Easy graph algorithms under hard constraints

GraphEx Symposium 2016

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U.S. National Security Agency
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Graphs are everywhere!

Why graph?

Graph-theoretic approaches are appealing to many fields

- simple data abstraction
  - binary relationships — nodes and links
- powerful algorithmic approaches

The expanding field of graph research

Results from Google Scholar

The number of articles containing "graph", "algorithm" and "vertex" or "edge" has more than *tripled* in the last ten years!

576,000 articles through 2006

2,020,000 articles through today

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Google Scholar results for the following terms added to first query

Up to four-fold increase across non-traditional disciplines

neuroscience 4× increase: 227 → 1,020

biology 4× increase: 2,000 → 7,720

chemistry 3× increase: 1570 → 4,580

Graphs in Biology

Pathways in Protein-Protein Interaction (PPI) networks

Finding signaling pathways in yeast is analogous to finding k-length simple paths in graphs [6]

- simple path has no repeated vertices

Comparing PPI networks

Comparing yeast and fly protein interaction networks [8]

- find the maximum common subgraph (subgraph isomorphism)

Graphs in Chemistry

Chemical reactions

Identify routes in chemical reactions [9]

- cyclic subgraphs — route of reaction

Dissociation pathways

Lowest-cost pathway for six-dimensional free energy surface of 1 million grid points [10]

- Dijkstra's shortest-path

N-body interactions

Enumerate n-body intramolecular interactions using line graphs [5]

Graphs in Neuroscience

Conscious awareness

Awareness is linked to the brain's functional connectivity [2]

- decreased modularity (functional segregation)
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- lower probability of hubs (high degree centrality)

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Greater self-awareness in Schizophrenia?

Graphs in Neuroscience

Alzheimer's disease (AD)

Alzheimer's disease (AD) exhibit aberrant brain network [3]

- longer shortest-paths (less effective information transfer)
- largest connected-component is smaller in AD patients

Technology shift

Google Scholar results for the following terms added to first query

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database 6× increase: 78,100 → 497,000

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Graph algorithms expressed in the language of linear algebra...

- sparse matrix products are natural for GPU acceleration

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Graph DB

Graphs are becoming the new relational model!

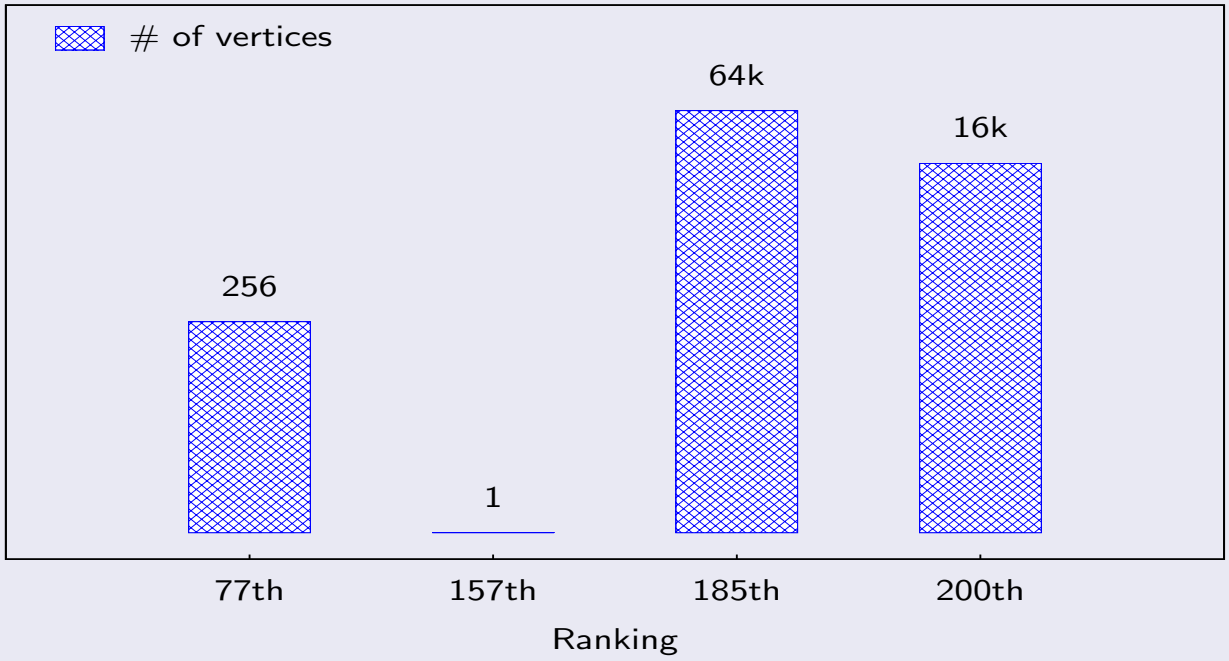
- graph databases
- semantic graphs

Who needs Big Graphs?

Graph500 scale ≤ 16

If only 64k vertices was more than anyone needed...

Source: Graph500 November 2015 List



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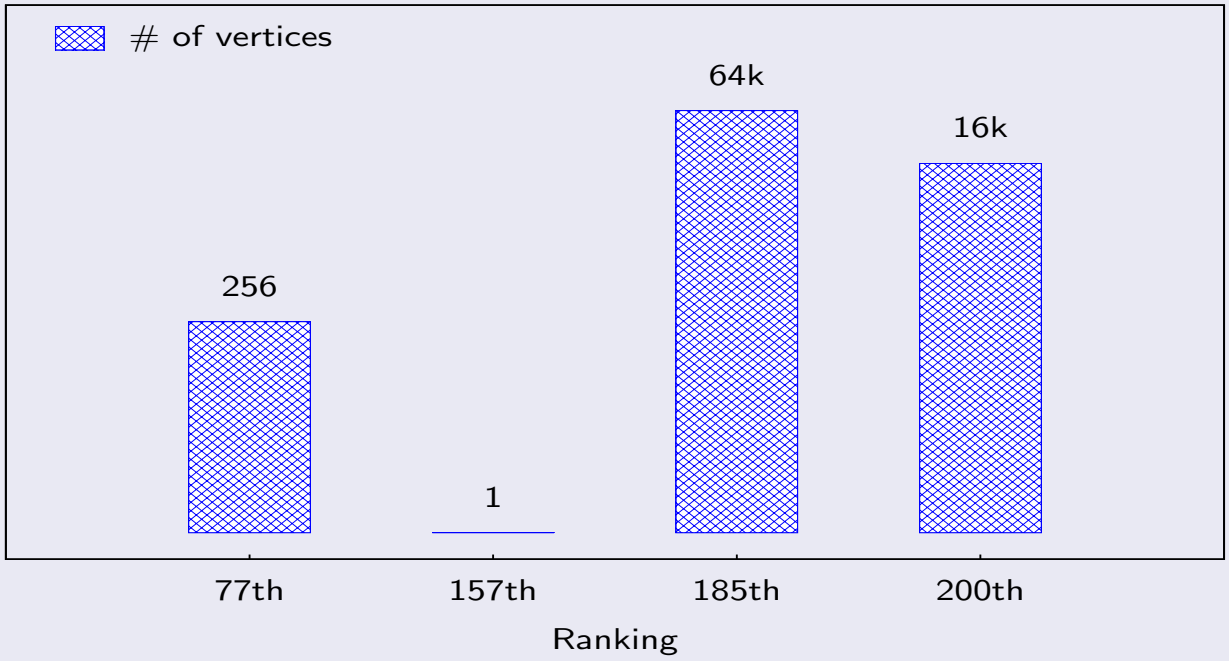

