Biostatistics 615/815
Statistical Computing

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Objectives

- Understanding computational aspects of statistical methods.
  - ✓ Estimate computational time and memory required
  - ✓ Understand how the method scales with data size
- Learning practical skills for efficient implementation of methods.
  - ✓ Determine appropriate data structure for implmentation
  - ✓ Make use of existing libraries when useful.
  - ✓ Implement one's own library / routine when necessary
- Developing algorithmic perspective for improving analytic methods.
  - ✓ Approximation algorithms for computationally intractable problems.
  - ✓ Computational improvement of existing methods

Why Study Statistical "Computing"?

- Statistical methods need to "compute" from data.
  - ✓ Need to understand computation for better interpretation of the results.
- Computational efficiency is critical for large-scale data analysis
  - ✓ In genomic data analysis, more accurate methods are often not used in practice due to prohibitive computational cost.
  - ✓ Many algorithms works "in principle", but almost impossible to run with large-scale data due to exponential time complexity with data size.
- Many statistical methods require "optimization" or "randomization"
  - ✓ Logistic regression
  - ✓ Maximum-likelihood estimation
  - ✓ Bootstrapping
  - ✓ Markov-chain Monte Carlo (MCMC) methods

What Will Be Covered?

1. Algorithms 101

- Computational Time Complexity
- Sorting
- Divide and Conquer Algorithms
- Searching
- Key Data Stucture
- Dynamic Programming

What Will Be Covered?

2. Matrices and Numerical Methods

- Matrix decomposition (LU, QR, SVD)
- Implementation of Linear Models
- Numerical optimizations

What Will Be Covered?

3. Advanced Statistical Methods

- Hidden Markov Models
- Expectation-Maximization
- Markov-Chain Monte Carlo (MCMC) Methods

Textbooks

Required Textbook

- *"Introduction to Algorithms"*
  - ✓ by Cormen, Leiserson, Rivest, and Stein (CLRS)
  - ✓ Third Edition, MIT Press, 2009

Optional Textbooks

- *"Numerical Recipes"*
  - ✓ by Press, Teukolsky, Vetterling, and Flannery
  - ✓ Third Edition, Cambridge University Press, 2007
- *"C++ Primer Plus"*
  - ✓ by Stephen Prata
  - ✓ Fifth Edition, Sams, 2004

Assignments

BIOSTAT615

- Weekly Assignments - 50%
- Midterm Exam - 20%
- Final Exam - 30%

BIOSTAT815

- Weekly Assignments - 33%
- Midterm Exam - 14%
- Final Exam - 20%
- Projects, to be completed in pairs - 33%

Target Audiences

BIOSTAT615

- Programming experience is not required
- Those who do not have previous programming experience should expect to spend additional time studying and learning to be familiar with a programming language during the coursework.

BIOSTAT815

- Students should be familiar with programming languages, so that they can accomplish class project.
- List of suggested projects will be announced shortly.

Choice of Programming Language

- C++ is preferred.
- C or Java is acceptable, but may require additional work.

More information

Office hours

- Fill-in doodle poll at *http://doodle.com/7z2mqvft8cdhh4bn*

Course Web Page

- Visit
  - ✓ *http://genome.sph.umich.edu/wiki/Biostatistics_615/815*
  - ✓ or *http://goo.gl/9DoFo*

Algorithms

An Informal Definition

- An **algorithm** is a sequence of well-defined computational steps
- that takes a set of values as **input**
- and produces a set of values as **output**

Key Features of Good Algorithms

- Correctness
  - ✓ Algorithms must produce correct outputs across all legitimate inputs
- Efficiency
  - ✓ Time efficiency : Consume as small computational time as possible.
  - ✓ Space efficiency : Consume as small memory / stroage as possible
- Simplicity
  - ✓ Concise to write down & Easy to interpret.

