6.172
Performance
Engineering
of Software
Systems

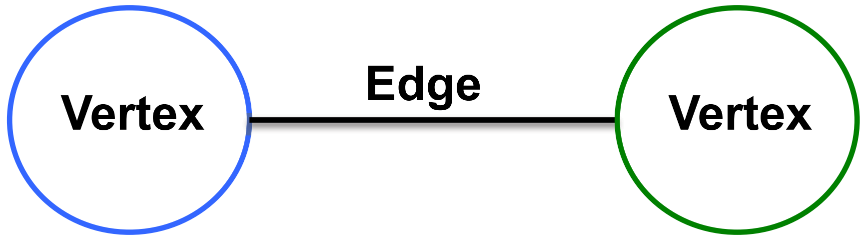
LECTURE 22
Graph Optimization

Julian Shun

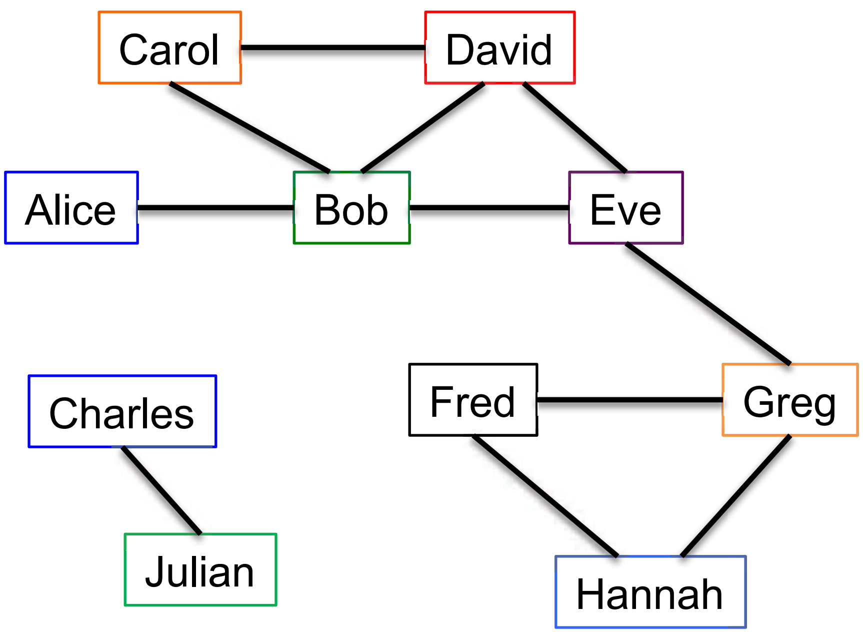
Outline

- What is a graph?
- Graph representations
- Implementing breadth-first search
- Graph compression/reordering

What is a graph?



- Vertices model objects
- Edges model relationships between objects



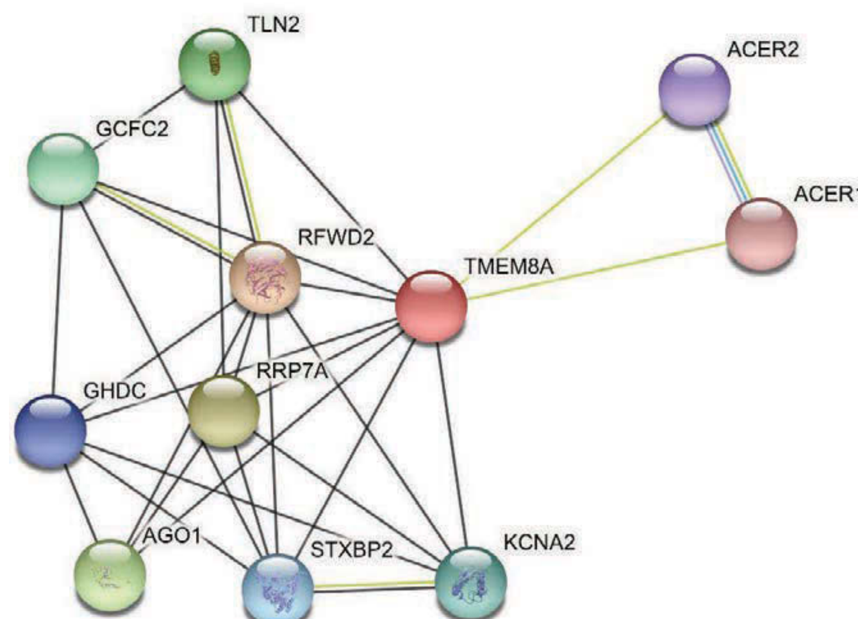


Image courtesy of STRING. Used under CC-BY.

What is a graph?

- Edges can be directed
  - Relationship can go one way or both ways

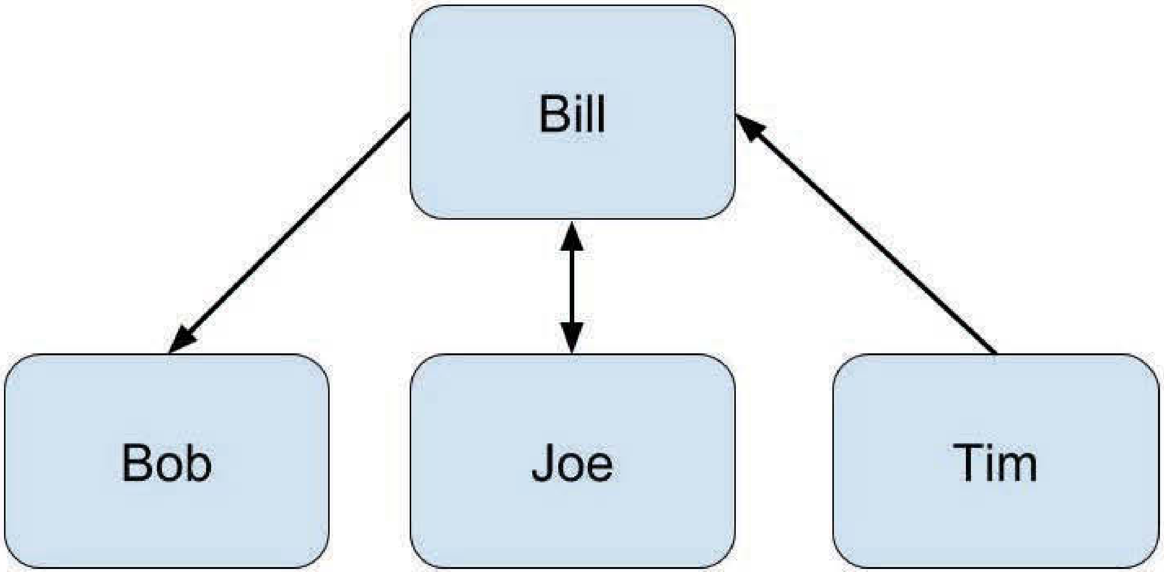
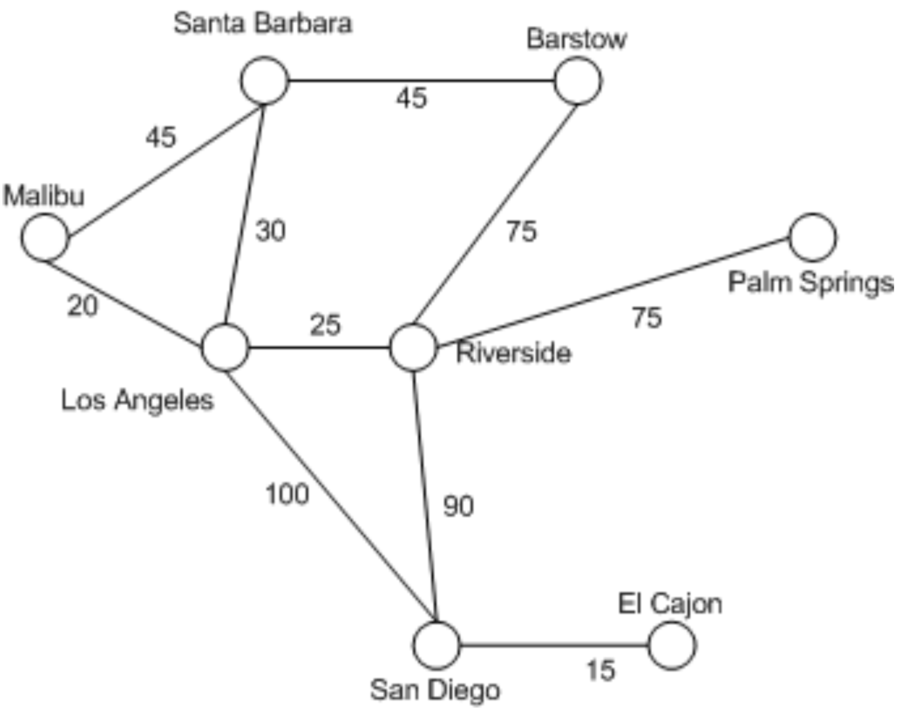


Image created by MIT OpenCourseWare.

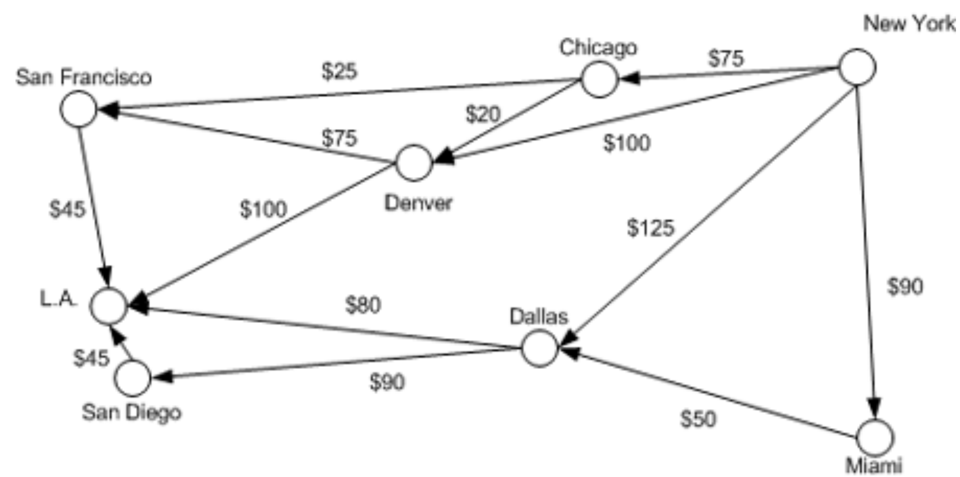
What is a graph?