The 77th ranked competitor can assign one thread to each vertex!

- Intel Xeon E5-2670 — 128 cores
- 256 threads with simultaneous multithreading (SMT)

More focus on increasing graph sizes

The challenge is with Big Graphs

Increasing data and problem sizes lead to bigger graphs. . .

- everything gets harder with increasing scale

Google Scholar results for the following terms added to first query

distributed 60× increase: 17,400 → 1,150,000

parallel 14× increase: 74,100 → 1,030,000

scalable 7× increase: 19,100 → 134,000

The need for graph analytics!

Trending

The increase in graph analysis across different domains can be due in part to

- simple and compact representation of complex data
- practical but powerful algorithms — many of which are easy to implement

Data as a graph

A graph is simple but not all data looks like a graph...

- some datasets are a natural fit, e.g. human brain
- other data has to be mapped...

Graph algorithms need a graph

Is your data a graph?

- Your data may not appear as a network. . .

Graph algorithms need a graph

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- But any pairwise collection of data points is a graph!

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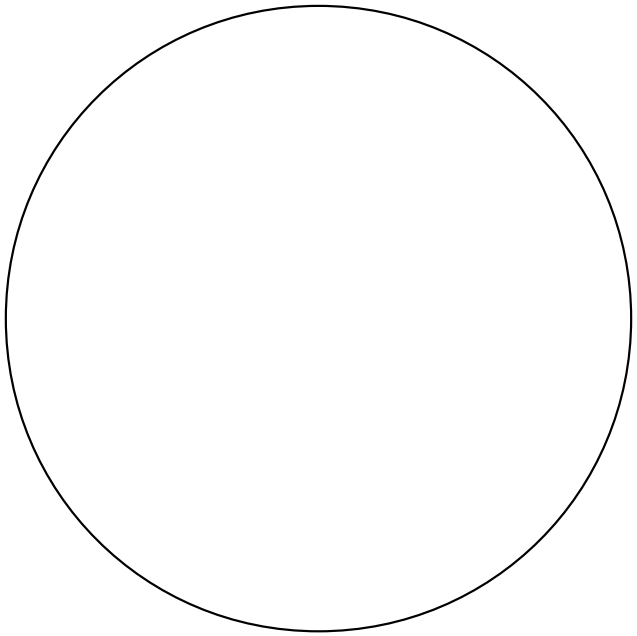
Let's play a game!

Graphing the Game of Darts

Example

Go to nearest pub and find a dartboard...



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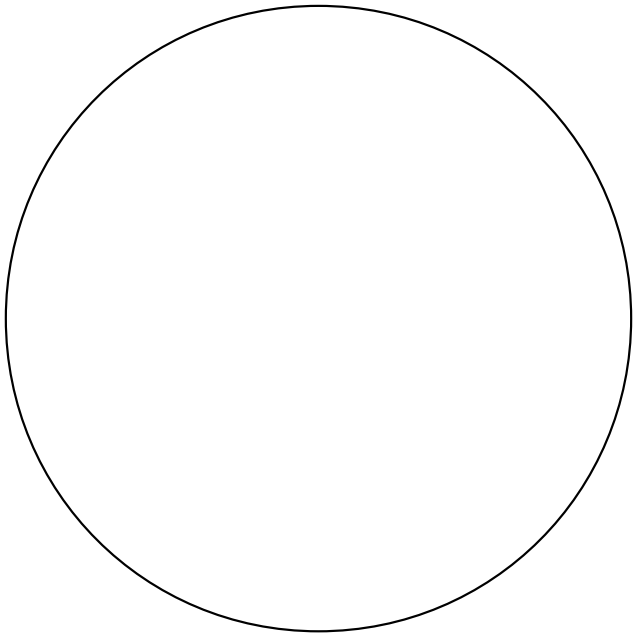

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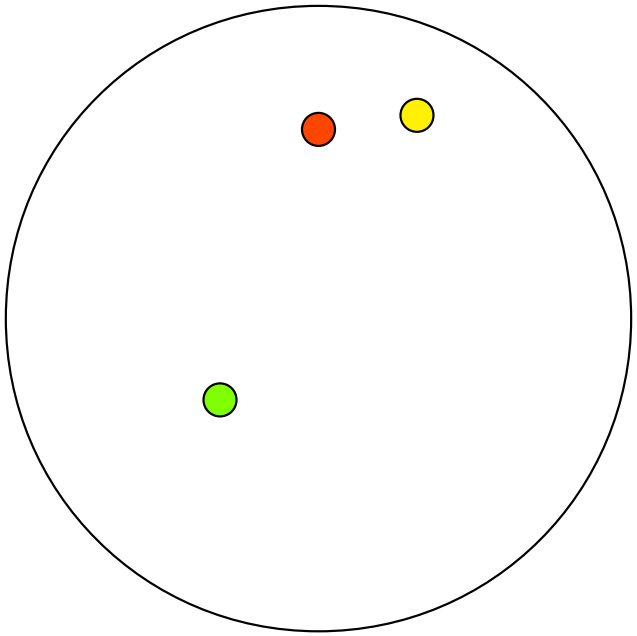

