Biostatistics 615/815 Lecture 10: Boost Library Graph Algorithms

Hyun Min Kang

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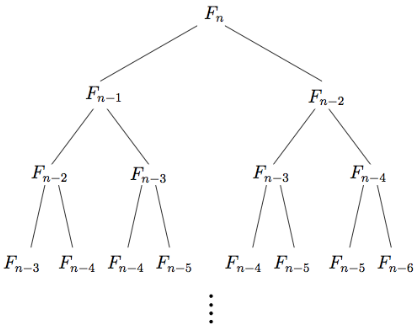
Recap : Simple vs smart recursion

Simple recursion of fibonacci numbers

```
int fibonacci(int n) {
  if ( n < 2 ) return n;
  else return fibonacci(n-1)+fibonacci(n-2);
}
```



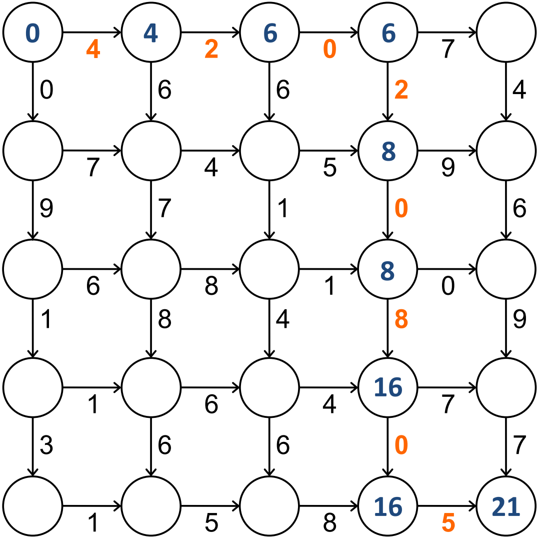
Top-down dynamic programming

```
int fibonacci(int n) {
  int* fibs = new int[n+1];
  fibs[0] = 0;
  fibs[1] = 1;
  for(int i=2; i <= n; ++i) {
    fibs[i] = fibs[i-1]+fibs[i-2];
  }
  int ret = fibs[n];
  delete [] fibs;
  return ret;
}
```

Bottom-up dynamic programming : smart recursion

```
int fibonacci(int* fibs, int n) {
  if ( fibs[n] > 0 ) {
    return fibs[n];     // reuse stored solution if available
  }
  else if ( n < 2 ) {
    return n;           // terminal condition
  }
  fibs[n] = fibonacci(n-1) + fibonacci(n-2); // store the solution once computed
  return fibs[n];
}
```

Recap: The Manhattan tourist problem



A "dynamic" structure of the solution

- Let $C(r, c)$ be the optimal cost from $(0, 0)$ to (r, c)
- Let $h(r, c)$ be the weight from (r, c) to $(r, c + 1)$
- Let $v(r, c)$ be the weight from (r, c) to $(r + 1, c)$
- We can recursively define the optimal cost as

$$C(r,c) = \begin{cases} \min \begin{cases} C(r-1,c) + v(r-1,c) \\ C(r,c-1) + h(r,c-1) \end{cases} & r > 0, c > 0 \\ C(r,c-1) + h(r,c-1) & r > 0, c = 0 \\ C(r-1,c) + v(r-1,c) & r = 0, c > 0 \\ 0 & r = 0, c = 0 \end{cases}$$

- Once $C(r, c)$ is evaluated, it must be stored to avoid redundant computation.

Recap: Edit distance

		A	L	G	O	R	I	T	H	M
	0	1	2	3	4	5	6	7	8	9
A	1	**0**	1	2	3	4	5	6	7	8
L	2	1	**0**	1	2	3	4	5	6	7
T	3	2	1	1	2	3	4	**4**	5	6
R	4	3	2	2	2	**2**	3	4	5	6
U	5	4	3	3	3	3	3	4	5	6
I	6	5	4	4	4	4	**3**	4	5	6
S	7	6	5	5	5	5	4	4	5	6
T	8	7	6	6	6	6	5	**4**	5	6
I	9	8	7	7	7	7	**6**	5	5	6
C	10	9	8	8	8	8	7	6	6	6

Today

- Boost library
- Graph algorithms
    - Dijkstra's algorithm
    - All-pair shortest path

Using boost C++ libraries

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- An extensive set of libraries for C++
- Supports many additional classes and functions beyond STL
- Useful for increasing productivity=

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Examples of useful libraries

- Math/Statistical Distributions
- Graph
- Regular expressions
- Tokenizer

Getting started with `boost` libraries

Download, Compile, and Install

- Follow instructions at *http://http://www.boost.org/users/download//*
- Note that compile takes a REALLY LONG time - up to hours!
- Everyone should try to install it, and let me know if it does not work for your environment.