- Edges can be weighted
  - Denotes "strength", distance, etc.

Distance between cities



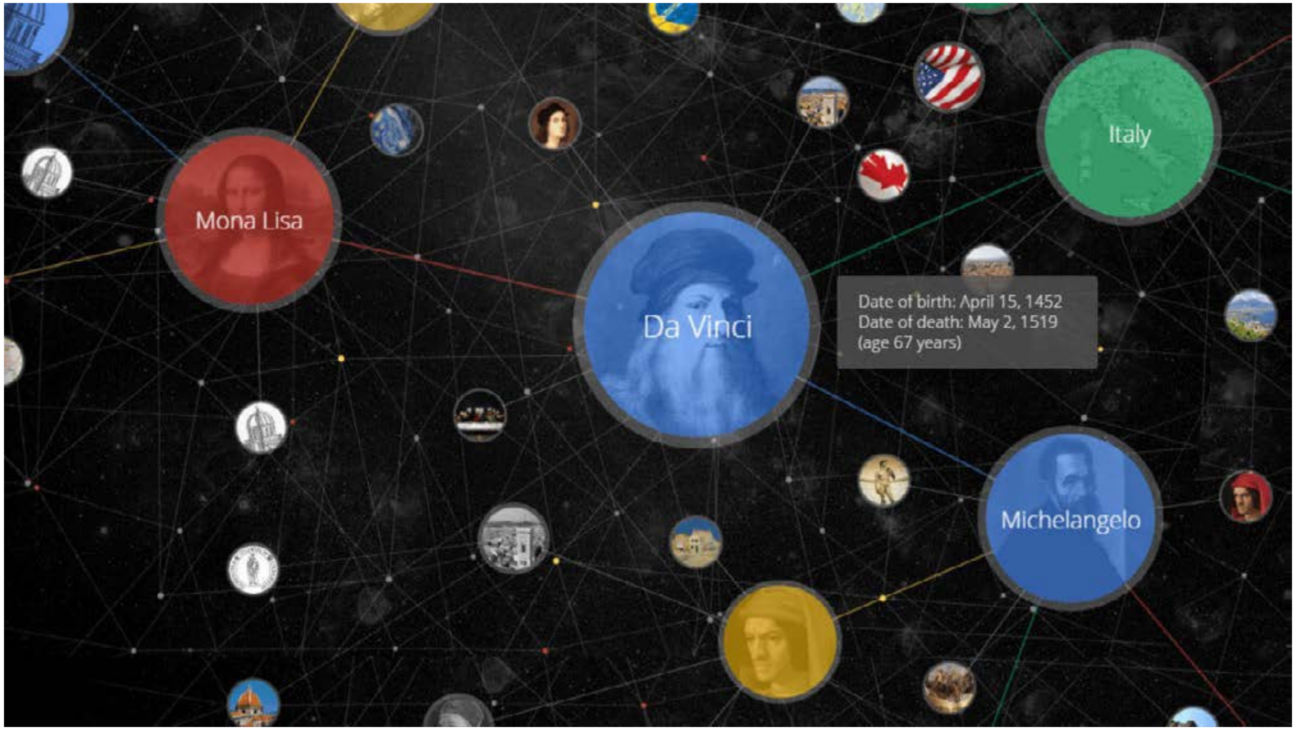
Flight costs



What is a graph?

- Vertices and edges can have types and metadata

Google Knowledge Graph

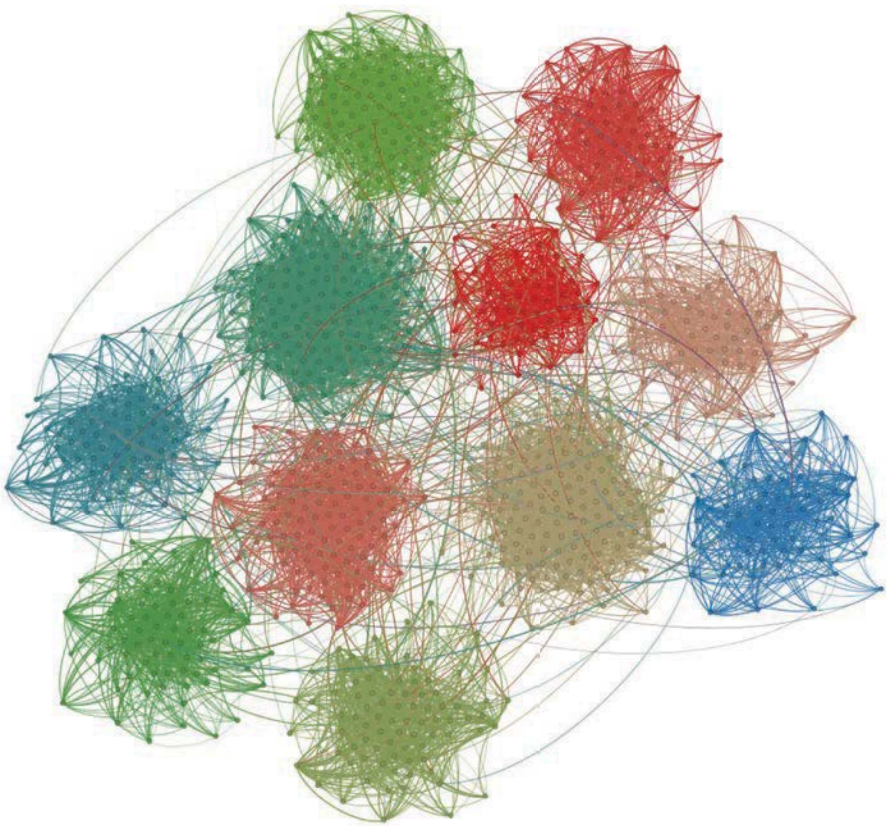


SOME MORE APPLICATIONS OF GRAPHS

Social network queries

- Examples:
  - Finding all your friends who went to the same high school as you
  - Finding common friends with someone
  - Social networks recommending people whom you might know
  - Product recommendation

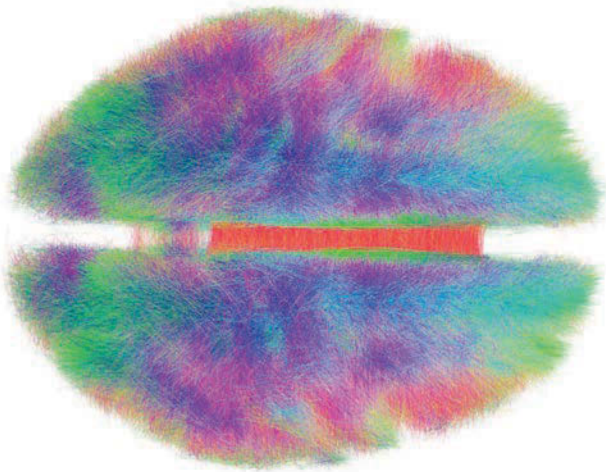
Finding good clusters



- Some applications
  - Finding people with similar interests
  - Detecting fraudulent websites
  - Document clustering
  - Unsupervised learning

- Finding groups of vertices that are "well-connected" internally and "poorly-connected" externally

More Applications



Connectomics

- Study of the brain network structure

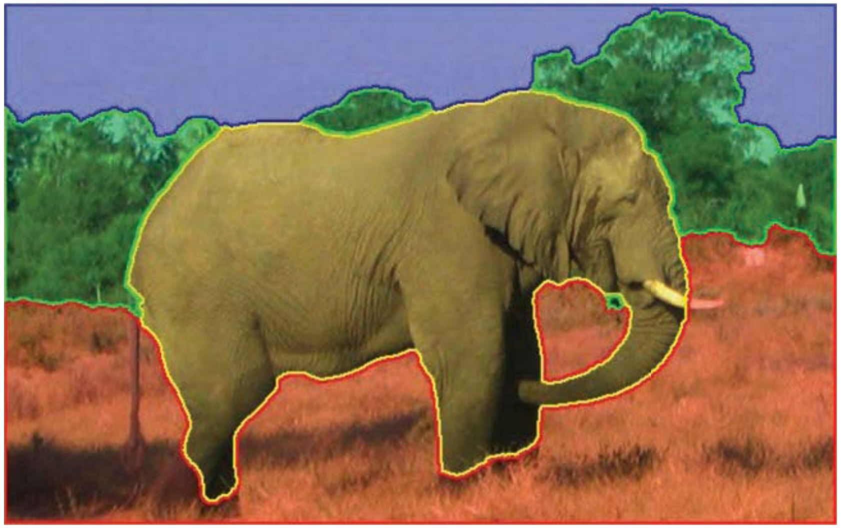


Image Segmentation

- Pixels correspond to vertices
- Edges between neighboring pixels with weight corresponding to similarity

Graph Representations

Graph Representations

- Vertices labeled from 0 to n–1

	0	1	2	3	4
0	0	1	0	0	0
1	1	0	0	1	1
2	0	0	0	1	0
3	0	1	1	0	0
4	0	1	0	0	0

Adjacency matrix
("1" if edge exists, "0" otherwise)

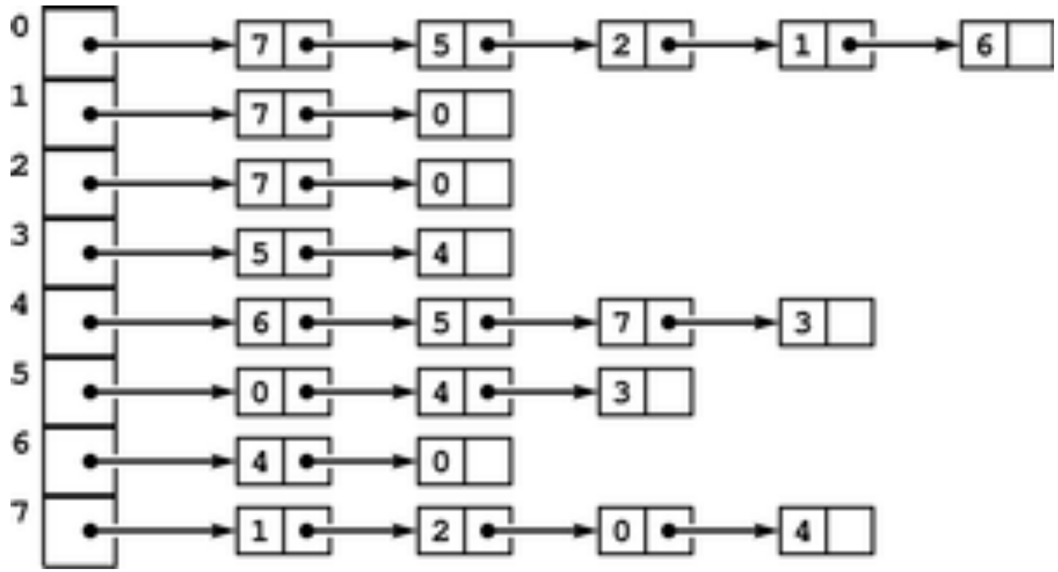
(0,1)
(1,0)
(1,3)
(1,4)
(2,3)
(3,1)
(3,2)
(4,1)

Edge list

- What is the space requirement for each in terms of number of edges (m) and number of vertices (n)?

