

*Biostatistics 615/815*  
*Statistical Computing*

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## Course Objective

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- Introduce skills required for executing statistical computing projects
- Applications and examples mostly in C.
  - Can be easily translated into R, etc.
- But the focus is on an algorithmic way of thinking!

# Part I: Key Algorithms

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- Connectivity
- Sorting
- Searching
- Hashing
- Key data structures

## Part II: Statistical Methods

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- Random Numbers
- Markov-Chain Monte-Carlo
  - Metropolis-Hastings
  - Gibbs Sampling
- Function Optimization
  - Naïve algorithms
  - Newton's Methods
  - E-M algorithm
- Numerical Integration

# Textbooks

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- Algorithms in C
  - Sedgewick (1998)
  - 3<sup>rd</sup> edition printed in 1998
- Numerical Recipes in C
  - Press, Teukolsky, Vetterling, Flannery
  - 2<sup>nd</sup> edition printed in 2002

# Assessment for 615

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- **Weekly Assignments**
  - About 50% of the final mark
- **2 Exams**
  - About 50% of the final mark

# Assessment for 815

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- **Weekly Assignments**
  - About 33% of the final mark
- **2 Exams**
  - About 33% of the final mark
- **Project, to be completed in pairs**
  - About 33% of the final mark

## Office Hours

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- Please fill out doodle poll with your availability:
  - [www.doodle.ch/tsuhaiage4ar5cer](http://www.doodle.ch/tsuhaiage4ar5cer)
- My office:
  - School of Public Health II, Crossroads Level 4
- My e-mail:
  - goncalo@umich.edu



# Algorithms

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- Methods for solving problems that are well suited to computer implementation
- Good algorithms make apparently impossible problems become simple

# Algorithms are ideas ...

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- Focus on approach to a problem
- Typically, the actual implementation could be take many different forms
  - Computer languages
  - Pen and paper

## Example: DNA Sequence Matches

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- When the Human Genome Project started, searching through the entire genome sequence seemed impractical...
- For example,
  - Searching for ~150 sequences of about 500bp each in ~3,000,000,000 bases of sequence would take ~3 hours with the original BLAST or FASTA3 algorithms

## Example: DNA Sequence Matches

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- Mullikin and colleagues (2001) described an improved algorithm, using hash tables, that could do this in  $< 2$  seconds
- Reference:
  - Ning, Cox and Mullikin (2001) *Genome Research* **11**:1725-1729

# Today's Lecture

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- Introduce a “Connectivity problem” and some alternative solutions
- If you haven't done much programming before, don't worry too much about implementation details.
  - We'll fill these in later lectures.

# The Connectivity Problem

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- **N objects**
  - Integer names  $0 \dots N - 1$
- **M connections between pairs of objects**
  - Each connection identifies a pair  $(p, q)$
- **Possible questions:**
  - Are all objects connected?
  - Are some connections redundant?
  - What are the groups of connected objects?

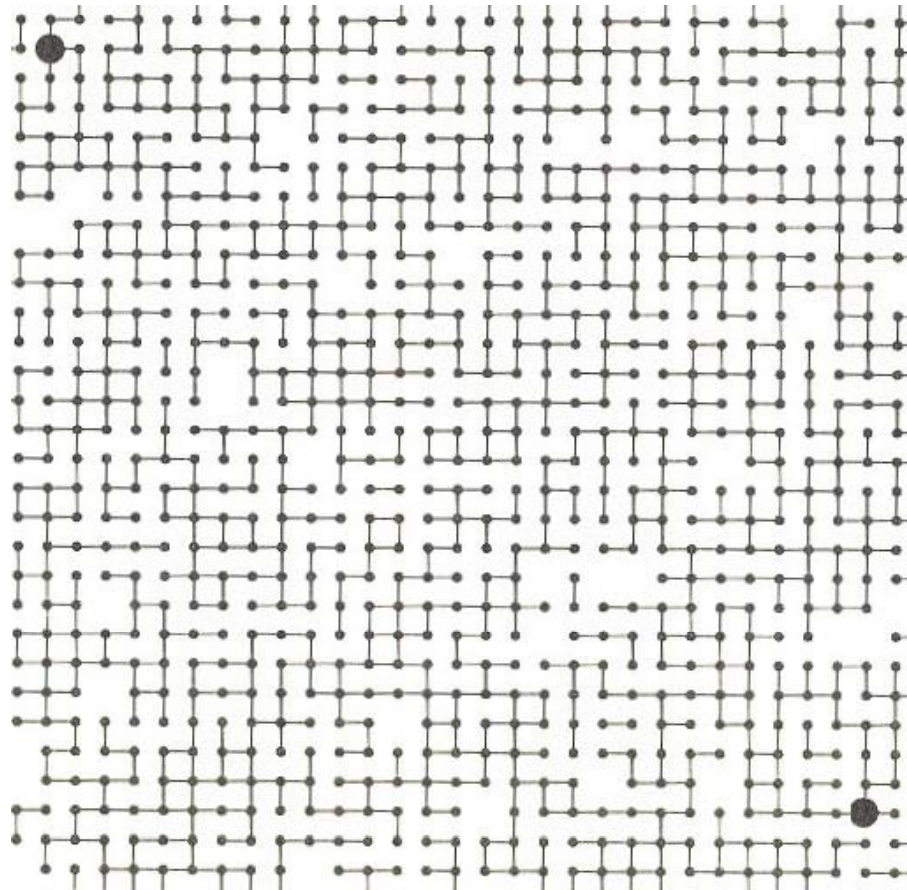
## Possible applications

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- Is a direct connection between two computers required in a network?
  - Or can we use some existing connections instead?
- Are two individuals part of the same extended family in a genetic study?
- Are two genes in the same regulatory network?