An Informal Example

Old MacDonald Song

http://www.youtube.com/watch?v=7_mol6B9z00

Algorithm SingOldMacDonald (from Jeff Erickson's notes)

Data: $animals[1 \cdots n]$, $noises[1 \cdots n]$
Result: An "Old MacDonald" Song with *animals* and *noises*

```
for i = 1 to n do
    Sing "Old MacDonald had a farm, E I E I O";
    Sing "And on this farm he had some animals[i], E I E I O";
    Sing "With a noises[i] noises[i] here, and a noises[i] noises[i] there";
    Sing "Here a noise[i], there a noise[i], everywhere a noise[i] noise[i]";
    for j = i - 1 downto 1 do
        Sing "noise[j] noise[j] here, noise[j] noise[j] there";
        Sing "Here a noise[j], there a noise[j], everywhere a noise[j] noise[j]";
    end
    Sing "Old MacDonald had a farm, E I E I O.";
end
```

Analysis of Algorithm SINGOLDMACDONALD

Correctness

- Need a formal definition of the "Old MacDonald" song for proof.
- Prove by showing the algorithm produces the same song with the formal definition

Time Complexity

- Count how many words the algorithm produces
- For each i
  - First four lines produces 41 words
  - Two lines of inner loop produces 16 words for each j
  - The last line produces 10 words
- $T(n) = \sum_{i=1}^{n} \left(51 + \sum_{j=1}^{i-1} 16\right) = 43n + 8n^2$ words are produced.
- Asymptotic complexity of $T(n) = \Theta(n^2)$.

Sorting - A Classical Algorithmic Problem

The Sorting Problem

Input A sequence of n numbers. $A[1 \cdots n]$

Output A permutation (reordering) $A'[1 \cdots n]$ of input sequence such that $A'[1] \leq A'[2] \leq \cdots \leq A'[n]$

Sorting Algorithms

- Insertion Sort
- Selection Sort
- Bubble Sort
- Shell Sort
- Merge Sort
- Heapsort
- Quicksort
- Counting Sort
- Radix Sort
- Bucket Sort
- And much more..

A Visual Overview of Sorting Algorithms

http://www.sorting-algorithms.com

Insertion Sort

http://www.sorting-algorithms.com/insertion-sort

Algorithm InsertionSort

Data: An unsorted list $A[1 \cdots n]$
Result: The list $A[1 \cdots n]$ is sorted
for $j = 2$ **to** n **do**
  $key = A[j]$;
  $i = j - 1$;
  while $i > 0$ *and* $A[i] > key$ **do**
    $A[i+1] = A[i]$;
    $i = i - 1$;
  end
  $A[i+1] = key$;
end

Correctness of InsertionSort

Loop Invariant

At the start of each iteration, $A[1 \cdots j-1]$ is loop invariant iff:

- $A[1 \cdots j-1]$ consist of elements originally in $A[1 \cdots j-1]$.
- $A[1 \cdots j-1]$ is in sorted order.

A Strategy to Prove Correctness

Initialization Loop invariant is true prior to the first iteration

Maintenance If the loop invariant is true at the start of an iteration, it remains true at the start of next iteration

Termination When the loop terminates, the loop invariant gives us a useful property to show the correctness of the algorithm

Correctness Proof (Informal) of InsertionSort

Initialization

- When $j = 2$, $A[1 \cdots j-1] = A[1]$ is trivially loop invariant.

Maintenance

If $A[1 \cdots j-1]$ maintains loop invariant at iteration j, at iteration $j+1$:

- $A[j+1 \cdots n]$ is unmodified, so $A[1 \cdots j]$ consists of original elements.
- $A[1 \cdots i]$ remains sorted because it has not modified.
- $A[i+2 \cdots j]$ remains sorted because it shifted from $A[i+1 \cdots j-1]$
- $A[i] \leq A[i+1] \leq A[i+2]$, thus $A[1 \cdots j]$ is sorted and loop invariant

Termination

- When the loop terminates $(j = n+1)$, $A[1 \cdots j-1] = A[1 \cdots n]$ maintains loop invariant, thus sorted.