Graph Representations

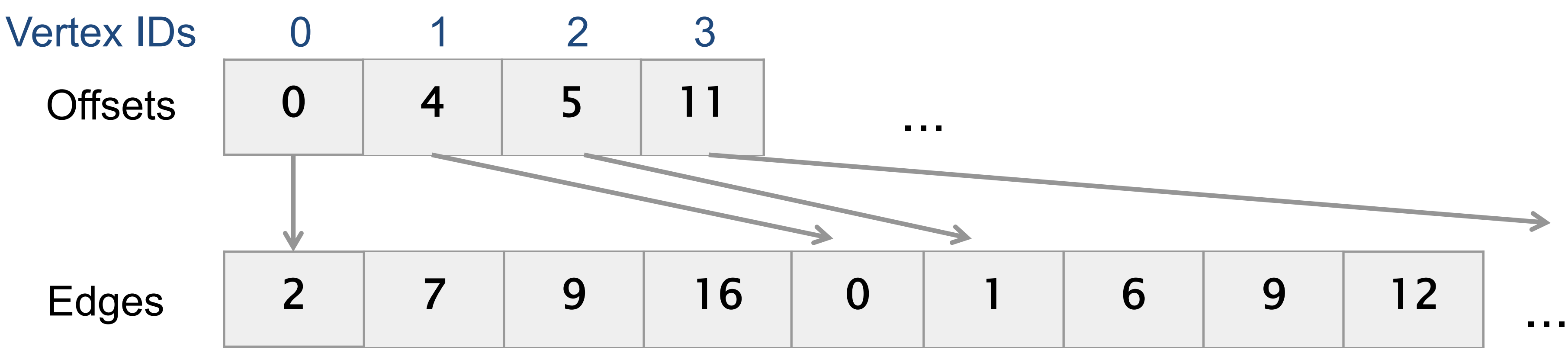
- Adjacency list
  - Array of pointers (one per vertex)
  - Each vertex has an unordered list of its edges



- What is the space requirement?
- Can substitute linked lists with arrays for better cache performance
  - Tradeoff: more expensive to update graph

Graph Representations

- Compressed sparse row (CSR)
  - Two arrays: Offsets and Edges
  - Offsets[i] stores the offset of where vertex i's edges start in Edges



- How do we know the degree of a vertex?
- Space usage?
- Can also store values on the edges with an additional array or interleaved with Edges

Tradeoffs in Graph Representations

- What is the cost of different operations?

	Adjacency matrix	Edge list	Adjacency list	Compressed sparse row
Storage cost / scanning whole graph	$O(n^2)$	$O(m)$	$O(m+n)$	$O(m+n)$
Add edge	$O(1)$	$O(1)$	$O(1)/O(deg(v))$	$O(m+n)$
Delete edge from vertex v	$O(1)$	$O(m)$	$O(deg(v))$	$O(m+n)$
Finding all neighbors of a vertex v	$O(n)$	$O(m)$	$O(deg(v))$	$O(deg(v))$
Finding if w is a neighbor of v	$O(1)$	$O(m)$	$O(deg(v))$	$O(deg(v))$

- There are variants/combinations of these representations

Graph Representations

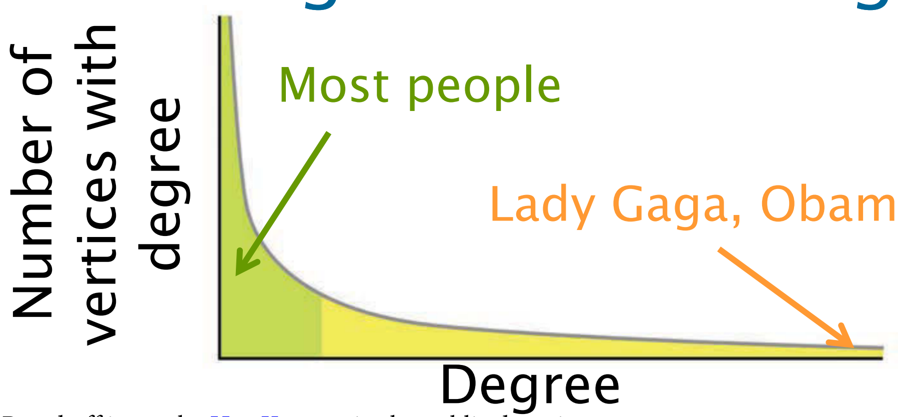
- The algorithms we will discuss today are best implemented with compressed sparse row (CSR) format
  - Sparse graphs
  - Static algorithms–no updates to graph
  - Need to scan over neighbors of a given set of vertices

Properties of real-world graphs

- They can be big (but not too big)

Social network	Web graph	Web graph
41 million vertices	1.4 billion vertices	3.5 billion vertices
1.5 billion edges	6.6 billion edges	128 billion edges
(6.3 GB)	(38 GB)	(540 GB)

- Sparse (m much less than n^2)
- Degrees can be highly skewed



Based off image by Hay Kranen, in the public domain.

Studies have shown that many real-world graphs have a power law degree distribution

#vertices with deg. $d \approx a \times d^{-p}$
$(2 < p < 3)$

Implementing a graph algorithm: Breadth-first search

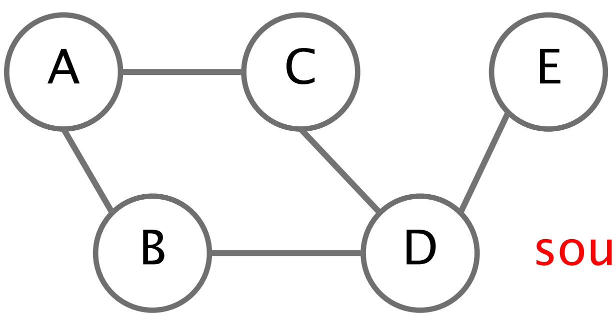
Breadth-First Search (BFS)

- Given a source vertex *s*, visit the vertices in order of distance from *s*
- Possible outputs:
  - Vertices in the order they were visited
    - D, B, C, E, A
  - The distance from each vertex to *s*

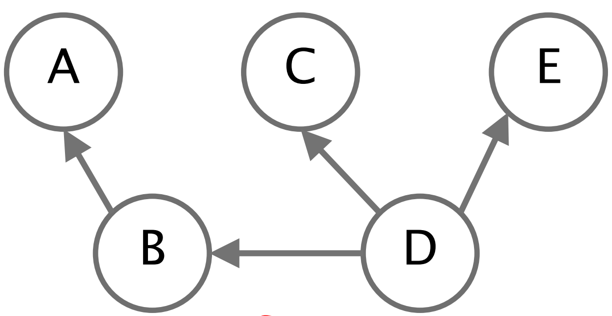
A	B	C	D	E
2	1	1	0	1

  - A BFS tree, where each vertex has a parent to a neighbor in the previous level

Applications
Betweenness centrality
Eccentricity estimation
Maximum flow
Web crawlers
Network broadcasting
Cycle detection
…



source = D



BFS tree

Serial BFS Algorithm

```
Breadth-First-Search(Graph, root):

    for each node n in Graph:
        n.distance = INFINITY
        n.parent = NIL
```

Source: https://en.wikipedia.org/wiki/Breadth-first_search

Serial BFS Algorithm

- Assume graph is given in compressed sparse row format
  - Two arrays: Offsets and Edges
  - n vertices and m edges (assume Offsets[n] = m)

```
int* parent =
 (int*) malloc(sizeof(int)*n);
int* queue =
 (int*) malloc(sizeof(int)*n);

for(int i=0; i<n; i++) {
   parent[i] = -1;
}

queue[0] = source;
parent[source] = source;

int q_front = 0, q_back = 1;
```

```
//while queue not empty
while(q_front != q_back) {
    int current = queue[q_front++]; //dequeue
    int degree =
         Offsets[current+1]-Offsets[current];
    for(int i=0;i<degree; i++) {
         int ngh = Edges[Offsets[current]+i];
         //check if neighbor has been visited
         if(parent[ngh] == -1) {
             parent[ngh] = current;
             //enqueue neighbor
             queue[q_back++] = ngh;
         }
    }
}
```

Total of m random accesses

- What is the most expensive part of the code?
  - Random accesses cost more than sequential accesses

Analyzing the program

```
int* parent =
 (int*) malloc(sizeof(int)*n);
int* queue =
 (int*) malloc(sizeof(int)*n);

for(int i=0; i<n; i++) {
   parent[i] = -1;
}

queue[0] = source;
parent[source] = source;

int q_front = 0; q_back = 1;
```

```
//while queue not empty
while(q_front != q_back) {
   int current = queue[q_front++]; //dequeue
   int degree =
        Offsets[current+1]-Offsets[current];
   for(int i=0;i<degree; i++) {
        int ngh = Edges[Offsets[current]+i];
        //check if neighbor has been visited
        if(parent[ngh] == -1) {
            parent[ngh] = current;
            //enqueue neighbor
            queue[q_back++] = ngh;
        }
   }
}
```

- (Approx.) analyze number of cache misses (cold cache; cache size << n; 64 byte cache line size; 4 byte int)
  - n/16 for initialization
  - n/16 for dequeueing
  - n for accessing Offsets array
  - ≤ 2n + m/16 for accessing Edges array
  - m for accessing parent array
  - n/16 for enqueueing