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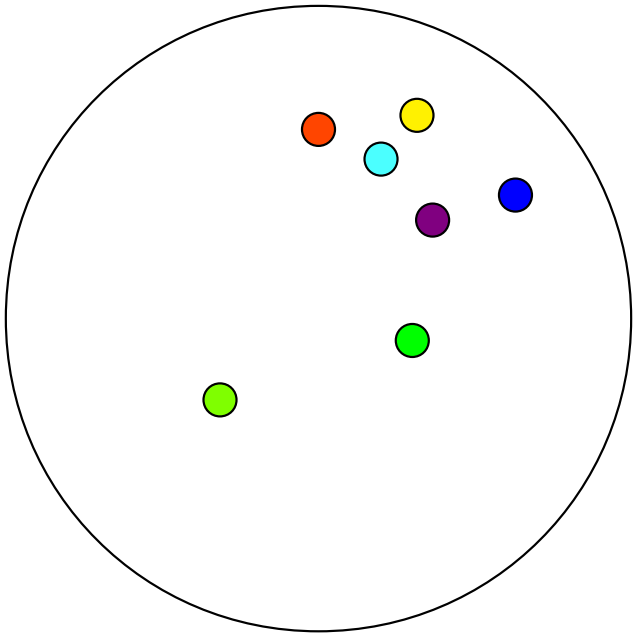

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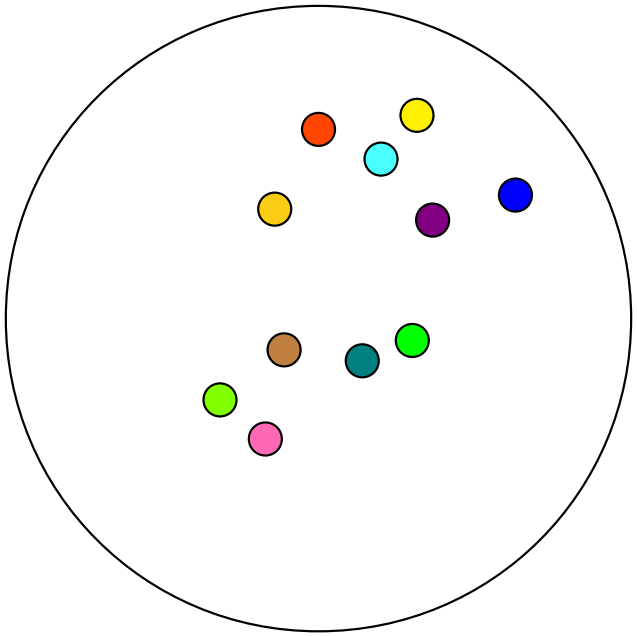

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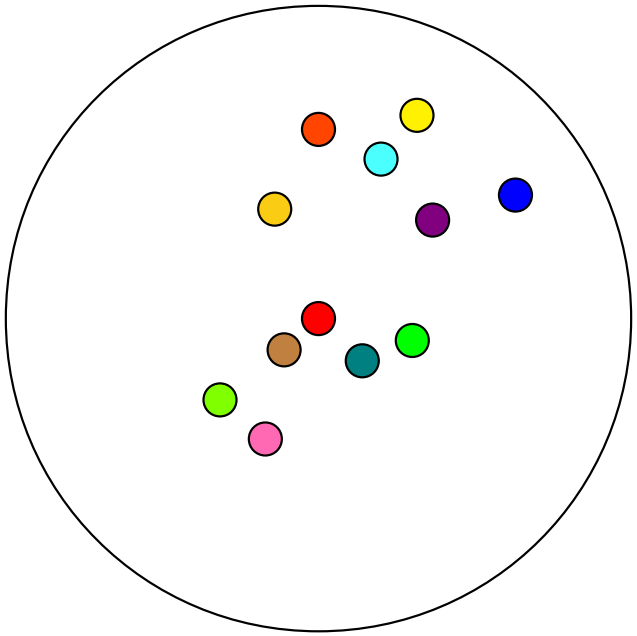

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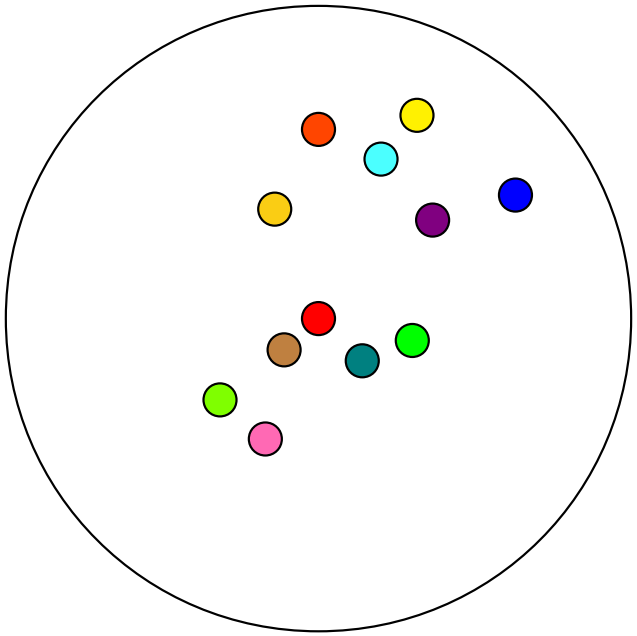

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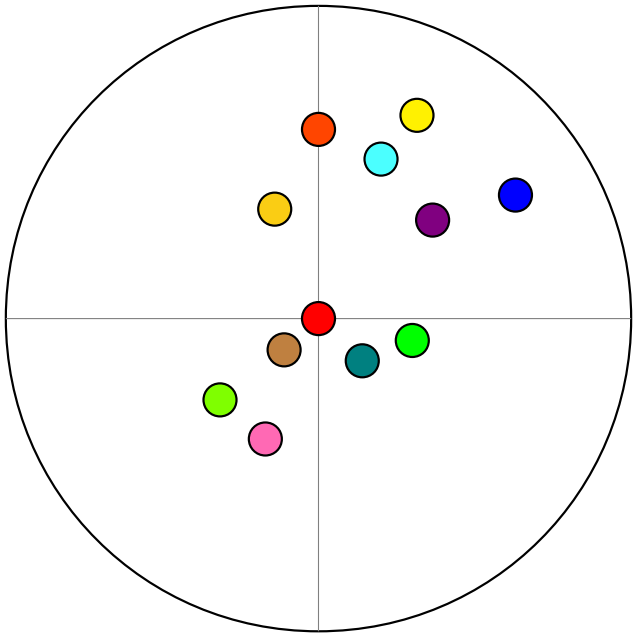