Quick boost installation guide

Check whether your system already has boost installed

- Type `ls /usr/include/boost` or `ls /usr/local/include/boost`
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Otherwise, in Linux or MacOS X

```
user@host:~/$ tar xzvf boost_1_45_0.tar.gz
user@host:~/$ cd boost_1_45_0
user@host:~/$ mkdir --p /home/[user]/devel
user@host:~/$ ./bootstrap.sh --prefix=/home/[user]/devel
              (exclude --prefix when you have superuser permission)
user@host:~/$ ./bjam install (or sudo ./bjam install if you are a superuser)
user@host:~/$ g++ -I/home/[user]/devel/include -o boostExample boostExample.cpp
```

In Windows with Visual Studio

http://www.boost.org/doc/libs/1_45_0/more/getting_started/windows.html

boost example 1 : Chi-squared test

```
#include <iostream>
#include <boost/math/distributions/chi_squared.hpp>
int main(int argc, char** argv) {
  if ( argc != 5 ) {
    std::cerr << "Usage: chisqTest [a] [b] [c] [d]" << std::endl;
    return -1;
  }
  int a = atoi(argv[1]);  // read 2x2 table from command line arguments
  int b = atoi(argv[2]);
  int c = atoi(argv[3]);
  int d = atoi(argv[4]);
  // calculate chi-squared statistic and p-value
  double chisq = (double)(a*d-b*c)*(a*d-b*c)*(a+b+c+d)/(a+b)/(c+d)/(a+c)/(b+d);
  boost::math::chi_squared chisqDist(1);         // chi-squared statistic
  double p = boost::math::cdf(chisqDist, chisq); // calculate cdf
  std::cout << "Chi-square statistic = " << chisq << std::endl;
  std::cout << "p-value = " << 1-p << std::endl; // output p-value
  return 0;
}
```

Running examples of chisqTest

```
user@host~:/$ ./chisqTest 2 7 8 2
Chi-square test statistic = 6.34272
p-value = 0.0117864

user@host~:/$ ./chisqTest 20 70 80 20
Chi-square test statistic = 63.4272
p-value = 1.66533e-15

user@host~:/$ ./chisqTest 200 700 800 200
Chi-square test statistic = 634.272
p-value = 0  (not very robust to small p-values)
```

Using namespace: save your wrists

```
#include <iostream>
#include <boost/math/distributions/chi_squared.hpp>
using namespace std;
using namespace boost::math;
int main(int argc, char** argv) {
  ...
  // calculate chi-squared statistic and p-value
  double chisq = (double)(a*d-b*c)*(a*d-b*c)*(a+b+c+d)/(a+b)/(c+d)/(a+c)/(b+d);
  chi_squared chisqDist(1);         // instead of boost::math::chi_squared
  double p = cdf(chisqDist, chisq); // instead of boost::math::cdf
  cout << "Chi-square statistic = " << chisq << endl; // instead of std::cout
  cout << "p-value = " << 1-p << endl;                // and std::endl;
  return 0;
}
```

boost Example 2 : Tokenizer

```
#include <iostream>
#include <boost/tokenizer.hpp>
#include <string>
using namespace std;
using namespace boost;

int main(int argc, char** argv) {
  // default delimiters are spaces and punctuations
  string s1 = "Hello, boost  library";
  tokenizer<> tok1(s1);
  for(tokenizer<>::iterator i=tok1.begin(); i != tok1.end() ; ++i) {
    cout << *i << endl;
  }
  // you can parse csv-like format
  string s2 = "Field 1,\"putting quotes around fields, allows commas\",Field 3";
  tokenizer<escaped_list_separator<char> > tok2(s2);
  for(tokenizer<escaped_list_separator<char> >::iterator i=tok2.begin();
       i != tok2.end(); ++i) {
    cout << *i << endl;
  }
  return 0;
}
```

A running example of tokenizerTest

```
user@host~:/$ ./tokenizerTest
Hello
boost
library
Field 1
putting quotes around fields, allows commas
Field 3
```

Introducing graphs

Graph is useful for representing

- Bayesian network
- Biological network
- Dependency between processes
- Phylogenetic tree

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Key components of a graph

- Vertices
- Edges
- Directionality (directed, undirected, bidirectional)
- Vertex properties (e.g. colors)
- Edge properties (e.g. weights)

Algorithmic problems with graphs

- Vertex coloring (k-coloring) problem
  - Minimum number of colors required to color all pairs of adjacent vertices with different colors
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- Traveling salesman problem
  - Determine whether there is a path to visit each vertex exactly once.
  - Another *NP-complete* problem
- Shortest path finding problem
  - Find shortest path from a source to destination
  - A polynomial time solution exists

Single-source shortest paths problem

Given

- A directed graph $G = (V, E)$
- With weight function $w : E \rightarrow \mathbb{R}$
- (u, v) : source and destination vertices.