Total ≤ (51/16)n + (17/16)m

Analyzing the program

```
int* parent =
 (int*) malloc(sizeof(int)*n);
int* queue =
 (int*) malloc(sizeof(int)*n);

for(int i=0; i<n; i++) {
   parent[i] = -1;
}

queue[0] = source;
parent[source] = source;

int q_front = 0; q_back = 1;
```

```
//while queue not empty
while(q_front != q_back) {
    int current = queue[q_front++]; //dequeue
    int degree =
          Offsets[current+1]-Offsets[current];
    for(int i=0;i<degree; i++) {
          int ngh = Edges[Offsets[current]+i];
          //check if neighbor has been visited
          if(parent[ngh] == -1) {
               parent[ngh] = current;
               //enqueue neighbor
               queue[q_back++] = ngh;
          }
    }
}
```

Check bitvector first before accessing parent array

n cache misses instead of m

- What if we can fit a bitvector of size n in cache?
  - Might reduce the number of cache misses
  - More computation to do bit manipulation

BFS with bitvector

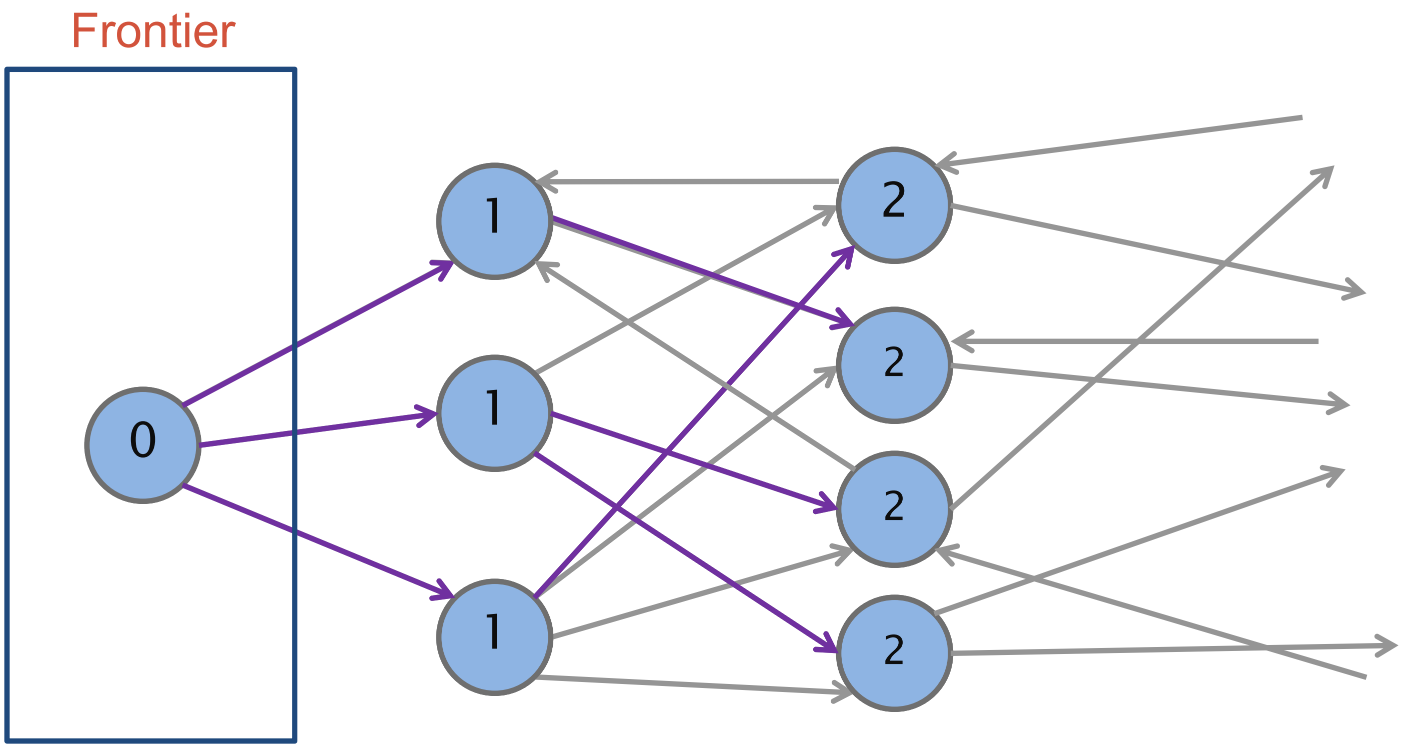
```
int* parent =
 (int*) malloc(sizeof(int)*n);
int* queue =
 (int*) malloc(sizeof(int)*n);
int nv = 1+n/32;
int* visited =
 (int*) malloc(sizeof(int)*nv);

for(int i=0; i<n; i++) {
   parent[i] = -1;
}

for(int i=0; i<nv; i++) {
   visited[i] = 0;
}

queue[0] = source;
parent[source] = source;
visited[source/32]
   = (1 << (source % 32));

int q_front = 0; q_back = 1;
```

```
//while queue not empty
while(q_front != q_back) {
    int current = queue[q_front++]; //dequeue
    int degree =
          Offsets[current+1]-Offsets[current];
    for(int i=0;i<degree; i++) {
       int ngh = Edges[Offsets[current]+i];
       //check if neighbor has been visited
       if(!((1 << ngh%32) & visited[ngh/32])){
          visited[ngh/32] |= (1 << (ngh%32));
          parent[ngh] = current;
          //enqueue neighbor
          queue[q_back++] = ngh;
       }
    }
}
```

- Bitvector version is faster for large enough values of m

Parallelizing Breadth-first search

Parallel BFS Algorithm



- Can process each frontier in parallel
  - Parallelize over both the vertices and their outgoing edges
- Races, load balancing

Parallel BFS Code

```
BFS(Offsets, Edges, source) {
  parent, frontier, frontierNext, and degrees are arrays
  cilk_for(int i=0; i<n; i++) parent[i] = -1;
  frontier[0] = source, frontierSize = 1, parent[source] = source;

  while(frontierSize > 0) {
    cilk_for(int i=0; i<frontierSize; i++)
        degrees[i] = Offsets[frontier[i]+1] – Offsets[frontier[i]];
    perform prefix sum on degrees array
    cilk_for(int i=0; i<frontierSize; i++) {
        v = frontier[i], index = degrees[i], d = Offsets[v+1]-Offsets[v];
        for(int j=0; j<d; j++) { //can be parallel
                ngh = Edges[Offsets[v]+j];
                if(parent[ngh] == -1 && compare-and-swap(&parent[ngh], -1, v)) {
                    frontierNext[index+j] = ngh;
                } else { frontierNext[index+j] = -1; }
        }
    }
    filter out "-1" from frontierNext, store in frontier, and update frontierSize to be
        the size of frontier (all done using prefix sum)
  }
}
```

frontierSize = 5

2	4	3	1	3

Prefix sum

(See problem 27-4 of CLRS)

0	2	6	9	10

v_1 v_2 v_3 v_4 v_5

frontier =

24	9	24	9	15	89	25	90	99	4	-1	-1	4

frontierSize = 8

BFS Work-Span Analysis

- Number of iterations <= diameter D of graph
- Each iteration takes Θ(log m) span for cilk_for loops, prefix sum, and filter (assuming inner loop is parallelized)

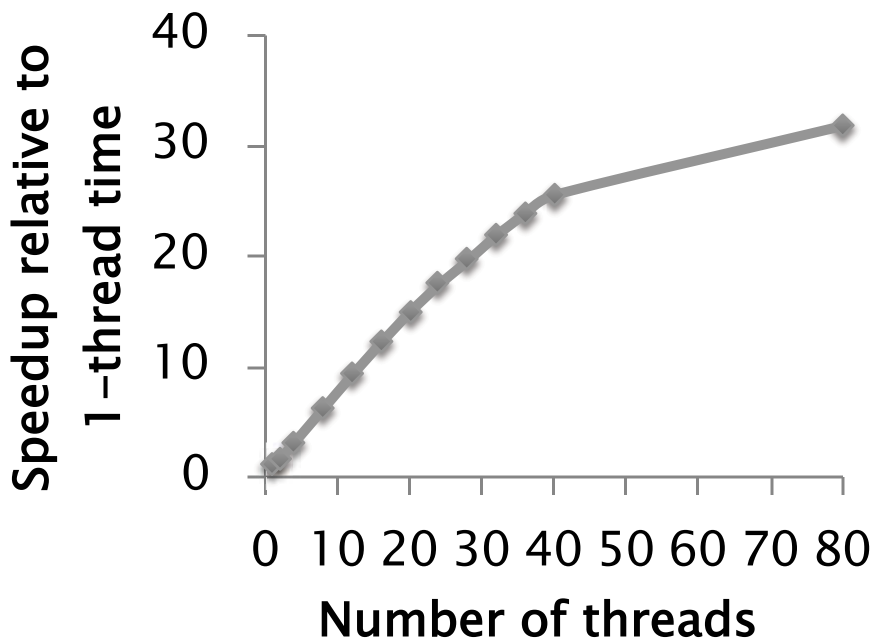
$$\text{Span} = \Theta(D \log m)$$

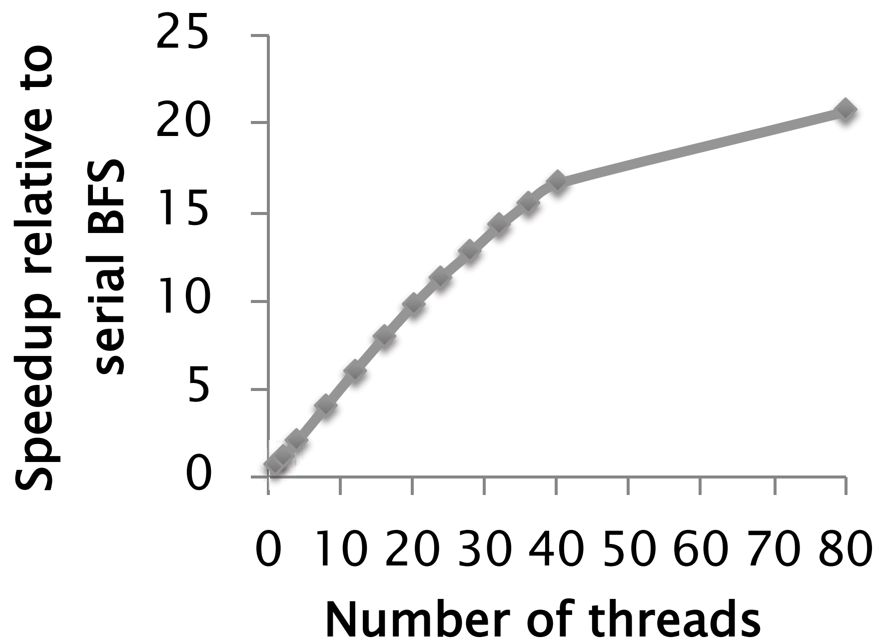
- Sum of frontier sizes = n
- Each edge traversed once -> m total visits
- Work of prefix sum on each iteration is proportional to frontier size -> Θ(n) total
- Work of filter on each iteration is proportional to number of edges traversed -> Θ(m) total

$$\text{Work} = \Theta(n+m)$$

Performance of Parallel BFS

- Random graph with $n=10^7$ and $m=10^8$
  - 10 edges per vertex
- 40-core machine with 2-way hyperthreading





- 31.8x speedup on 40 cores with hyperthreading
- Serial BFS is 54% faster than parallel BFS on 1 thread

Golden Rule of Parallel Programming

Never write nondeterministic parallel programs.