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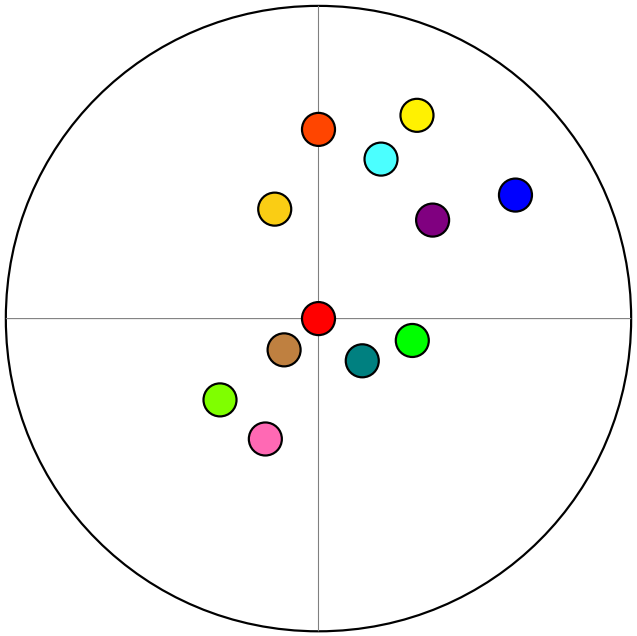

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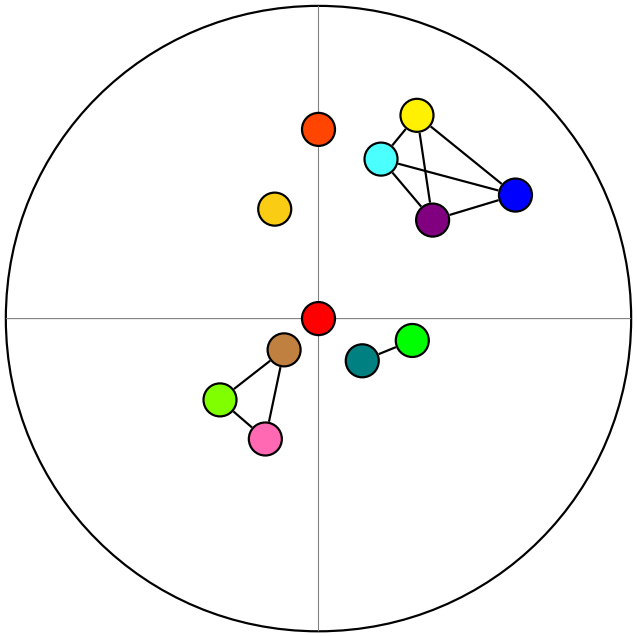

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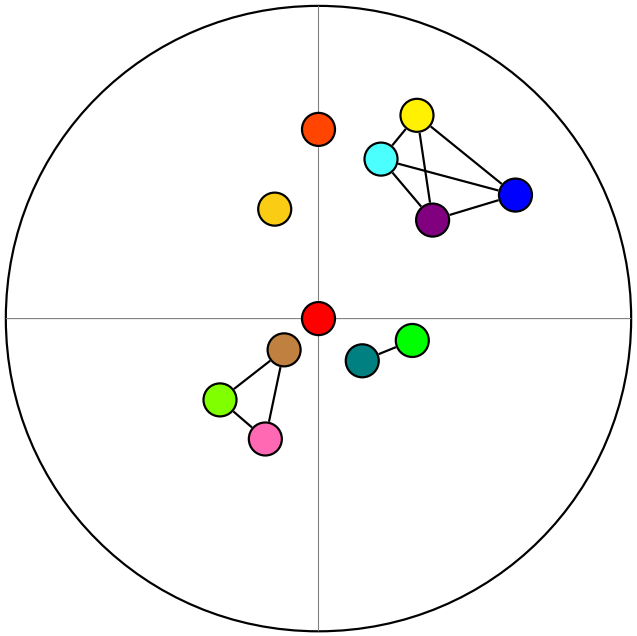

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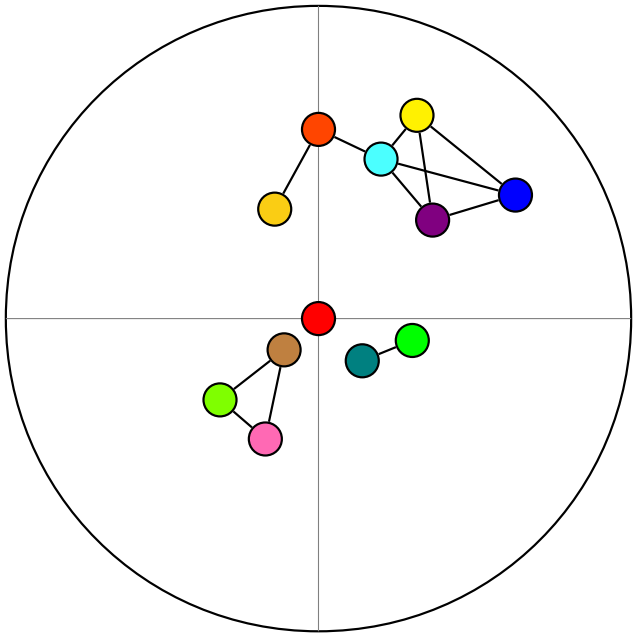

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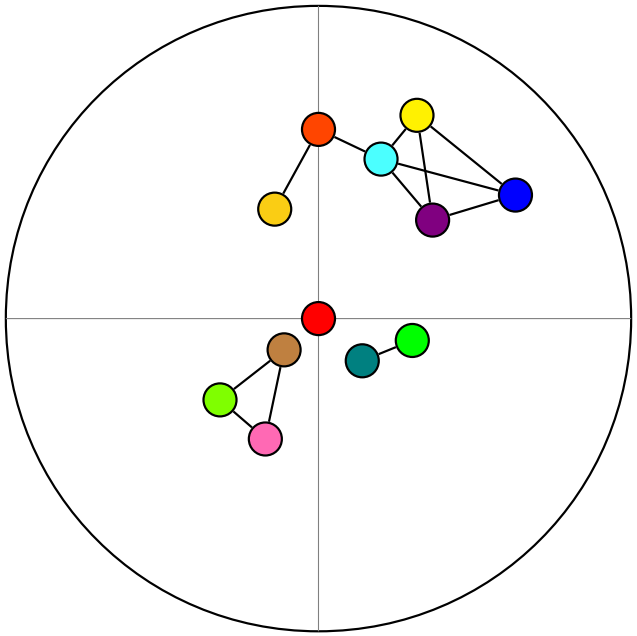