Want

A path $p =< x_0, x_1, \cdots, x_k > (x_0 = u, x_k = v)$ whose weight $w(p) = \sum_{i=1}^{k} w(x_{i-1}, x_i)$ is minimum among all possible paths

Shortest path algorithms

- Single-source shortest paths problems
  - Bellman-Ford algorithm : allowing negative weights
    - $\Theta(|V||E|)$ complexity
  - Dijkstra's algorithm : non-negative weights only
    - $\Theta(|V|\log|V| + |E|)$ complexity
- All-pair shortest paths algorithms
  - Floyd-Warshall algorithm
    - $\Theta(|V|^3)$ complexity

Elementary functions

Algorithm InitializeSingleSource

Data: G : graph, s : source
for $v \in G.V$ **do**
    $v.d = \infty$;
    $v.\pi =$ NIL;
end
$s.d = 0$;

Algorithm Relax

Data: u : vetex, v : vertex, w : weights
if $v.d > u.d + w(u, v)$ **then**
    $v.d = u.d + w(u, v)$;
    $v.\pi = u$;
end

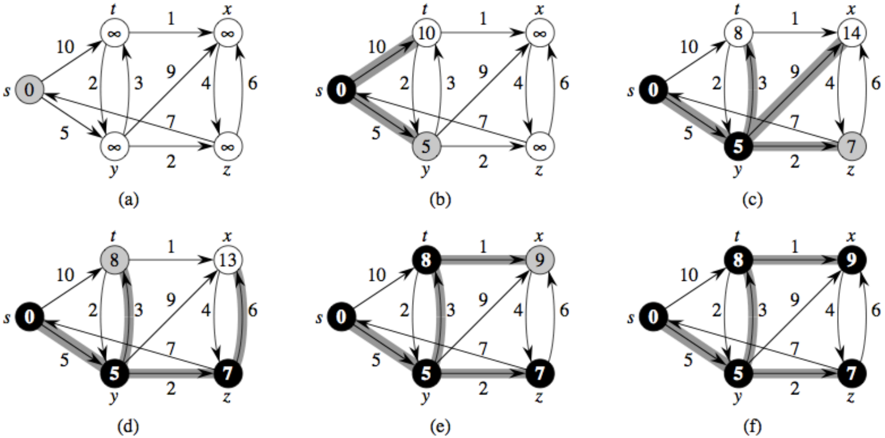
Dijkstra's algorithm

Algorithm Dijkstra

Data: G : graph, w : weight, s : source
Result: Each vertex contains the optimal weight from s

InitializeSingleSource(G,s);
$S = \emptyset$;
$Q = G.V$;
while $Q \neq \emptyset$ **do**
  $u =$ExtractMin(Q);
  $S = S \cup \{u\}$;
  for $v \in G.Adj[u]$ **do**
    Relax(u, v, w);
  end
end

Illustration of DIJKSTRA's algorithm



Time complexity of DIJKSTRA's algorithm

- The total number of `while` iteration is $|V|$
- EXTRACTMIN takes $\Theta(\log |Q|) \leq \Theta(\log |V|)$ time
- The total number of `for` iteration if $|E|$ because RELAX is called only once per edge
- The total time complexity is $\Theta(|V| \log |V| + |E|)$.

Using boost library for Manhattan Tourist Problem

```
int main(int argc, char** argv) {
  // defining a graph type
  // 1. edges are stored as std::list internally
  // 2. verticies are stored as std::vector internally
  // 3. the graph is directed (undirectedS, bidirectionalS can be used)
  // 4. vertices do not carry particular properties
  // 5. edges contains weight property as integer value
  typedef adjacency_list< listS, vecS, directedS, no_property,
                          property< edge_weight_t, int> > graph_t;

  // vertex_descriptor is a type for representing vertices
  typedef graph_traits< graph_t >::vertex_descriptor vertex_descriptor;
  // a nodes is represented as an integer, and an edge is a pair of integers
  typedef std::pair<int, int> E;

  // Connect between verticies as in the Manhattan Tourist Problem
  // Each node is labled as a two-digit integer of [#row] and [#col]
  enum { N11, N12, N13, N14, N15,
         N21, N22, N23, N24, N25,
         N31, N32, N33, N34, N35,
         N41, N42, N43, N44, N45,
         N51, N52, N53, N54, N55 };
```