Time Complexity of InsertionSort

Worst Case Analysis

for $j = 2$ **to** n	$c_1 n$
do	
$\quad key = A[j]$;	$c_2(n-1)$
$\quad i = j - 1$;	$c_3(n-1)$
$\quad$ **while** $i > 0$ *and* $A[i] > key$	$c_4 \sum_{j=2}^{n} j$
$\quad$ **do**	
$\quad\quad A[i+1] = A[i]$;	$c_5 \sum_{j=2}^{n} (j-1)$
$\quad\quad i = i - 1$;	$c_6 \sum_{j=2}^{n} (j-1)$
$\quad$ **end**	
$\quad A[i+1] = key$;	$c_7(n-1)$
end	

$$
\begin{aligned}
T(n) &= \frac{c_4 + c_5 + c_6}{2} n^2 + \frac{2(c_1 + c_2 + c_3 + c_7) + c_4 - c_5 - c_6}{2} n - (c_2 + c_3 + c_4 + c_7) \\
&= \Theta(n^2)
\end{aligned}
$$

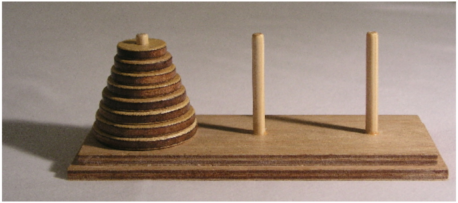
Tower of Hanoi

Problem

Input
- A (leftmost) tower with n disks, ordered by size, smallest to largest
- Two empty towers

Output Move all the disks to the rightmost tower in the original order

Condition
- One disk can be moved at a time.
- A disk cannot be moved on top of a smaller disk.



How many moves are needed?

A Working Example

http://www.youtube.com/watch?v=aGlt2G-DC8c

Think Recursively

Key Idea

- Suppose that we know how to move $n-1$ disks from one tower to another tower.
- And concentrate on how to move the largest disk.

How to move the largest disk?

- Move the other $n-1$ disks from the leftmost to the middle tower
- Move the largest disk to the rightmost tower
- Move the other $n-1$ disks from the middle to the rightmost tower

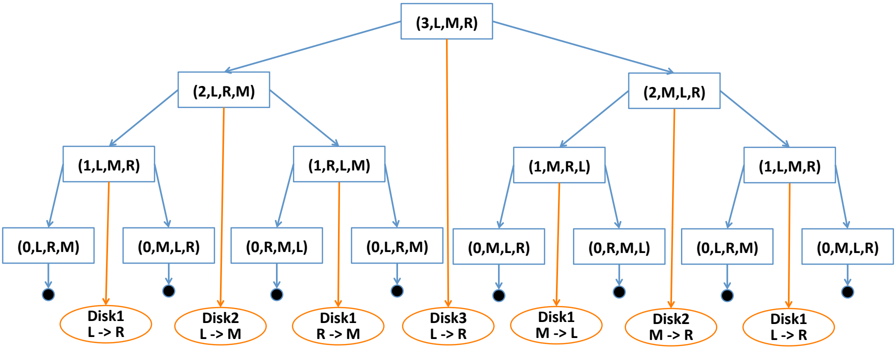
A Recursive Algorithm for the Tower of Hanoi Problem

Algorithm TowerOfHanoi

Data: n : # disks, (s, i, d) : source, intermediate, destination towers
Result: n disks are moved from s to d

```
if n == 0 then
    do nothing;
else
    TowerOfHanoi(n − 1, s, d, i);
    move disk n from s to d;
    TowerOfHanoi(n − 1, i, s, d);
end
```

How the Recursion Works



Analysis of TowerOfHanoi Algorithm

Correctness

- Proof by induction - Skipping

Time Complexity

- $T(n)$: Number of disk movements required
  - ✓ $T(0) = 0$
  - ✓ $T(n) = 2T(n-1) + 1$
- $T(n) = 2^n - 1$
- If $n = 64$ as in the legend, it would require $2^{64} - 1 = 18,446,744,073,709,551,615$ turns to finish, which is equivalent to roughly 585 billon years if one move takes one second.