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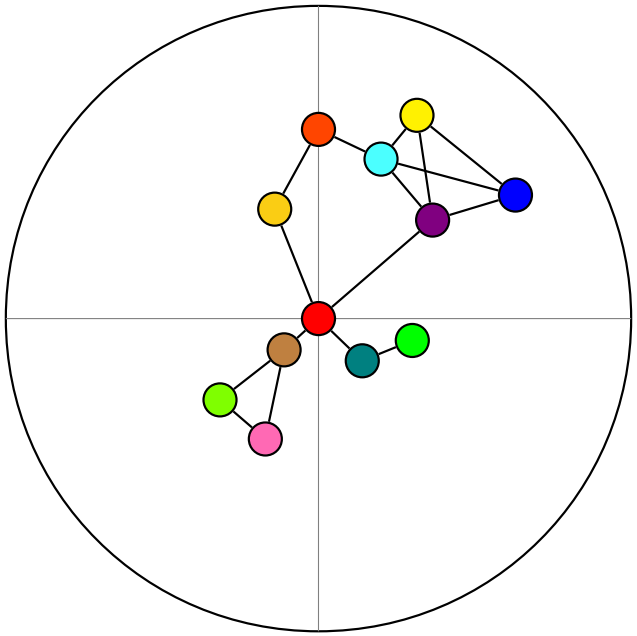

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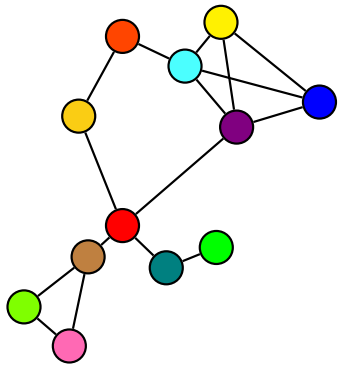
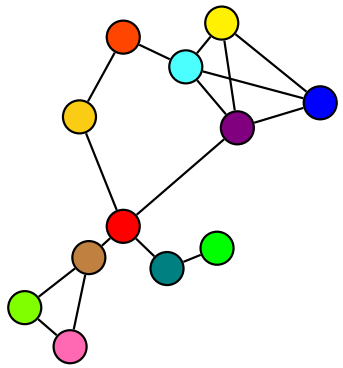


Dart Graph

Simple graph generator

Our game was a simple graph generator. . . not unlike other generators

- we created some recognizable structures. . .
- cycles, cliques, cores, components, clusters. . .



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Graph analysis

What can we learn from simple graph analysis?

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But we'll do this at a larger scale and under hard constraints. . .

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New algorithms

We'll describe our easy algorithms under hard constraints

Graph data is hard. . . really hard!

Real-world graphs represent irregular data

- topology is irregular thus. . .
- difficult to leverage computer memory hierarchy leading to. . .
- increasing latency and bandwidth costs and. . .
- high degree vertices cause hot-spots

Hard constraints for graph algorithms

Big Data constraints

Constraints commonly encountered with Big Data.

- graph does not fit in memory
- share nothing (no globally-shared data)
- no random access

Harder constraints. . .

For good measure we'll add the following constraints

state-less	tasks cannot save local information between steps
constant-memory	tasks have fixed memory with respect to input
data-stream	tasks cannot re-read input within the same step

Hardest constraint of all!

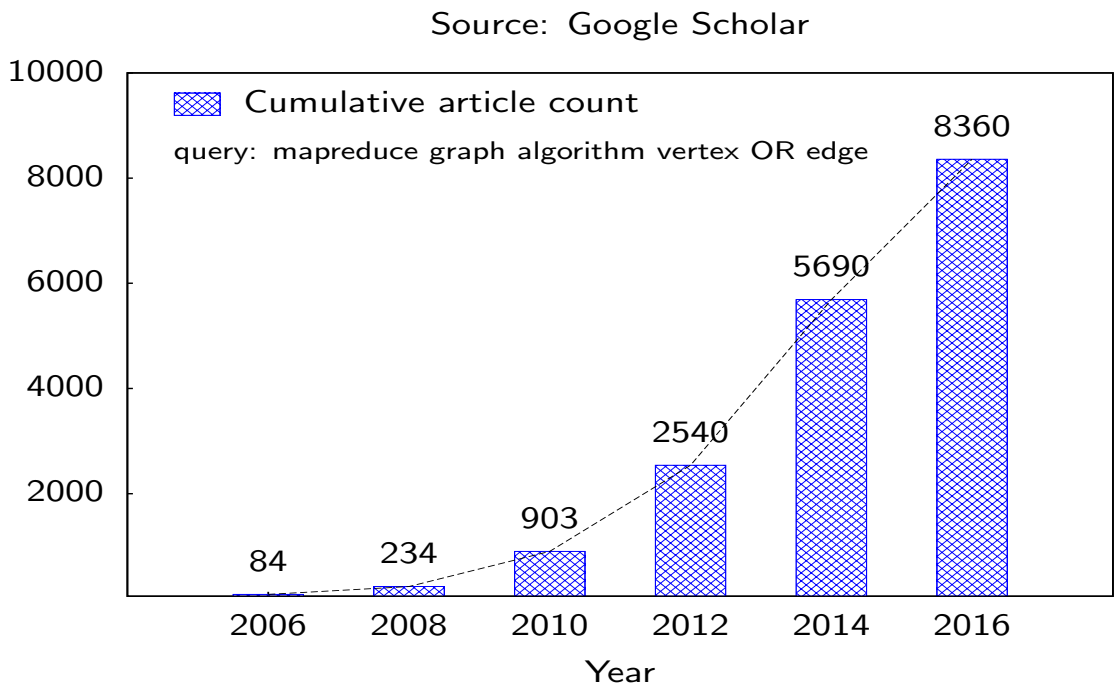
Hardest constraint of all!

We'll design the algorithms in MapReduce!

Results from Google Scholar

100-fold increase in MapReduce graph algorithm articles in the last ten years!

- spike is common in early phase of new technology. . .
- but still an active research area



Why MapReduce?

Benefits

The MapReduce computational model provides many benefits

- distributed computation
- compute migration
- overlap of communication with computation
- not memory-bound
- fault-tolerant. . .

Growing research interest

- improvements in theoretical model of computation
- increase in algorithm development

Exercising constraint

Limitations for a gain. . .