Using boost library for Manhattan Tourist Problem

```
// model edges for Manhattan tourist problem
E edges [] = { E(N11,N12), E(N12,N13), E(N13,N14), E(N14,N15),
               E(N21,N22), E(N22,N23), E(N23,N24), E(N24,N25),
               E(N31,N32), E(N32,N33), E(N33,N34), E(N34,N35),
               E(N41,N42), E(N42,N43), E(N43,N44), E(N44,N45),
               E(N51,N52), E(N52,N53), E(N53,N54), E(N54,N55),
               E(N11,N21), E(N12,N22), E(N13,N23), E(N14,N24), E(N15,N25),
               E(N21,N31), E(N22,N32), E(N23,N33), E(N24,N34), E(N25,N35),
               E(N31,N41), E(N32,N42), E(N33,N43), E(N34,N44), E(N35,N45),
               E(N41,N51), E(N42,N52), E(N43,N53), E(N44,N54), E(N45,N55) };
// Assign weights for each edge
int weight [] = { 4, 2, 0, 7,     // horizontal weights
                  7, 4, 5, 9,
                  6, 8, 1, 0,
                  1, 6, 4, 7,
                  1, 5, 8, 5,
                  0, 6, 6, 2, 4,  // vertical weights
                  9, 7, 1, 0, 6,
                  1, 8, 4, 8, 9,
                  3, 6, 6, 0, 7 };
```

Using Dijkstra's algorithm to solve the MTP

```
// define a graph as an array of edges and weights
graph_t g(edges, edges + sizeof(edges) / sizeof(E), weight, 25);
// vectors to store predecessors and shortest distances from source
std::vector<vertex_descriptor> p(num_vertices(g));
std::vector<int> d(num_vertices(g));
vertex_descriptor s = vertex(N11, g); // specify source vertex
// Run Dijkstra's algorithm and store paths and distances to p and d
dijkstra_shortest_paths(g, s, predecessor_map(&p[0]).distance_map(&d[0]));
graph_traits < graph_t >::vertex_iterator vi, vend;

std::cout << "Backtracking the optimal path from the destination to source" << std::endl;
for(int node = N55; node != N11; node = p[node]) {
  std::cout << "Path: N" << getNodeID(p[node]) << " -> N"
    << getNodeID(node) << ", Distance from origin is " << d[node] << std::endl;
}
return 0;
```

The remainder - beginning of DijkstraMTP.cpp

```
// Note that this code would not work with VC++
#include <iostream>                          // for input/output
#include <boost/graph/adjacency_list.hpp> // for using graph type
#include <boost/graph/dijkstra_shortest_paths.hpp> // for dijkstra algorithm
using namespace std;   // allow to omit prefix 'std::'
using namespace boost; // allow to omit prefix 'boost::'

// converts 0,1,2,3,4,5,6,...,25 to 11,12,13,14,15,21,22,....,55
int getNodeID(int node) {
  return ((node/5)+1)*10+(node%5+1);
}

int main(int argc, char** argv) {
  ...
```

Running example of `DijkstraMTP`

```
user@host~/$ ./DijkstraMTP
Backtracking the optimal path from the destination to source
Path: N54 -> N55, Distance from origin is 21
Path: N44 -> N54, Distance from origin is 16
Path: N34 -> N44, Distance from origin is 16
Path: N24 -> N34, Distance from origin is 8
Path: N14 -> N24, Distance from origin is 8
Path: N13 -> N14, Distance from origin is 6
Path: N12 -> N13, Distance from origin is 6
Path: N11 -> N12, Distance from origin is 4
```

DIJKSTRA's algorithm : summary

- An efficient algorithm for shortest-path finding
- Using `boost` library
- Transformed Manhattan Tourist Problem (simpler) to a shortest-path finding problem (more complex).

Calculating all-pair shortest-path weights

A dynamic programming formulation

Let $d^{(}_{ij}k)$ be the weight of shortest path from vertex i to j, for which intermediate vertices are in the set $\{1, 2, \cdots, k\}$.

$$d_{ij}^{(k)} = \begin{cases} w_{ij} & k = 0 \\ \min(d_{ij}^{(k-1)}, d_{ik}^{(k-1)} + d_{kj}^{k-1}) & k = 1 \end{cases}$$

Floyd-Warshall Algorithm

Algorithm FLOYDWARSHALL

Data: W : $n \times n$ weight matrix

$D^{(0)} = W$;

for $k = 1$ **to** n **do**

  for $i = 1$ **to** n **do**

    for $j = 1$ **to** n **do**

      $d_{ij}^{(k)} = \min(d_{ij}^{(k-1)}, d_{ik}^{(k-1)} + d_{kj}^{(k-1)})$;

    end

  end

end

return $D^{(n)}$;

Graphs and Statistical Models

- Graphs are useful in modeling dependency between random variables, especially in Bayesian networks
  - Each node represents a random variable
  - A directed edge can represent conditional dependency
  - A undirected edge can represents joint probability distribution.
- Inference in Bayesian network directly correspond to particular graph algorithms
- For example, Viterbi algorithm in Hidden Markov Models (HMMs) is equivalentlt represented as Dijkstra's algorithm.

Next Lecture

- Random numbers
- Hidden Markov Models