Are the two points connected?

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## A possible approach ...

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- Process connections one-by-one
- First, check whether a connection links two previously unconnected items
  - If not, proceed to the next connection
  - If yes, update list of connected items
- With  $N$  items, no more than  $N-1$  updates to the list of connected items required...
  - After  $N-1$  updates, all items connected to each other!

# A simple example ...

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- Connections

- 3-4

- 4-9

- 8-0

- 2-3

- 5-6

- 2-9

- 4-8

- 0-2

## A simple example ...

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- Connections

- 3-4 ✓
- 4-9 ✓
- 8-0 ✓
- 2-3 ✓
- 5-6 ✓
- 2-9 Redundant: 2-3 ; 3-4 ; 4-9
- 4-8 ✓
- 0-2 Redundant: 0-8; 8-4; 4-3; 3-2

## Specific Tasks

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- As we proceed through list of connections, conduct two tasks:
  - Decide if each connection is new.
  - Incorporate information about new connections.

# The Fundamental Operations

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- The *Find* operation
  - Identify the set containing a particular item or items.
- The *Union* operation
  - Replace the sets containing two groups of objects by their union

# The First Step

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- Developing a solution that works
  - Easy to verify correctness
  - May not be most efficient
  - Should be simple
- Useful as check of “better” solutions...

# Arrays of Integers

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- Simple data structure
  - Analogous to a vector
- The notation  $a[i]$  refers to the  $i^{\text{th}}$  integer in the array
  - When programming, we typically pre-specify the total number of entries in a array

# Quick Find Algorithm

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- Data
  - Array of  $N$  integers
  - Objects  $p$  and  $q$  connected iff  $a[p] == a[q]$
- Setup
  - Initialize  $a[i] = i$ , for  $0 \leq i < N$
- For each pair
  - If  $a[p] == a[q]$  objects are connected (FIND)
  - Move all entries in set  $a[p]$  to set  $a[q]$  (UNION)



# A Simple C Implementation

```
#define N 1000

int main()
{
    int i, p, q, set, a[N];           // Variable declarations
    int unique_connections = 0;

    for (i = 0; i < N; i++)          // Data Initialization
        a[i] = i;

    while (read_connection(p, q))    // Loop through connections
    {
        if (a[p] == a[q]) continue; // FIND operation

        set = a[p];                 // UNION operation
        for (i = 0; i < N; i++)
            if (a[i] == set)
                a[i] = a[q];

        print_connection(p, q);
        unique_connections++;
    }
    return 0;
}
```

# A Simple C Implementation

```
bool read_connection(int &a, int &b)
{
    // The scanf function is a standard C function for processing input
    // data. It processes input fields (each marked with a % sign)
    // according to a type qualifier. For example, %d fields are stored
    // in integer variables.

    bool success = scanf(" %d %d ", &a, &b) == 2;

    return success;
}

void print_connection(int a, int b)
{
    // The printf function is a standard C function for processing
    // output. It processes fields (each marked with a % sign)
    // according to a type qualifier. For example, %d fields are
    // replaced with the contents of corresponding integer variables.

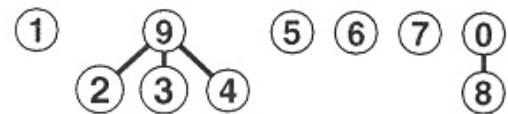
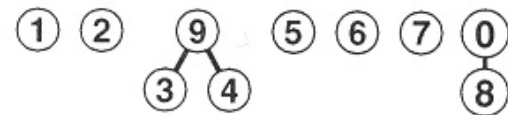
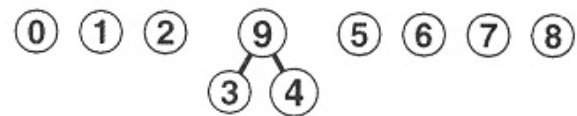
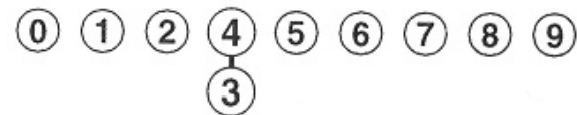
    printf("The connection from %d to %d is non-redundant.\n", a, b);
}
```

# Pictorial Representation

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- Array as connections are added:

- 3-4
- 4-9
- 8-0
- 2-3
- 2-9 \* Redundant \*



## How efficient is Quick Find?

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- If there  $N$  objects and  $M$  connections\*, the Quick Find algorithm requires on the order of  $MN$  operations
- Not feasible for very large numbers of objects...