In this exercise the hard constraints will limit algorithm design choices but help to

- maximize scalability
- improve parallelism
- conserve compute resources
- support streaming computation

Terms and Definitions

For a simple, undirected graph $G = (V, E)$

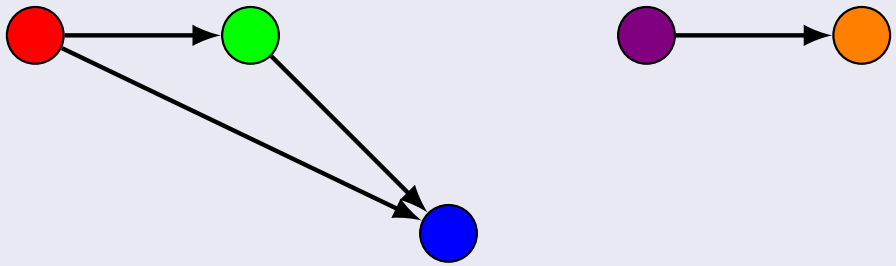
- with $n = |V|$ vertices and $m = |E|$ edges where ...
- $A \in \mathbb{R}^{n \times n}$ is the adjacency matrix of G; $A^T = A$
- $N(v) = \{u \in V \mid (v, u) \in E\}$ is the neighborhood of v
- $d(v) = |N(v)|$ is the degree of v
- $d_{max} = max\{d(v) \mid v \in V\}$ is the maximum degree
- $d(u, v)$ is the distance, i.e. shortest-path, from u to v
- $D(G)$ is the diameter of G, i.e. longest shortest-path in G

Connected Components in graphs

Group by connectivity

Group vertices that are reachable by a path, albeit not necessarily mutually reachable.

How many components do you see?



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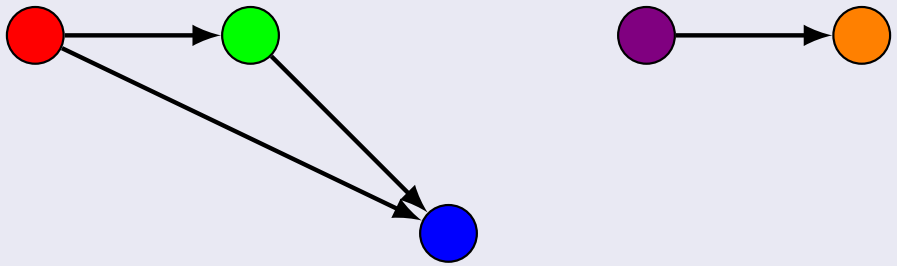
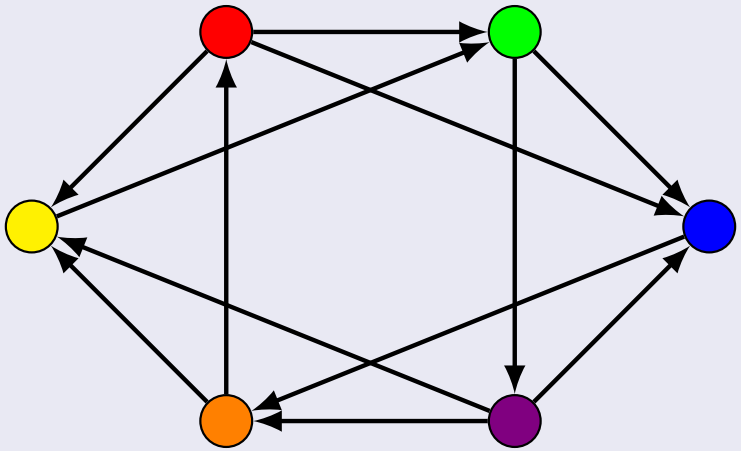


Is it 2 or 5?

Strongly Connected Component

Definition

A connected component in which a path exists between every pair of vertices.



Trivial path...

A singleton vertex is a connected component because it is trivially connected to itself; $d(v, v) = 0$

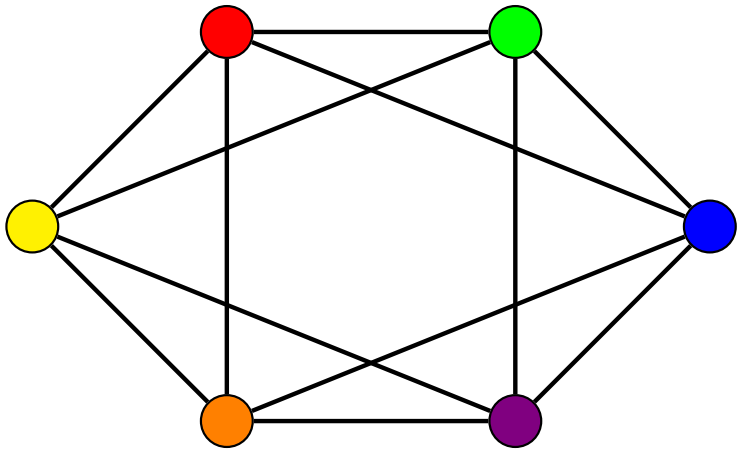
Connected Components in Undirected Graphs

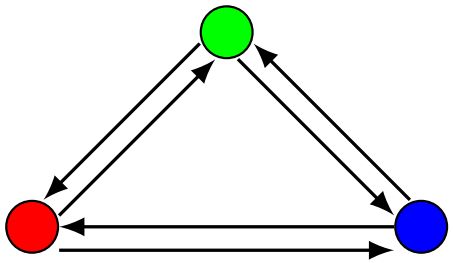
Strongly connected

Paths are symmetric in an undirected graph, thus a connected component in an undirected graph is strongly connected.

Undirected G. . .

The remainder of this presentation will focus on undirected graphs.





Easy Connected Components under hard constraints

Theorem 1

Given an edge list of G and a list L then the algorithm in Listing 1 takes $O(m \log^2 n)$ time.

Proof.

The edges are sorted so (v, w) is first where w is the minimum vertex ID for all endpoints of v. The time to sort all edges is

$$O(\sum_v d_v \log d_v) \leq O(m \log d_{max}) \leq O(m \log n)$$

There are $O(m)$ tests for each edge in L, and all other operations including inserts into L' take $O(1)$ time where L' is a temporary list. The time for each step is then $O(m + m \log n) \in O(m \log n)$. Every vertex v with a neighbor u, where $u \prec v$, will receive the minimum from $N(u)$. This contracts the graph by half after each step. Thus the overall time for $O(\log n)$ steps is $O(m \log^2 n)$! □

Listing 1: Label propagation Connected Components

```
L ← sorted E
count ← 1
while count > 0 do
    count ← 0
    create new list L'
    last ← ∞
    for all (v, u) ∈ L do
        if v ≠ last then
            w ← u
            last ← v
            if w < v then
                add (v, w), (w, v) to L'
            end if
        else if w < v then
            add (u, w) to L'
            count ← count + 1
        end if
    end for
    sort L'
    L ← L'
end while
```

Connected components under hard constraints. . .