They can exhibit anomalous behaviors, and it's hard to debug them.

Silver Rule of Parallel Programming

Never **write nondeterministic parallel programs**

— but if you must —*

always devise a test strategy to control the nondeterminism!

Typical test strategies

- Turn off nondeterminism.
- Encapsulate nondeterminism.
- Substitute a deterministic alternative.
- Use analysis tools.

---

*E.g., for performance reasons.

Dealing with nondeterminism

```
BFS(Offsets, Edges, source) {
  parent, frontier, frontierNext, and degrees are arrays
  cilk_for(int i=0; i<n; i++) parent[i] = -1;
  frontier[0] = source, frontierSize = 1, parent[source] = source;

  while(frontierSize > 0) {
    cilk_for(int i=0; i<frontierSize; i++)
          degrees[i] = Offsets[frontier[i]+1] – Offsets[frontier[i]];
    perform prefix sum on degrees array
    cilk_for(int i=0; i<frontierSize; i++) {
          v = frontier[i], index = degrees[i], d = Offsets[v+1]-Offsets[v];
          for(int j=0; j<d; j++) {
                ngh = Edges[Offsets[v]+j];
                if(parent[ngh] == -1 && compare-and-swap(&parent[ngh], -1, v)) {
                   frontierNext[index+j] = ngh;
                } else { frontierNext[index+j] = -1; }
          }
    }
    filter out "-1" from frontierNext, store in frontier, and update frontierSize to be
          the size of frontier (all done using prefix sum)
  }
}
```

Nondeterministic!

Deterministic parallel BFS

```
writeMin(addr, newval):
   oldval = *addr
   while(newval < oldval):
         if(CAS(addr, oldval, newval)): return
         else: oldval = addr*
```

On 32 cores, (an optimized version of) deterministic BFS is 5—20% slower than nondeterministic BFS

```
                                              x sum
   cilk_for(int i=0; i<frontierSize; i++) {  //phase
         v = frontier[i], index = degrees[i], d = Of
         for(int j=0; j<d; j++) {  //can be parallel
               ngh = Edges[Offsets[v]+j];
               writeMin(&parent[ngh], v); }
   }
   cilk_for(int i=0; i<frontierSize; i++) {  //phase 2
         v = frontier[i], index = degrees[i], d = Offsets[v+1]-Offsets[v];
         for(int j=0; j<d; j++) {  //can be parallel
               ngh = Edges[Offsets[v]+j];
               if(parent[ngh] == v)  {
                     parent[ngh] = -v; //to avoid revisiting
                     frontierNext[index+j] = ngh; }
               else { frontierNext[index+j] = -1; }}
   }
   filter out "-1" from frontierNext, store in frontier, and update frontierSize
}}
```

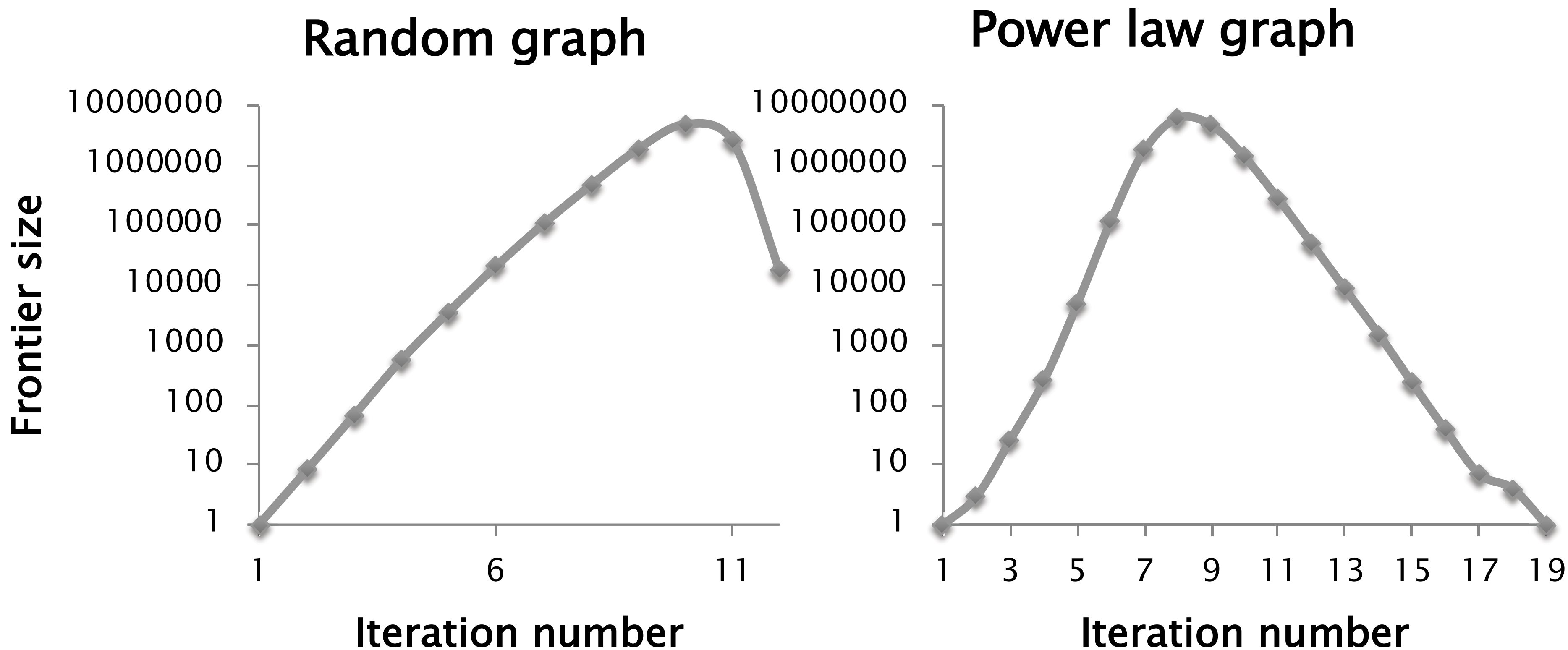
Smallest value gets written

Check if "won"

Source: G. Blelloch, P. Gibbons, J, Fineman, and J. Shun. *Internally Deterministic Parallel Algorithms Can Be Fast.* PPoPP 2012.

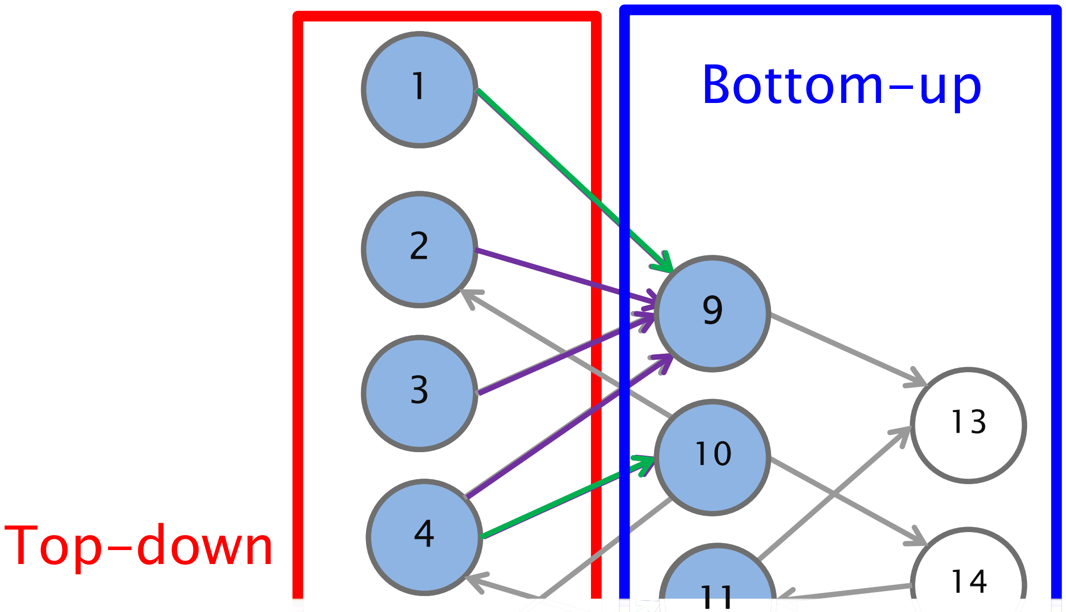
DIRECTION-OPTIMIZING BREADTH-FIRST SEARCH

