Complex Network Analysis using Parallel Approximate Motif Counting

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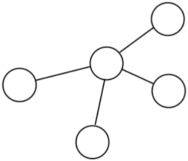
Our Contributions

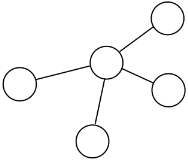
- New distributed-memory parallelization of a dynamic programming-based subgraph counting scheme
  - memory-efficient
  - complementary to prior shared-memory parallelism
- Comparative network analysis using relative subgraph counts as graph signatures
  - find motifs in networks
  - detect local structure in network snapshots
  - cluster networks into categories
- Open-source tool: fascia-psu.sf.net

Talk Outline

- **Introduction**: Color-coding for subgraph counting
- **Background**: Why fast subgraph counting?
- **Algorithms**: New distributed-memory parallelization
- **Results**: Parallel performance and scalability
- **Analysis**: Large network collection using subgraph counts


Template

Introduction
Subgraph Counting



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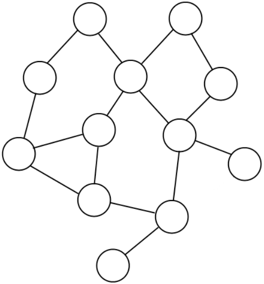

Larger Network

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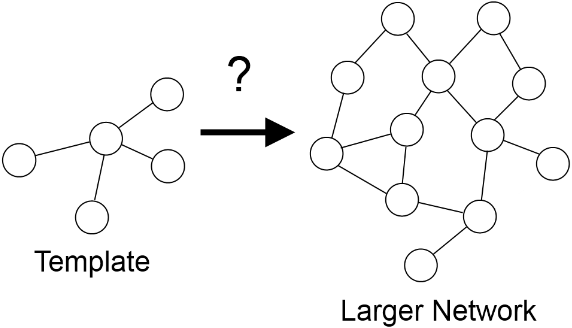

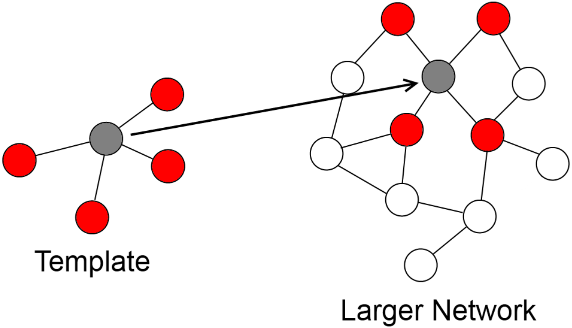
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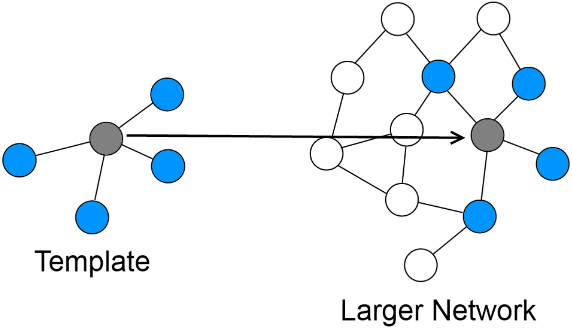
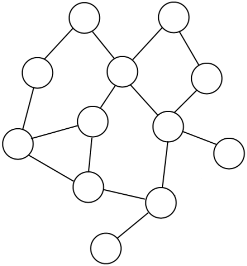


Introduction

Color-coding [Alon et al., 1995] for Approximate Subgraph Counting

- Color-coding: randomized method to get approximate counts of *tree-structured non-induced subgraphs*, termed as **treelets**



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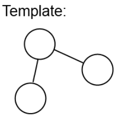

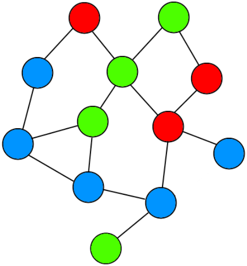

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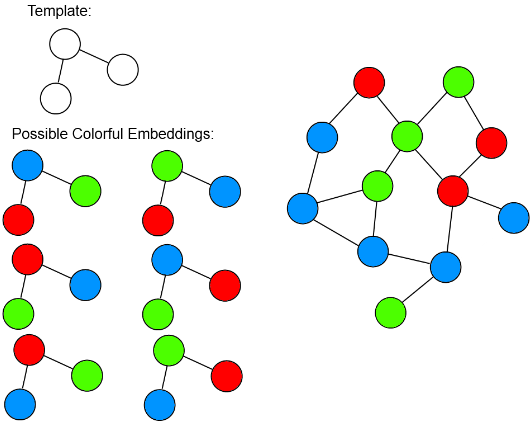