Benefits

- does not re-read the entire graph at each step
- fast drop-off in output size
- neighborhood of a vertex is ignored if the vertex ID is less than the minimum of all neighbors. . .
- completes in $O(\log n)$ rounds

MapReduce Connected Components

Connected Components algorithm

- $N[v]$ is the sorted set of neighbors of v
- Constant, $O(1)$, working memory

Round $1..O(\log n)$

Map: Ordered vertex pair for secondary-sort

$$\langle v, u \rangle \longrightarrow \langle (v, u), u \rangle$$

Reduce: Values are sorted so the first value, w, is the minimum

$$\langle v, \{u \in N[v]\} \rangle \longrightarrow \langle v, w \rangle, \langle w, v \rangle, \{\langle u, w \rangle\} \iff w \prec v, w = \min N[v]$$

Final Round

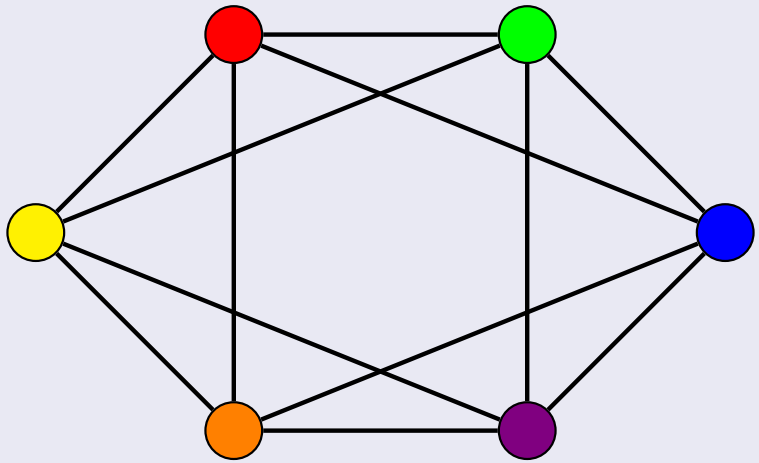
Map: Organize (v, u) pairs

$$\langle v, u \rangle \longrightarrow \langle v \prec u, u \rangle \iff v \prec u$$

Cores in Graphs

(loose) Definition

A core is a maximal subgraph in which vertices are well-connected



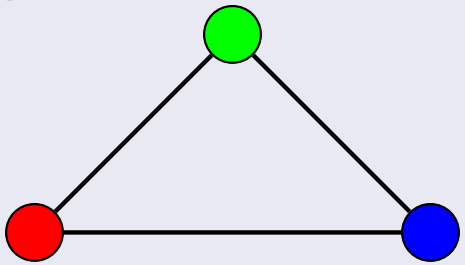
Cores are cohesive networks

Significant number of vertices must be removed for the core to become disconnected. . . cliques are maximally connected

Recall the definition of a clique...

Definition

A clique is a graph in which all pairs of vertices are connected, e.g. triangle



Completeness

A n-clique is a maximally complete graph of order n

- all degrees = n-1
- graph diameter = 1
- number of edges = n(n-1)/2

Cores are a relaxation of cliques

Cores are more loose then cliques...

Less strict in degree, connectivity, reachability, etc.

Types of cores

k-plex	each vertex is not connected to at most k-1 other vertices
k-club	diameter is at most k
γ-quasi-clique	density is at least γ
k-core	each vertex has degree at least k
k-truss	endpoints of each edge share at least k-2 neighbors

Reviewing the k-core

Introduced by Stephen B. Seidman in 1983 [7]

A k-core is a maximal connected subgraph with minimum degree k.

Hierarchy of k-cores

A k-core is a subset of the $[1..(k-1)]$-cores

$$\text{k-core} \subseteq \text{(k-1)-core} \subseteq \text{(k-2)-core} \ldots \subseteq \text{1-core}$$

Easy k-Core under hard constraints

Theorem 2

Given a sorted edge list of G, a list L, and $k \in O(\sqrt{m})$, then the k-core algorithm in Listing 2 is possible in $O(md_{max})$ time, and if d_{max} is constant the time is $O(m)$.

Proof.

At each step, all operations take $O(1)$ time including inserting an edge into the temporary list T_v and inserting T_v into the temporary list L'. Therefore the first pass takes $O(m)$ time, leaving at most $O(m/k)$ vertices remaining with $O(\frac{m}{k} d_{max})$ edges. All $O(m/k)$ passes take no more than $O(\frac{m}{k}(\frac{m}{k} d_{max})) \in O((\frac{m}{k})^2 d_{max})$ time, and if $k \in O(\sqrt{m})$ then the time is $O(md_{max})$. Thus the total time is,

$$O(m + md_{max}) \in O(md_{max})$$

If $d_{max} \in O(1)$ then the time complexity is $O(m)$. □

Listing 2: k-core algorithm

```
L ← sorted edges
count ← 1
while count ≠ 0 do
    count ← 0; degree ← 0
    create new L'
    for all (v, u) ∈ L do
        if done with edges for a v then
            if degree ≥ k then
                add T_v to L'
            else
                count ← count + 1
            end if
            create new T_v
            degree ← 0
        else
            add (u, v) to T_v
            degree ← degree + 1
        end if
    end for
    L = L'                ▷ L remains locally sorted
end while
```

MapReduce k-Core algorithm

Round 1 given $(v, (u, d_u))$ input

Map: Identity

$$\langle v, (u, d_u) \rangle \longrightarrow \langle v, (u, d_u) \rangle$$

Reduce: Output reverse edges

$$\langle v, \{(u, d_u) \mid u \in N(v)\} \rangle \longrightarrow \{\langle u, v \rangle\} \iff d_v, d_u \geq k$$

Rounds $[2..O(n)]$

Map: Identity

$$\langle v, u \rangle \longrightarrow \langle v, u \rangle$$

Reduce: Output reverse edges

$$\langle v, \{u \mid u \in N(v)\} \rangle \longrightarrow \{\langle u, v \rangle\} \iff d_v \geq k$$