Getting Started with C++

Writing helloWorld.cpp

```
#include <iostream> // import input/output handling library
int main(int argc, char** argv) {
  std::cout << "Hello, World" << std::endl;
  return 0; // program exits normally
}
```

Compiling helloWorld.cpp

Install Cygwin (Windows), Xcode (MacOS), or nothing (Linux).

```
user@host:~/$ g++ -o helloWorld helloWorld.cpp
```

Running helloWorld

```
user@host:~/$ ./helloWorld
Hello, World
```

Implementing TowerOfHanoi Algorithm in C++

towerOfHanoi.cpp

```
#include <iostream>
// recursive function of towerOfHanoi algorithm
void towerOfHanoi(int n, int s, int i, int d) {
  if ( n > 0 ) {
    towerOfHanoi(n-1,s,d,i); // recursively move n-1 disks from s to i
    // Move n-th disk from s to d
    std::cout << "Disk " << n << " : " << s << " -> " << d << std::endl;
    towerOfHanoi(n-1,i,s,d); // recursively move n-1 disks from i to d
  }
}
// main function
int main(int argc, char** argv) {
  int nDisks = atoi(argv[1]); // convert input argument to integer
  towerOfHanoi(nDisks, 1, 2, 3); // run TowerOfHanoi(n=nDisks, s=1, i=2, d=3)
  return 0;
}
```

Running TowerOfHanoi Implementation

Running towerOfHanoi

```
user@host:~/$ ./towerOfHanoi 3
Disk 1 : 1 -> 3
Disk 2 : 1 -> 2
Disk 1 : 3 -> 2
Disk 3 : 1 -> 3
Disk 1 : 2 -> 1
Disk 2 : 2 -> 3
Disk 1 : 1 -> 3
```

Implementing InsertionSort Algorithm

insertionSort.cpp - main() function

```
#include <iostream>
#include <vector>
void printArray(std::vector<int>& A);    // declared here, defined later
void insertionSort(std::vector<int>& A); // declared here, defined later
int main(int argc, char** argv) {
  std::vector<int> v; // contains array of unsorted/sorted values
  int tok;            // temporary value to take integer input
  while ( std::cin >> tok ) // read an integer from standard input
    v.push_back(tok)        // and add to the array
  std::cout << "Before sorting:";
  printArray(v);    // print the unsorted values
  insertionSort(v); // perform insertion sort
  std::cout << "After sorting:";
  printArray(v);    // print the sorted values
  return 0;
}
```

Implementing InsertionSort Algorithm

insertionSort.cpp - printArray() function

```
// print each element of array to the standard output
void printArray(std::vector<int>& A) { // call-by-reference : will explain later
  for(int i=0; i < A.size(); ++i) {
    std::cout << " " << A[i];
  }
  std::cout << std::endl;
}
```

Implementing INSERTIONSORT Algorithm

insertionSort.cpp - insertionSort() function

```
// perform insertion sort on A
void insertionSort(std::vector<int>& A) { // call-by-reference
  for(int j=1; j < A.size(); ++j) { // 0-based index
    int key = A[j];  // key element to relocate
    int i = j-1;     // index to be relocated
    while( (i >= 0) && (A[i] > key) ) { // find position to relocate
      A[i+1] = A[i]; // shift elements
      --i;           // update index to be relocated
    }
    A[i+1] = key;    // relocate the key element
  }
}
```

Running INSERTIONSORT Implementation

Test with small-sized data (in Linux)

```
user@host:~/$ seq 1 20 | shuf | ./insertionSort
Before sorting:  18 9 20 3 1 8 5 19 7 16 17 12 2 15 14 10 13 6 11 4
After sorting:  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
```

Running time evaluation with large data

```
user@host:~/$ time sh -c 'seq 1 100000 | shuf | ./insertionSort > /dev/null'
real 0m24.615s
user 0m24.650s
sys 0m0.000s
user@host:~/$ time sh -c 'seq 1 100000 | shuf | /usr/bin/sort -n > /dev/null'
real 0m0.238s
user 0m0.250s
sys 0m0.020s
```

/usr/bin/sort is orders of magnitude faster than insertionSort

Summary

- Algorithms are sequences of computational steps transforming inputs into outputs
- Insertion Sort
  - ✓ An intuitive sorting algorithm
  - ✓ Loop invariant property
  - ✓ $\Theta(n^2)$ time complexity
  - ✓ Slower than default `sort` application in Linux.
- A recursive algorithm for the Tower of Hanoi problem
  - ✓ Recursion makes the algorithm simple
  - ✓ Exponential time complexity
- C++ Implementation of the above algorithms.

For the Next Lecture

Reading Materials

- CLRS Chapter 1-2 (pp. 3-42)

What to expect

- C++ Programming 101
- Fisher's exact test