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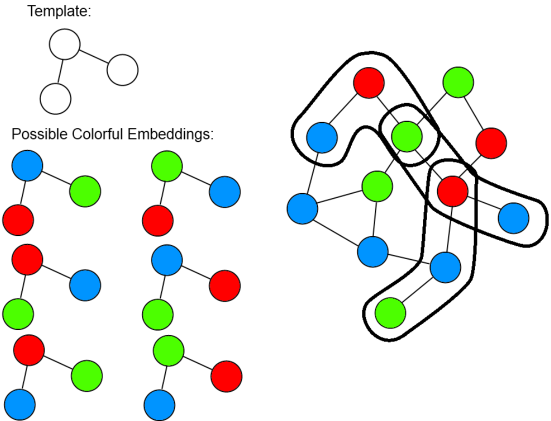
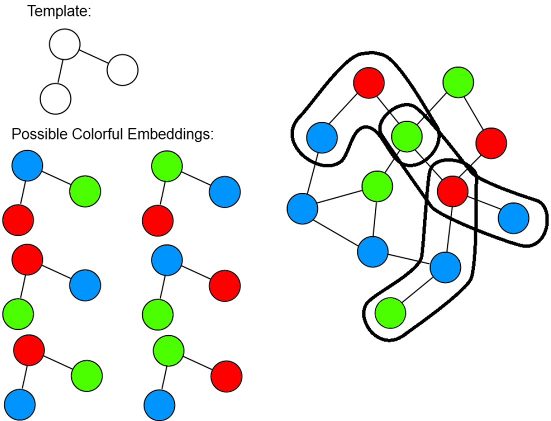


- Color-coding: randomized method to get approximate counts of *tree-structured non-induced subgraphs*, termed as **treelets**
- $cnt_{colorful} = 3$, $C_{total} = 3^3$, $C_{colorful} = 3!$, $P = \frac{3!}{3^3}$
- $cnt_{estimate} = \frac{cnt_{colorful}}{P} = \mathbf{13.5}$



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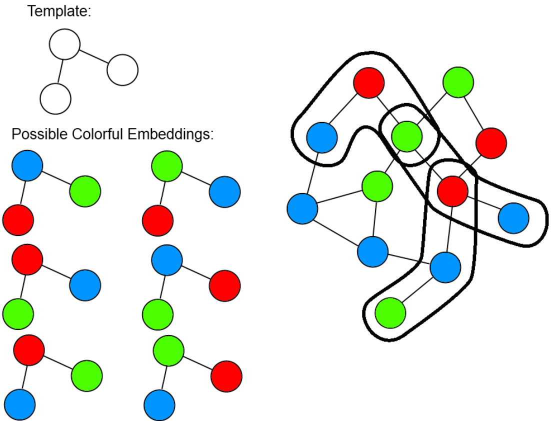
- $cnt_{estimate} = \frac{cnt_{colorful}}{P} = \mathbf{13.5}$
- Use multiple coloring iterations. Each iteration is $O(m2^k)$ work.



Motivation

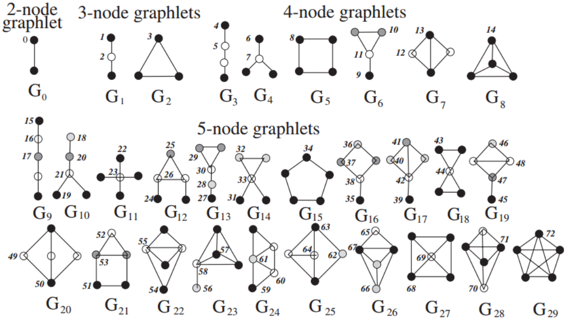
Why do we want fast algorithms for subgraph counting?

- Important uses in bioinformatics, chemoinformatics, social network analysis, communication network analysis, etc.
- Counts form basis for more complex analyses:
  - Motif finding
  - Graphlet frequency distances (GFD)
  - Graphlet degree distributions (GDD) and agreements (GDDA)
  - Graphlet degree signatures (GDS)
- Counting and enumeration on large networks is very expensive, $O(n^k)$ complexity for naïve algorithm. Color-coding reduces this to $O(m2^k n_{\text{iter}})$.