Evaluation of degree

Evaluating $d_v \geq k$ is possible in $O(1)$ memory by using a k-element buffer

- reducer reads u values into buffer
- if buffer is filled then d_v is at least k so...
- output the u already in the buffer and then output all remaining u

Preliminary exercise

Experiment

Test the easy MapReduce algorithms on real datasets

Datasets

Stanford Network Analysis Project (SNAP)

as-Skitter	Autonomous Systems Internet topology graph
com-Orkut	Orkut online social network
com-Friendster	Friendster online social network

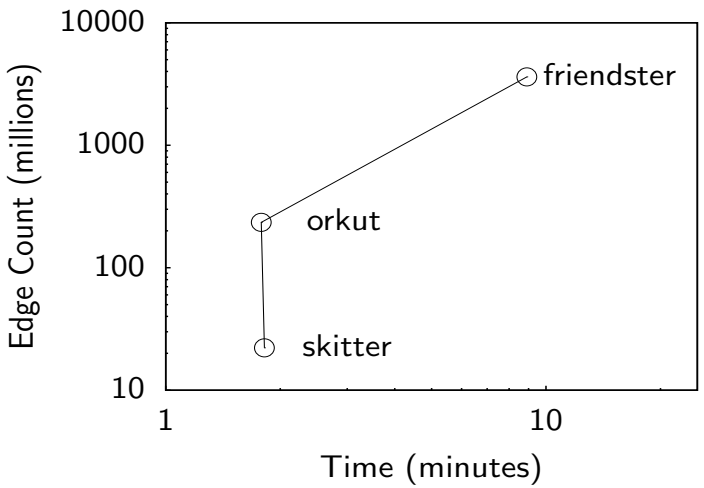
Hadoop Yarn Cluster

1200 nodes
32 cores per node
128 GB RAM per node

Connected Component Benchmarks on SNAP datasets

SNAP Graphs (undirected)

	n (vertices)	2m (edges)	# of concom
Skitter	1,696,415	22,190,596	756
Orkut	3,072,441	234,370,166	1
Friendster	65,608,366	3,612,134,270	1



	time (minutes)	rounds
Skitter	1.82	10
Orkut	1.78	7
Friendster	8.90	10

A post-step to organize labels is included

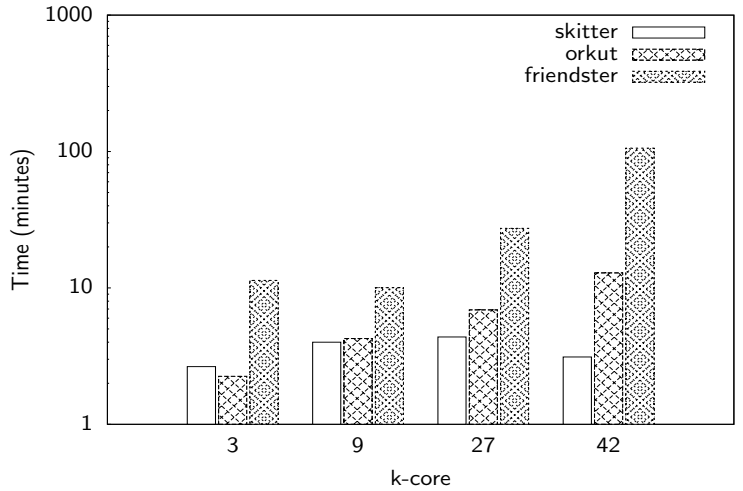
k-Core Benchmarks on SNAP datasets

SNAP Graphs (undirected)

	n (vertices)	2m (edges)	# of concom
Skitter	1,696,415	22,190,596	756
Orkut	3,072,441	234,370,166	1
Friendster	65,608,366	3,612,134,270	1

	Skitter	Orkut	Friendster
3-core	2.65	2.25	11.35
9-core	4.00	4.25	10.03
27-core	4.37	6.90	27.37
42-core	3.12	12.87	105.95

Time (minutes)



	Skitter	Orkut	Friendster
3-core	11	6	17
9-core	18	11	15
27-core	22	18	41
42-core	16	37	172

# of rounds

A pre-step round for degree annotation is included

Conclusion

Results

Demonstrated very easy algorithms under hard constraints.

- no part of the graph is stored in memory
- data access per step is single-pass and sequential
- no saved state either globally or locally — tasks perish after each step
- very minimal memory per task
- simple implementations
- room for improvement

Bibliography I

[1] A. F. Alexander-Bloch, N. Gogtay, et al.
Disrupted modularity and local connectivity of brain functional networks in childhood-onset schizophrenia.
Frontiers in Systems Neuroscience, 4(147), 2010.

[2] D. Godwin, R. L. Barry, and R. Marois.
Breakdown of the brain's functional network modularity with awareness.
PNAS, 112(12):3799–3804, March 2015.

[3] Y. He, Z. Chen, and A. Evans.
Structural insights into aberrant topological patterns of large-scale cortical networks in alzheimer's disease.
The Journal of Neuroscience, 28(18):4756–4766, 2008.

[4] M.-E. Lynall, D. S. Bassett, R. Kerwin, et al.
Funtional connectivity and brain networks in schizophrenia.
The Journal of Neuroscience, 30(29):9447–9487, 2010.

[5] R. Penfold and P. J. Wilde.
Enumerating and indexing many-body intramolecular interactions: a graph theoretic approach.
Journal of mathematical chemistry, 53(7):1634–1648, 2015.

[6] J. Scott, T. Ideker, and R. M. Karp.
Efficient algorithms for detecting signaling pathways in protein interaction networks.
Journal of Computational Biology, 13(2):133–144, 2006.

[7] S. B. Seidman.
Network structure and minimum degree.
Social Networks, 5:269–287, 1983.

[8] R. Singh, J. Xu, and B. Berger.
Pairwise global alignment of protein interaction networks by matching neighborhood topology.
In *Proceedings of the 11th annual international conference on research in computational molecular biology*, RECOMB'07, pages 16–31. Springer-Verlag, 2007.

Bibliography II

[9] S. Spivak, A. Ismagilova, and I. Khamitova.
Graph-theoretical method for determining routes of complex chemical reactions.
In *Doklady Physical Chemistry*, volume 434, pages 169–171. Springer, 2010.

[10] L. Wang, B. Stumm, and V. Helms.
Graph-theoretical identification of dissociation pathways on free energy landscapes of biomolecular interaction.
Journal of computational chemistry, 31(4):847–854, 2010.