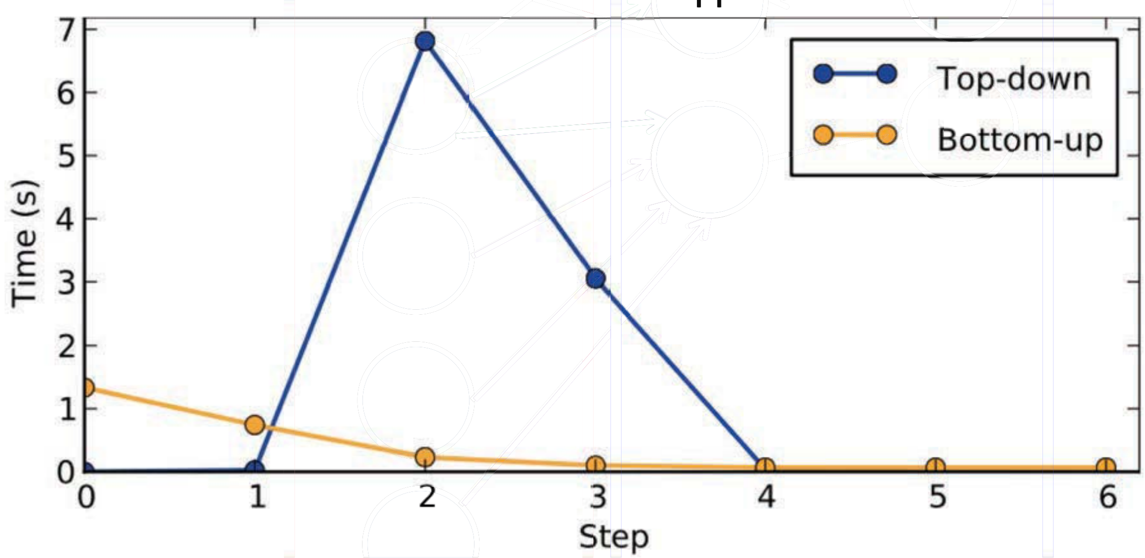
Growth of frontiers



- For many graphs, frontier grows rapidly and then shrinks
- Most of the work done with frontier (and sum of out-degrees) is large

Two ways to do BFS





- Bottom–up is better when frontier is large and many vertices have been visited
  - Reduces number of edges traversed
- Top–down is better when frontier is small

Which one to use?

Direction-optimizing BFS

- Choose based on frontier size *(Idea by Beamer, Asanovic, and Patterson in Supercomputing 2012)*

Top-down

- Loop through frontier vertices and explore unvisited neighbors

- Efficient for small frontiers
- Updates to parent array is atomic

Bottom-up

```
for all vertices v in parallel:
  if parent[v] == -1:
    for all neighbors ngh of v:
      if ngh on frontier:
        parent[v] = ngh;
        place v on frontierNext;
        break;
```

- Efficient for larger frontiers
- Update to parent array need not be atomic

- Threshold of frontier size > n/20 works well in practice
  - Can also consider sum of out-degrees
- Need to generate "inverse" graph if it is directed

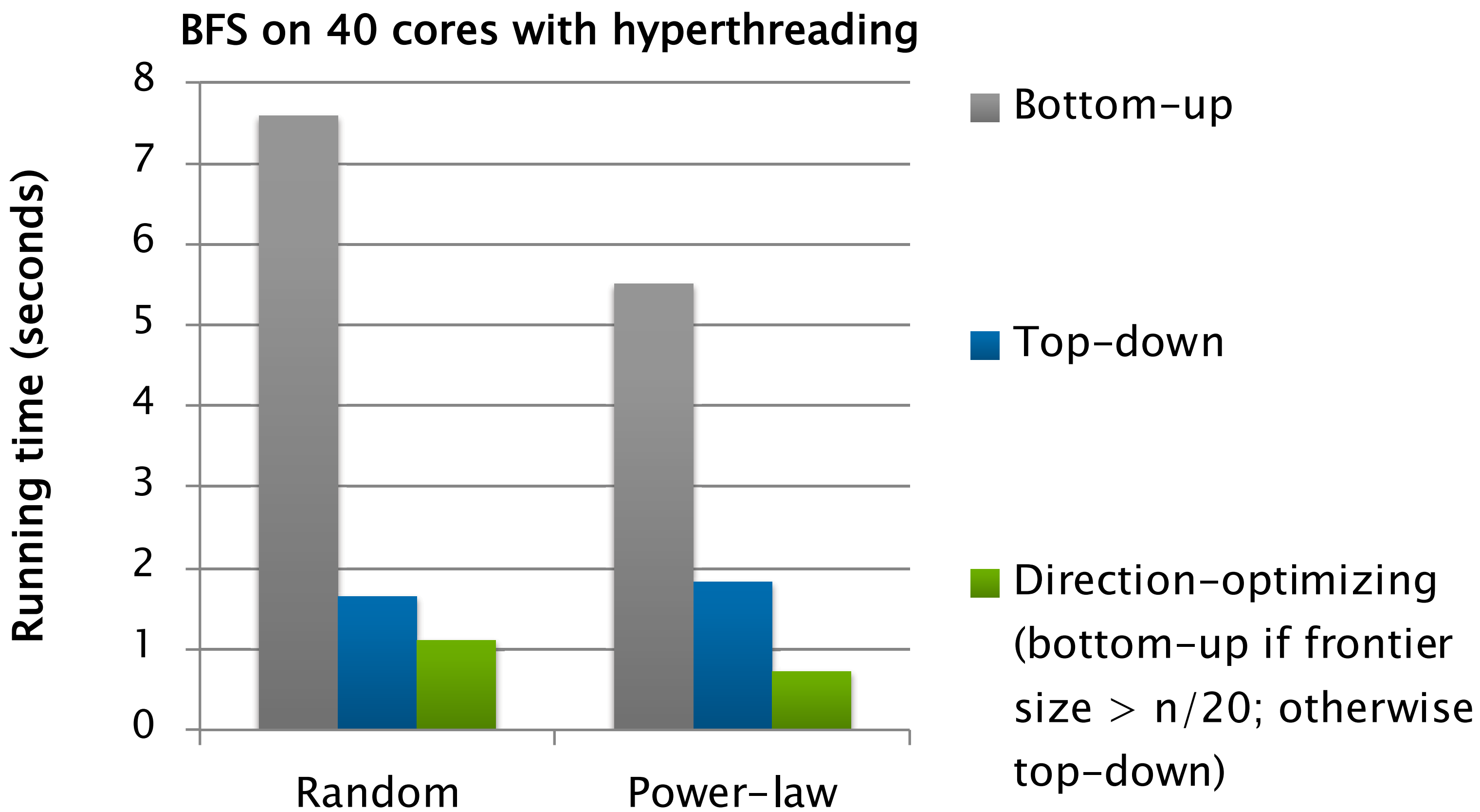
Representing the frontier

- Sparse integer array
  - For example, [1, 4, 7]
- Dense byte array
  - For example, [0, 1, 0, 0, 1, 0, 0, 1] *(n=8)*
  - Can further compress this by using 1 bit per vertex and using bit-level operations to access it

- Sparse representation used for top-down
- Dense representation used for bottom-up

- Need to convert between representations when switching methods

Direction-optimizing BFS performance



- Benefits highly dependent on graph
- No benefits if frontier is always small (e.g., on a grid graph or road network)

Ligra Graph Framework

```
procedure EDGEMAP(G, frontier, Update, Cond):
    if (size(frontier) + sum of out-degrees > threshold) then:
            return EDGEMAP_DENSE(G, frontier, Update, Cond);
    else:
            return EDGEMAP_SPARSE(G, frontier, Update, Cond);
```

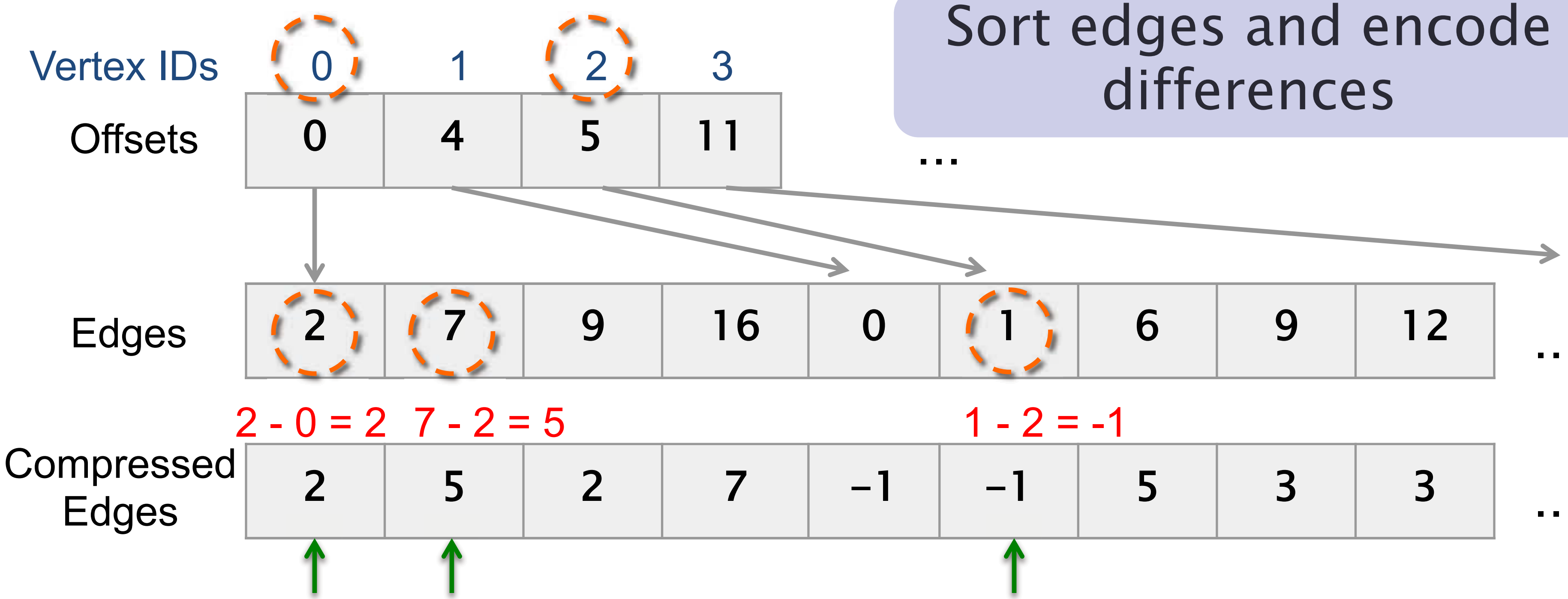
- More general than just BFS!
- Ligra framework generalizes direction-optimization to many other problems
  - For example, betweenness centrality, connected components, sparse PageRank, shortest paths, eccentricity estimation, graph clustering, k-core decomposition, set cover, etc.