Background

Network analysis using graphlet counts

- Graphlets: all possible 2-5 vertex undirected subgraphs



[Milo et al., 2002, Alon et al., 2008, Pržulj, 2004, 2007, Milenkovič and Pržulj, 2008]

Background
Network analysis using graphlet counts

- Graphlets: all possible 2-5 vertex undirected subgraphs
- Graphlet frequency distance

$$S_i(G) = -\log\left(\frac{C_i(G)}{\sum_{i=1}^{\mathrm{n}} C_i(G)}\right)$$

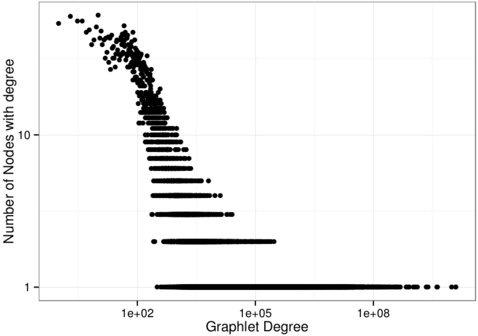
$$D(G,H) = \sum_{i=1}^{\mathrm{n}} |S_i(G) - S_i(H)|$$

[Milo et al., 2002, Alon et al., 2008, Pržulj, 2004, 2007, Milenkovič and Pržulj, 2008]

Background

Network analysis using graphlet counts

- Graphlets: all possible 2-5 vertex undirected subgraphs
- Graphlet frequency distance
- Graphlet degree distribution and agreement



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- Graphlet degree distribution and agreement

$$S_G^j(k) = \frac{d_G^j(k)}{k}$$

$$N_G^j(k) = \frac{S_G^j(k)}{\sum_{k=1}^{\infty} S_G^j(k)}$$

$$A^j(G,H) = 1 - \frac{1}{\sqrt{2}}(\sum_{k=1}^{\infty}[N_G^j(k) - N_H^j(k)]^2$$

[Milo et al., 2002, Alon et al., 2008, Pržulj, 2004, 2007, Milenkovič and Pržulj, 2008]

Background
Network analysis using graphlet counts

- Graphlets: all possible 2-5 vertex undirected subgraphs
- Graphlet frequency distance
- Graphlet degree distribution and agreement
- Graphlet degree signature

$$S_i(u,v) = 1 - w_i \times \frac{|\log(u_i+1) - \log(v_i+1)|}{\log(\max\{u_i, v_i\} + 2}$$

[Milo et al., 2002, Alon et al., 2008, Pržulj, 2004, 2007, Milenkovič and Pržulj, 2008]

Background

Network analysis using treelet counts

- Can we use treelets instead of graphlets? Are they more/less powerful?
- Goals of this work:
  - Create distributed-memory subgraph counting program to produce counts on larger networks, and faster counts on smaller networks.
  - Quantitative analyses using GFD and GDD with treelets to evaluate efficacy.
  - Evaluate effect of noise on treelet counts by deleting vertices and edges, as well as rewiring edges in various networks.

FASCIA

Fast Approximate Subgraph Counting (for In-memory/Insightful/I* Analytics)

- Previous work: FASCIA for shared-memory color-coding treelet counting [Slota and Madduri, 2013].
  - Memory reduction through efficient table and color set representations
  - Work reduction through template partitioning
  - Multilevel algorithm parallelization
- Present work: FASCIA for distributed memory
  - Further memory and communication reductions through CSR-like representation of table
  - Partitioned counting allowing counts for larger networks
  - Distributed counting for faster counts on smaller networks

FASCIA

Color-coding algorithm overview

1: Partition input template T (k vertices) into subtemplates S_i using *single edge cuts*.
2: Determine $Niter \approx \frac{e^k \log 1/\delta}{\epsilon^2}$, the number of iterations to execute. δ and ϵ are input parameters that control approximation quality.
3: **for** $it = 1$ to $Niter$ **do**
4: Randomly assign to each vertex v in graph G a color between 0 and $k - 1$.
5: Use a dynamic programming scheme to count *colorful* non-induced occurrences of T.
6: Take average of all $Niter$ counts to be final count.

