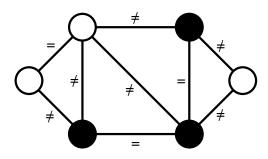
Minimum-Weight Path experiments

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Balanced graphs

Definition



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Characterization of balance

Special case

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

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Experiments with Parameterized Approaches to Hard Graph Problems

18/33

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Balanced Subgraph experiments

Characterization of balance

Special case

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

Theorem (Kőnig 1936)

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

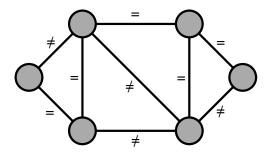
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Balanced Subgraph



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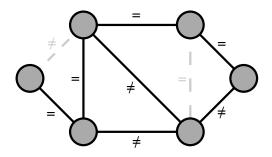
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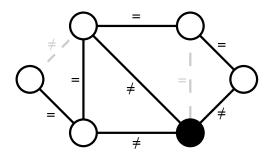
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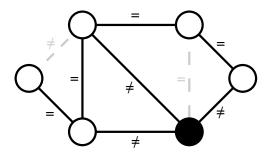
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Minimum-Weight Path experiments

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Balanced Subgraph



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.

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Minimum-Weight Path experiments

Balanced Subgraph

Balanced Subgraph experiments

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 ≠)
- 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]

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Minimum-Weight Path experiments

Balanced Subgraph

Balanced Subgraph experiments

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]

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Minimum-Weight Path experiments

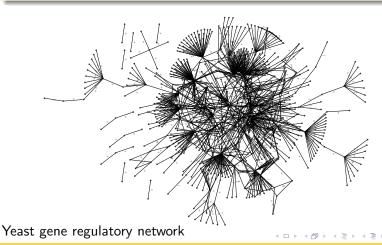
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Graph structure

Idea

Exploit the structure of the relevant networks



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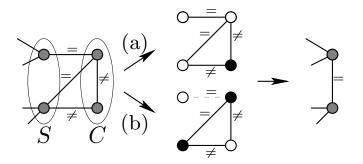
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Vertex cut-based data reduction



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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 ∪ C]
- Replace in G the subgraph $G[S \cup C]$ by an equivalent smaller gadget

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Minimum-Weight Path experiments

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- Replace in G the subgraph $G[S \cup C]$ by an equivalent smaller gadget

Subsumes all 8 data reduction rules given by $_{\rm [Wernicke,\ 2003]}$ for Edge Bipartization

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Minimum-Weight Path experiments

Balanced Subgraph

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Filling in the data reduction scheme

• Need to restrict both |S| and |C|: we use $|S| \le 4$ and $|C| \le 32$

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Minimum-Weight Path experiments

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Filling in the data reduction scheme

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

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Gadget construction

Idea

Use atomic gadgets and describe their effect by cost vectors.

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Minimum-Weight Path experiments

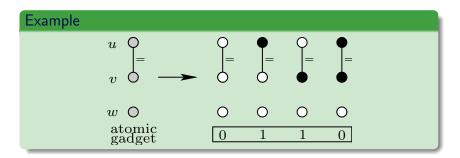
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Gadget construction

Theorem

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

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Gadget construction

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

Theorem

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

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Minimum-Weight Path experiments

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

• 4-cuts: 2948 atomic gadgets

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Gadget construction

Problem

How to determine an appropriate set of atomic cost vectors for a given cost vector?

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Balanced Subgraph

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Gadget construction

Problem

How to determine an appropriate set of atomic cost vectors for a given cost vector?

Vector Sum Problem

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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Minimum-Weight Path experiments

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Balanced Subgraph experiments

Gadget construction

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Vector Sum Problem

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.

• "Equality-constrained multidimensional knapsack"

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Gadget construction

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- "Equality-constrained multidimensional knapsack"
- In our implementation: simple branch & bound

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Minimum-Weight Path experiments

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Gadget construction

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How to determine an appropriate set of atomic cost vectors for a given cost vector?

Vector Sum Problem

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.

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

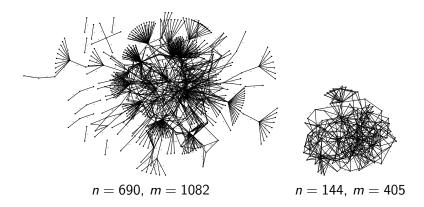
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Minimum-Weight Path experiments

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Reduction... and then?



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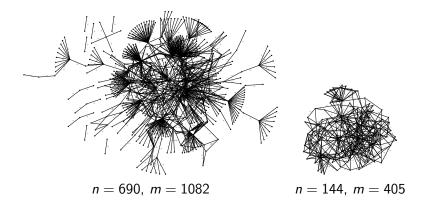
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Reduction... and then?



After data reduction, a hard "core" remains.

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Minimum-Weight Path experiments

Balanced Subgraph

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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].

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Minimum-Weight Path experiments

Balanced Subgraph

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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.

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Minimum-Weight Path experiments

Balanced Subgraph

Balanced Subgraph experiments •00

Experimental results

			A	Approximation			Exact alg.	
Data set	п	т	$k \ge$	$k \leq$	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	

Experiments with Parameterized Approaches to Hard Graph Problems

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Minimum-Weight Path experiments

Balanced Subgraph

Balanced Subgraph experiments •00

Experimental results

			Approximation			Exact alg.	
Data set	n	т	$k \ge$	$k \leq$	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

• Yeast is not solvable without reducing 4-cuts

• A real-world network with 688 vertices and 2208 edges could not be solved

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Minimum-Weight Path	Minimum-Weight Path experiments	Balanced Subgraph	Balanced Subgraph experiments
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)

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Minimum-Weight Path	Minimum-Weight Path experiments	Balanced Subgraph	Balanced Subgraph experiments
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