Source: Julian Shun and Guy Blelloch. *Ligra: A Lightweight Graph Processing Framework for Shared Memory,* ACM Symposium on Principles and Practice of Parallel Programming 2013

GRAPH COMPRESSION AND REORDERING

Graph Compression on CSR

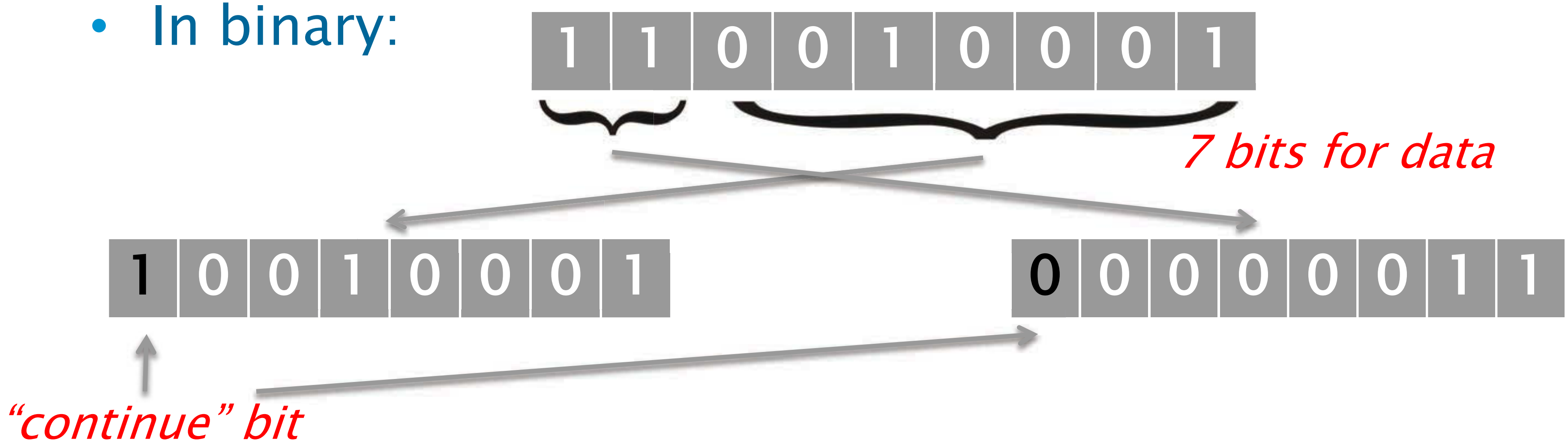
Sort edges and encode differences



- For each vertex v:
  - First edge: difference is Edges[Offsets[v]]−v
  - i'th edge (i>1): difference is Edges[Offsets[v]+i]−Edges[Offsets[v]+i−1]
- Want to use fewer than 32 or 64 bits to store each value

Variable-length codes

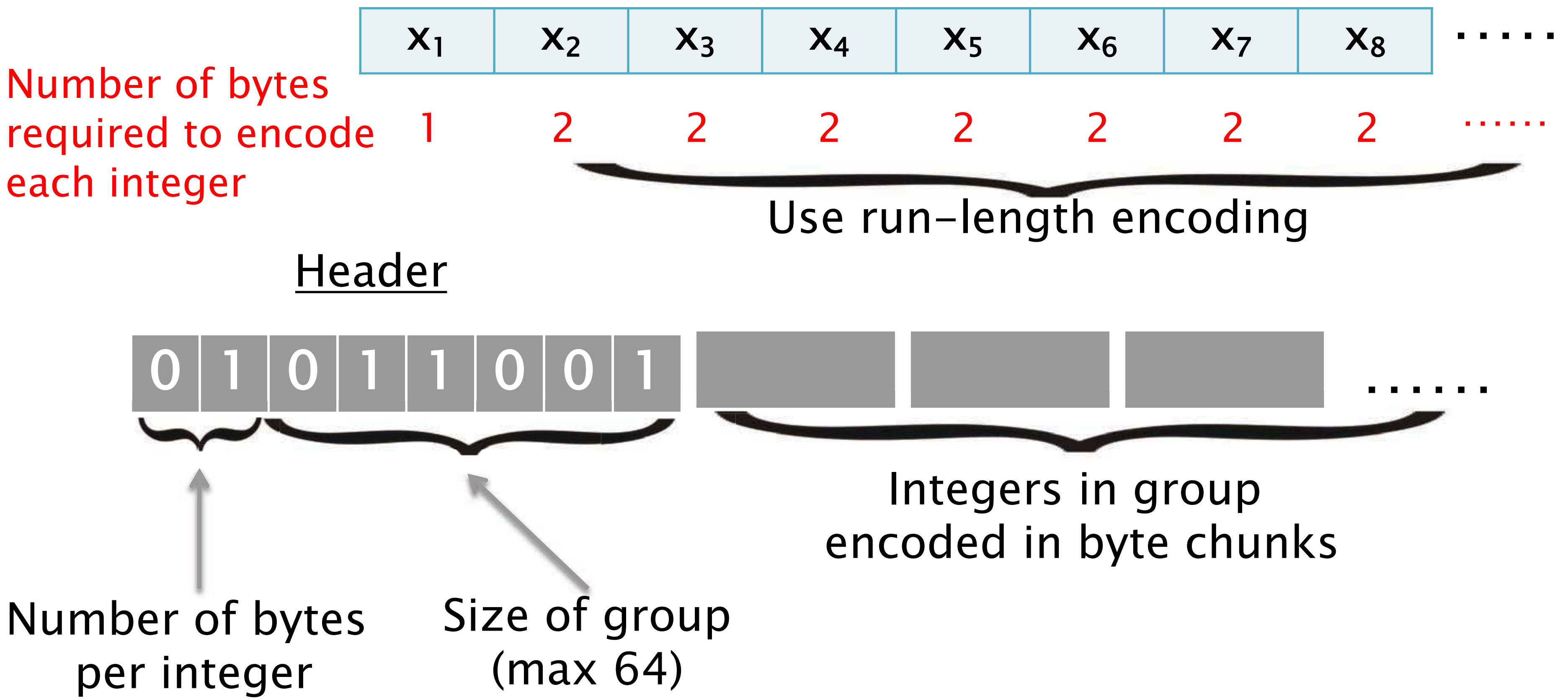
- k-bit (variable-length) codes
  - Encode value in chunks of k bits
  - Use k-1 bits for data, and 1 bit as the “continue” bit
- Example: encode “401” using 8-bit (byte) codes
- In binary:



- Decoding is just encoding “backwards”
  - Read chunks until finding a chunk with a “0” continue bit
  - Shift data values left accordingly and sum together
- Branch mispredictions from checking continue bit

Encoding optimization

- Another idea: get rid of "continue" bits

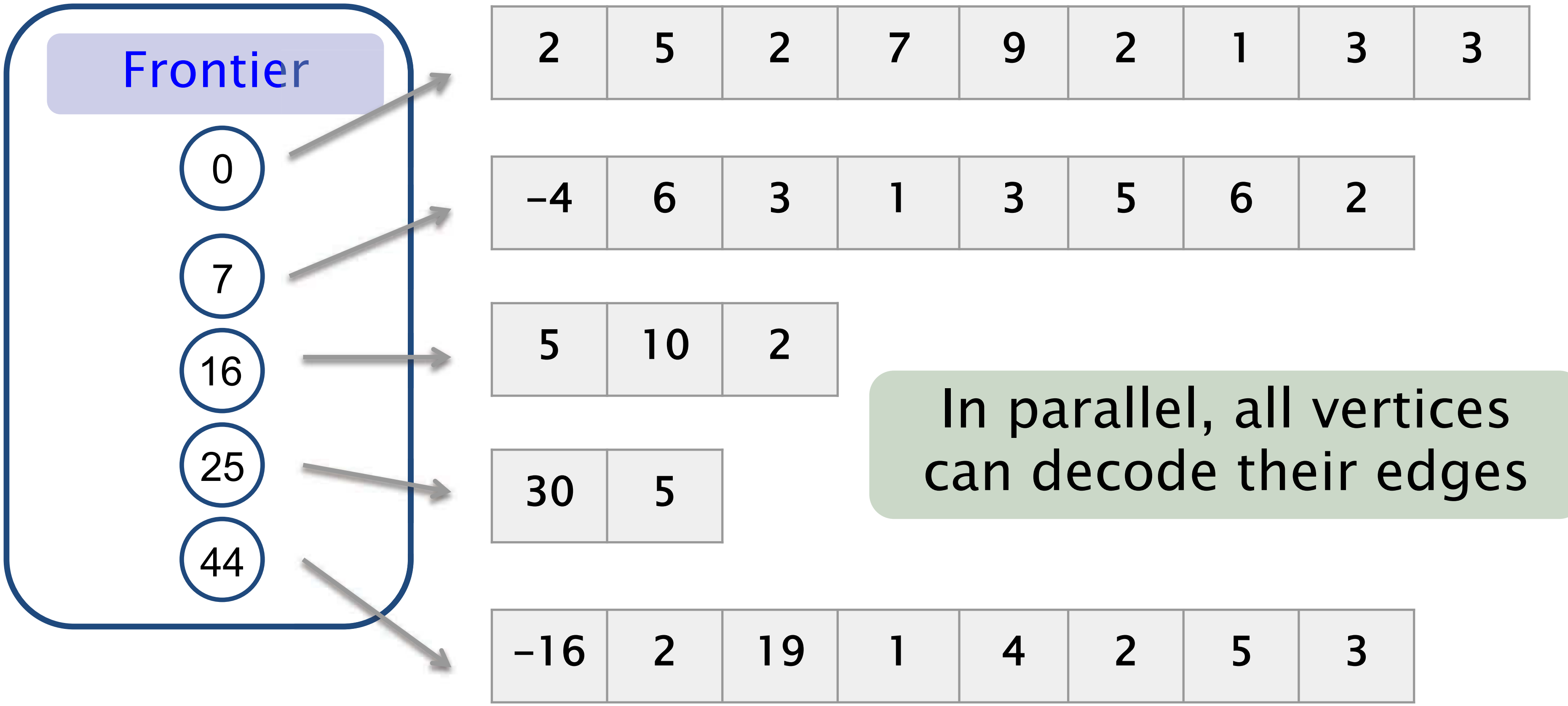


- Increases space, but makes decoding cheaper (no branch misprediction from checking "continue" bit)

Source: Julian Shun, Laxman Dhulipala and Guy Blelloch. *Smaller and Faster: Parallel Processing of Compressed Graphs with Ligra+*, IEEE Data Compression Conference 2015

Decoding on–the–fly

- Need to decode during the algorithm
  - If we decoded everything at the beginning we would not save any space!