FASCIA

New partitioned counting approach

- Each task gets a subset of $v \in G$, counts for this subset are further computed in parallel for each task
- Semi-partitioned: Each task holds full table for child subtemplates

for $it = 1$ to $Niter$ **do**
  Color $G(V, E)$ with k colors
  for all subtemplates S_i in reverse order of partitioning **do**
    Init $Table_{i,d}$ for V_d (vertex partition on task d)
    for all $v \in V_d$ **do in parallel** ▷ Multithreaded parallelism
      for all $c \in C_i$ **do**
        Compute all $Count_{S_i,c,v}$
    $N_d, I_d, B_d \leftarrow \text{Compress}(Table_{i,d})$
    for all $d = 1$ to $NumTasks$ **do**
      $N_i, I_i, B_i \leftarrow Bcast(N_d, I_d, B_d)$
  $$Count_d + = \sum_{v}^{V_d} \sum_{c}^{C_T} Count_{T,c,v}$$
$Count \leftarrow \text{Reduce}(Count_d)$
Scale $Count$ based on Niter and colorful embed prob.

- Dynamic programming table corresponding to each subtemplate can be represented as a $n \times C_i$ rectangular matrix (n: number of graph vertices, C_i: number of possible color sets of subtemplate i).
- We represent the table in a CSR-like format using three arrays:
  - N: count values in table
  - I: color set indexes
  - B: offsets for each vertex

FASCIA

Distributed counting (assign multiple iterations to each process)

for all $it = 1$ to $Niter$ **in parallel do** ▷ MPI task-level
  Color $G(V, E)$ with k colors
  Initialize 3D count table
  for all S_i in reverse order of partitioning **do**
    for all $v \in V$ **in parallel do** ▷ multithreaded
      Update count table for template S_i
      using child subtemplate counts

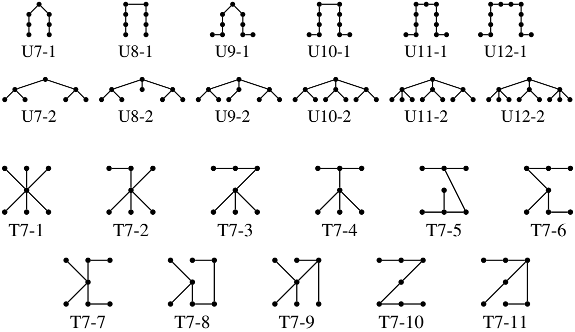
Results

Experimental setup - systems and graphs

- Performance results on *Compton*, a Sandia cluster with dual-socket Intel Xeon E5-2670 (Sandy Bridge) nodes and 64 GB main memory per node.
- Studies also performed on Cyberstar and Hammer clusters at Penn State.
- Networks from SNAP, Konect, DIMACS, UF sparse matrix, and Virginia Tech NDSSL collections; GTgraph and igraph generators.

Network Type	Count	n $(\times 10^3)$ min	n $(\times 10^3)$ max	m $(\times 10^3)$ min	m $(\times 10^3)$ max
Collaboration	6	26	425	14	1050
Communication	4	30	63	87	855
$G(n, p)$	4	10	100	100	1000
Peer-to-peer	9	6	63	9.7	77
Bio PPI	4	0.7	22	1.3	22
Road	5	440	1970	530	2800
Scale-free	4	10	100	100	1000
Social	6	60	150	214	5400
Small-world	4	10	100	100	1000
Web Crawl	4	280	875	761	3900
Orkut	-	3100	-	117000	-
Portland	-	1620	-	31000	-

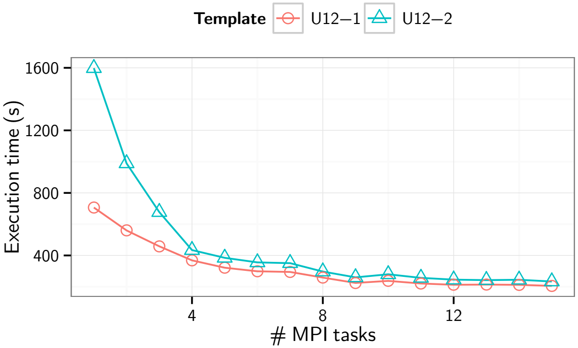
- UX-1 indicates chain or simple path, UX-2 indicates more complex tree
- T7-X indicates all 7 vertex treelets, used for evaluating effects of network noise on relative counts



Results

Running times and parallel scaling

- Parallel speedup on 15 nodes; 3.5× (U12-1) and 7× (U12-1) for Orkut crawl



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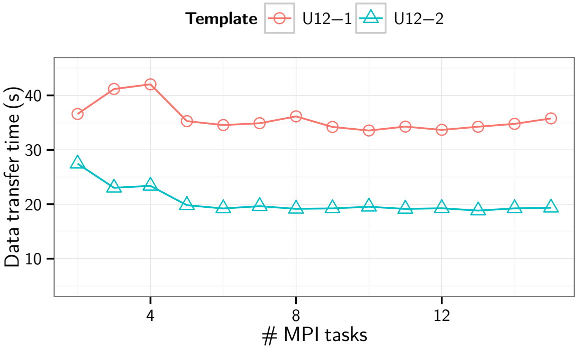
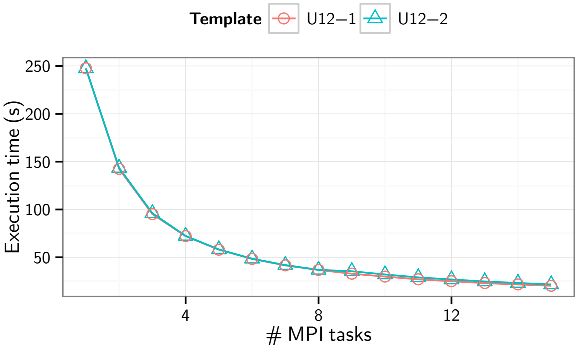
- Communication time is about 15-25% of total time



Results

Running times and parallel scaling

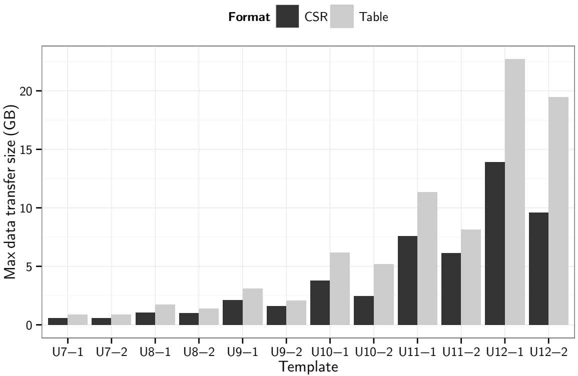
- Parallel speedup on 15 nodes; 3.5× (U12-1) and 7× (U12-1) for Orkut crawl
- Communication time is about 15-25% of total time
- Near-linear speedup for distributed counting on C.elegans PPI network



Results

Communication volume reduction

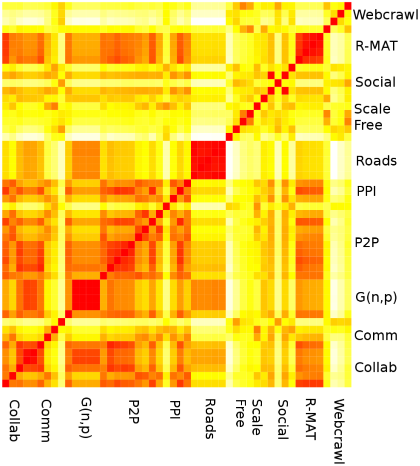
- Maximal data transfer during counting on Orkut for templates from 7 to 12 vertices
- About 35% mean reduction in transfer costs with CSR compression



Results

Graphlet frequency distance analysis

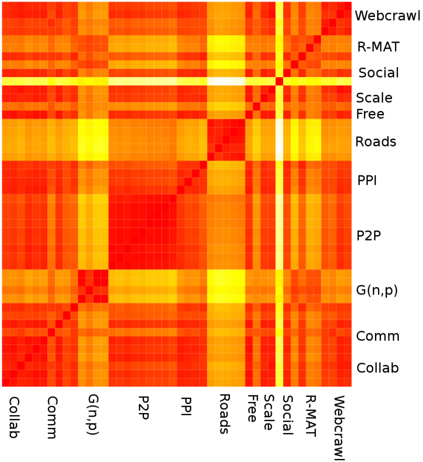
- Treelet frequency distance, GFD calculated with counts of all 4-9 vertex treelets (92 total)
- Intra-class mean agreements highest for 5/10 classes