- Each vertex decodes its edges sequentially
  - What about high degree vertices?

Parallel decoding

High-degree vertex

-1	2	4	3	16	2	1	5	8	19	4	1	23	14	12	1	9	10	3	5

…

Chunks of size T

…

-1	2	4	3	16	2

27	5	8	19	4	1

87	14	12	1	9	10

…

Encode first entry relative to source vertex

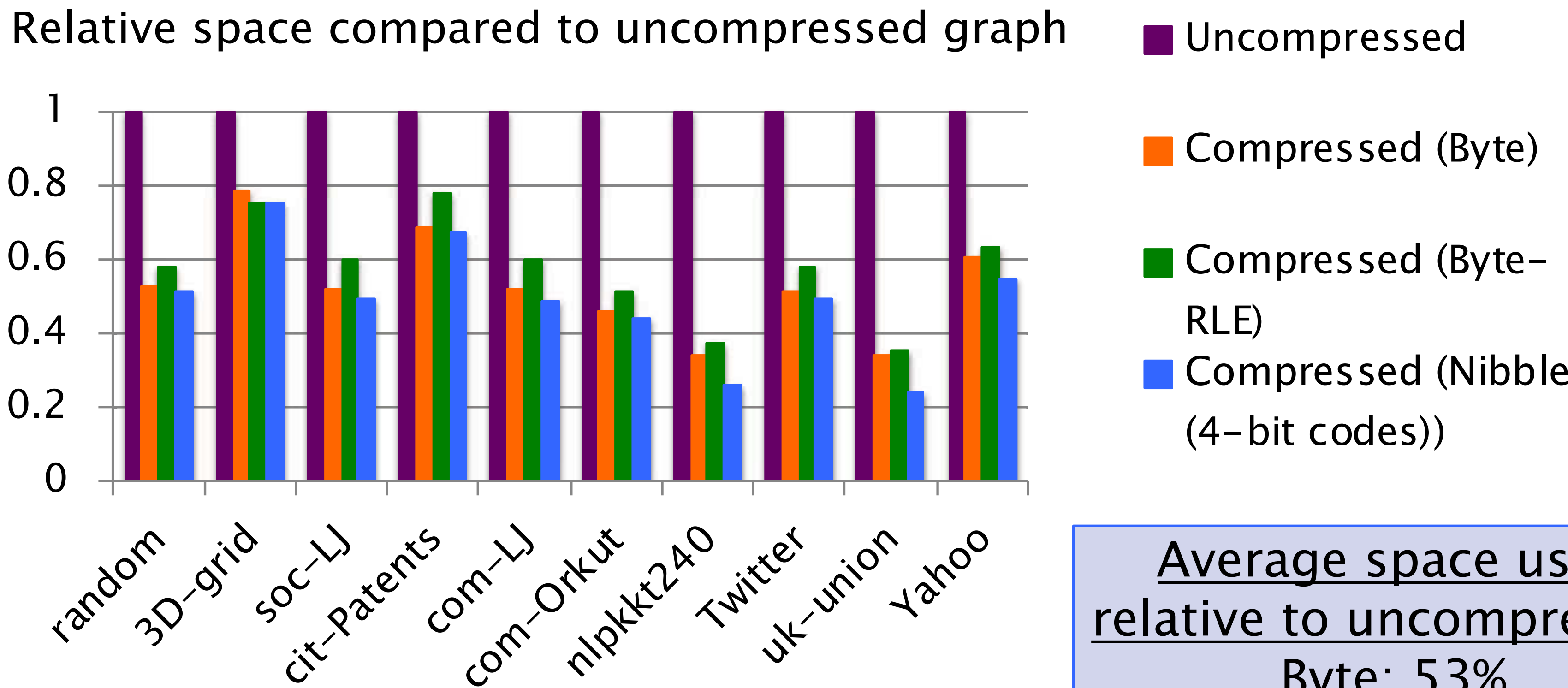
All chunks can be decoded in parallel!

- T=100 to 10,000 works well in practice

Source: Julian Shun, Laxman Dhulipala and Guy Blelloch. *Smaller and Faster: Parallel Processing of Compressed Graphs with Ligra+*, IEEE Data Compression Conference 2015

Good compression for most graphs

- Space to store graph, which dominates the actual space usage for most graphs

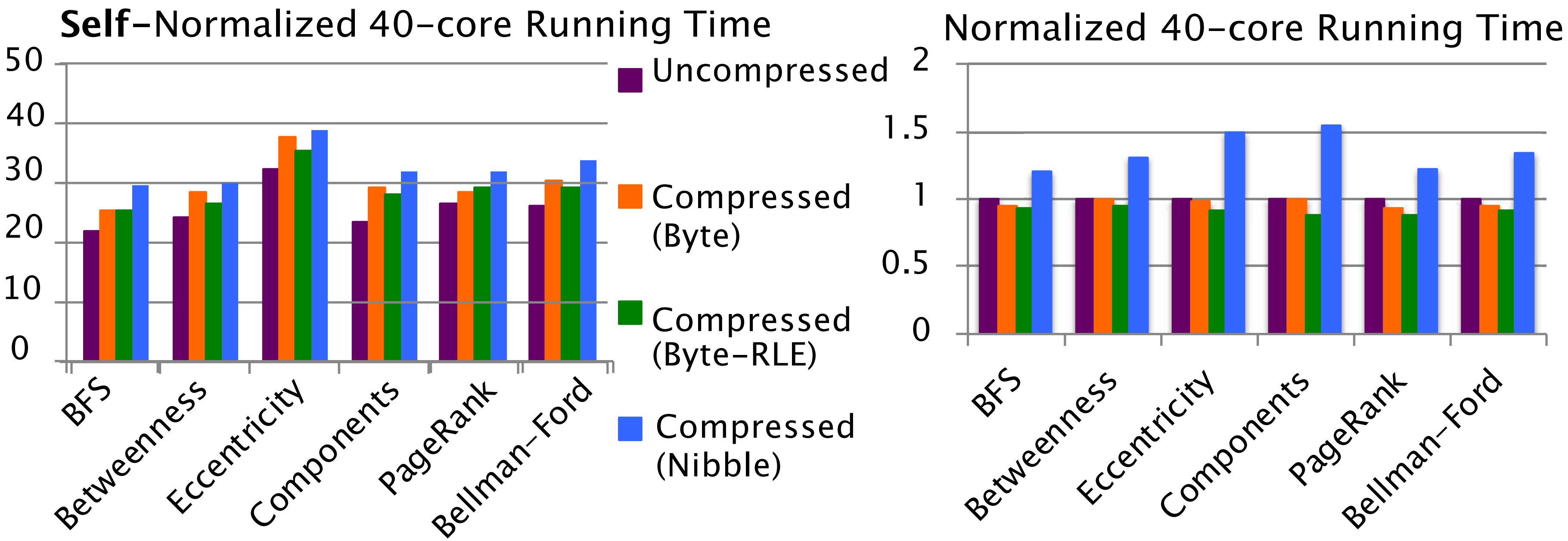


- Can further reduce space but need to ensure decoding is fast

<u>Average space used relative to uncompressed</u>
Byte: 53%
Byte-RLE: 56%
Nibble: 49%

Source: Julian Shun, Laxman Dhulipala and Guy Blelloch. *Smaller and Faster: Parallel Processing of Compressed Graphs with Ligra+*, IEEE Data Compression Conference 2015

What is the cost of decoding on-the-fly?

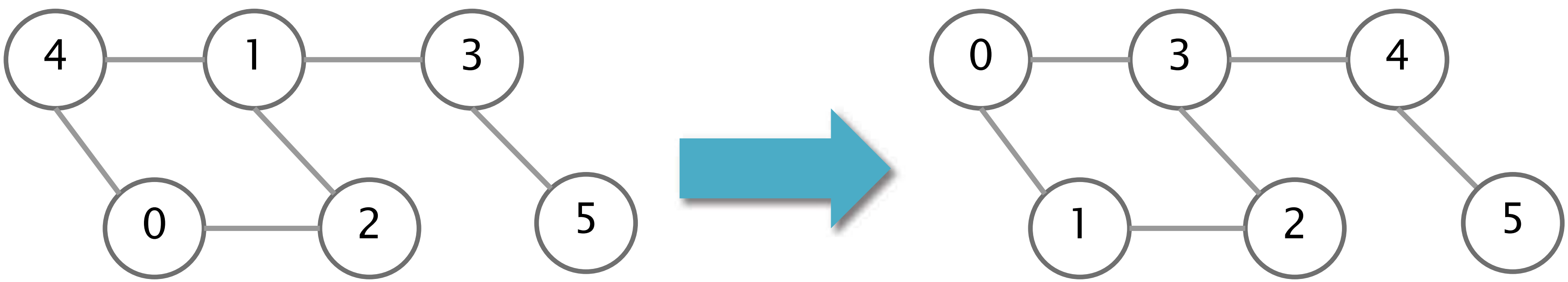


- In parallel, compressed can outperform uncompressed
  - These graph algorithms are memory-bound and memory subsystem is a bottleneck in parallel (contention for resources)
  - Spends less time on memory operations, but has to decode
- Decoding has good speedup so overall speedup is higher
- All techniques integrated into Ligra framework

Source: Julian Shun, Laxman Dhulipala and Guy Blelloch. *Smaller and Faster: Parallel Processing of Compressed Graphs with Ligra+*, IEEE Data Compression Conference 2015

Graph Reordering

- Reassign IDs to vertices to improve locality
  - Goal: Make vertex IDs close to their neighbors' IDs and neighbors' IDs close to each other



Sum of differences = 21

Sum of differences = 19

- Can improve compression rate due to smaller "differences"
- Can improve performance due to higher cache hit rate
- Various methods: BFS, DFS, METIS, by degree, etc.

Summary

- Real-world graphs are large and sparse
- Many graphs algorithms are irregular and involve many memory accesses
- Improve performance with algorithmic optimizations and by creating/exploiting locality
- Optimizations may work for some graphs, but not others