Results

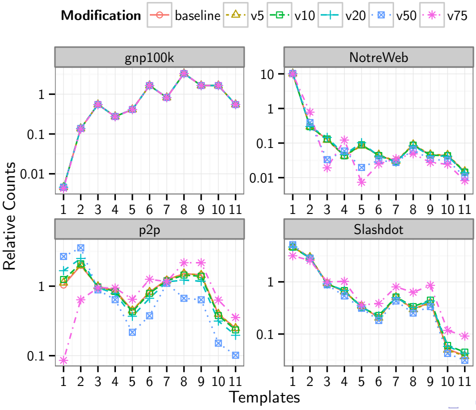
Graphlet degree distribution agreement analysis

- Treelet degree distribution agreements, GDDA calculated with counts of orbits of all 3-7 vertex treelets (83 total)
- Similar observations as with GFD, intra-class mean highest 6/10 classes



Results
Vertex deletion

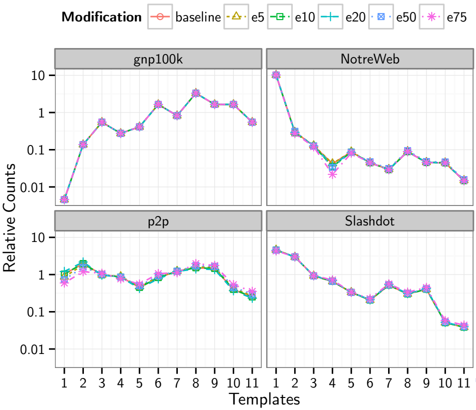
- 5, 10, 20, 50, and 75% vertices deleted, evaluated based on GFD for **only** 7 vertex templates, relative counts shown
- Largest disagreement for Notre Dame webcrawl, value of 4.1
- Mean disagreement between networks is 9.2



Results

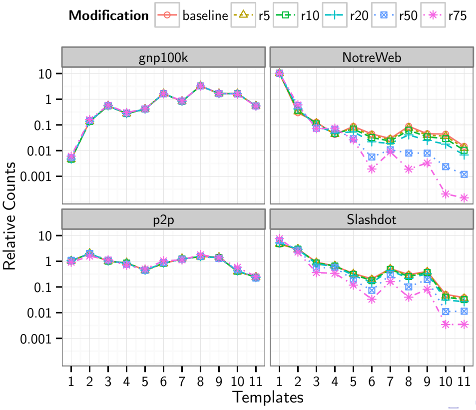
Edge deletion

- 5, 10, 20, 50, and 75% edges deleted
- Max disagreement value of 1.2 with Gnutella p2p snapshot
- Demonstrated relative treelet counts are useful analytic even on networks with a relatively high proportion of known vertices to known edges (e.g. PPI networks)



Results
Edge rewiring

- 5, 10, 20, 50, and 75% edges rewired
- 6.6 and 10.4 disagreements with Slashdot and Notre Dam webcrawl
- Minimal change with random and Gnutella networks; less inherent structure?



Conclusions

- Partitioned subgraph counting (i.e., partitioned dynamic programming table) makes it feasible to analyze large-scale networks on clusters.
- Distributed subgraph counting accelerates subgraph counting for small networks.
- Treelets counts seem to be as powerful as graphlets for network analysis.
- Relative treelet counts more sensitive to vertex sampling than edge sampling.

Bibliography

N. Alon, R. Yuster, and U. Zwick. Color-coding. *J. ACM*, 42(4):844–856, 1995.

N. Alon, P. Dao, I. Hajirasouliha, F. Hormozdiari, and S.C. Sahinalp. Biomolecular network motif counting and discovery by color coding. *Bioinformatics*, 24(13):i241–i249, 2008.

T. Milenkovič and N. Pržulj. Uncovering biological network function via graphlet degree signatures. *Cancer Informatics*, 6:257–273, 2008.

R. Milo, S. Shen-Orr, S. Itzkovitz, N. Kashtan, D. Chklovskii, and U. Alon. Network motifs: Simple building blocks of complex networks. *Science*, 298(5594):824–827, 2002.

N. Pržulj. Modeling interactome, scale-free or geometric? *Bioinformatics*, 20(18):3508–3515, 2004.

N. Pržulj. Biological network comparison using graphlet degree distribution. *Bioinformatics*, 23(2):e177–83, 2007.

G. M. Slota and K. Madduri. Fast approximate subgraph counting and enumeration. In *Proc. 42nd Int'l. Conf. on Parallel Processing (ICPP)*, pages 210–219, 2013.

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Questions?

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