\* In this case only non-redundant connections actually count

# Quick-Union Algorithm I

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- Complementary to Quick Find
- More complex data organization
  - Each object points to “parent” object in the same set

## Quick-Union Algorithm II

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- For each pair
  - Follow pointers until we reach object that points to itself
  - If  $a[p]$  and  $a[q]$  eventually lead to the same object, we are in the same set (FIND)
  - Otherwise, link the object to which  $a[p]$  leads to the object which  $a[q]$  leads (UNION)

# C Implementation

---

```
// Loop through connections
while (read_connection(p, q))
{
    // Check that input is within bounds
    if (p < 0 || p >= N || q < 0 || q >= N) continue;

    // FIND operation
    i = a[p];
    while (a[i] != i)
        i = a[i];

    j = a[q];
    while (a[j] != j)
        j = a[j];

    if (i == j) continue;

    // UNION operation
    a[i] = j;

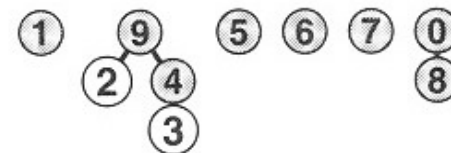
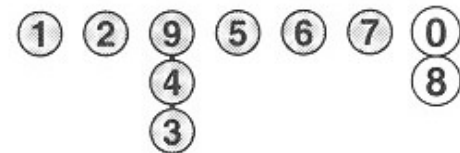
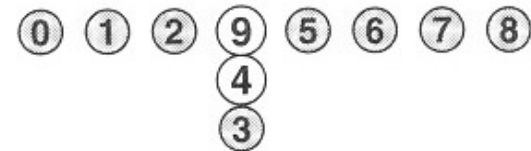
    print_connection(p, q);
    unique_connections++;
}
```

# Pictorial Representation

---

- Array as connections are added:

- 3-4
- 4-9
- 8-0
- 2-3
- 2-9 \* Redundant \*





## How efficient is Quick Union?

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- Quick Union is typically faster than Quick Find.
- However, the data can conspire to make things difficult:
  - If objects are paired 1-2; 2-3; 3-4; 4-5; ... we'll build long chains which slow down FIND operations
- In the worst case, we might even need more than MN operations

# Weighted Quick Union

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- A smarter version of Quick Union, that avoids long chains
- Keep track of the number of elements in each set (using a separate array)
- Link smaller set to larger set
  - Union increases length of chains in smaller set by 1

# C Implementation

```
// Initialize weights
for (i = 0; i < N; i++)
    weight[i] = 1;

// Loop through connections
while (read_connection(p, q))
{
    // Check that input is within bounds
    if (p < 0 || p >= N || q < 0 || q >= N) continue;

    // FIND operation
    for (i = a[p]; a[i] != i; i = a[i] ) ;
    for (j = a[q]; a[j] != j; j = a[j] ) ;
    if (i == j) continue;

    // UNION operation
    if (weight[i] < weight[j])
        { a[i] = j; weight[j] += weight[i]; }
    else
        { a[j] = i; weight[i] += weight[j]; }

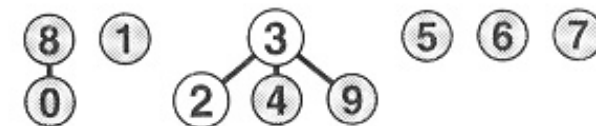
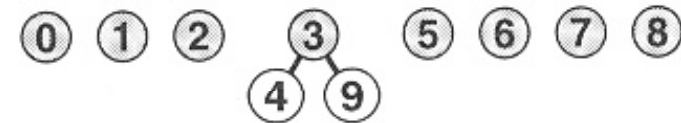
    print_connection(p, q);
    unique_connections++;
}
```

# Pictorial Representation

---

- Array as connections are added:

- 3-4
- 4-9
- 8-0
- 2-3
- 2-9 \* Redundant \*



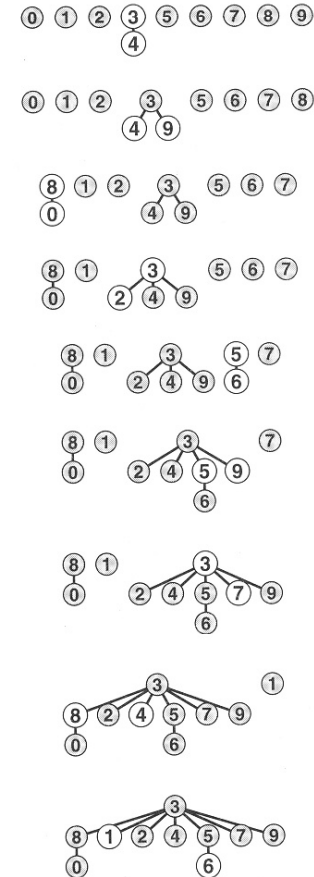
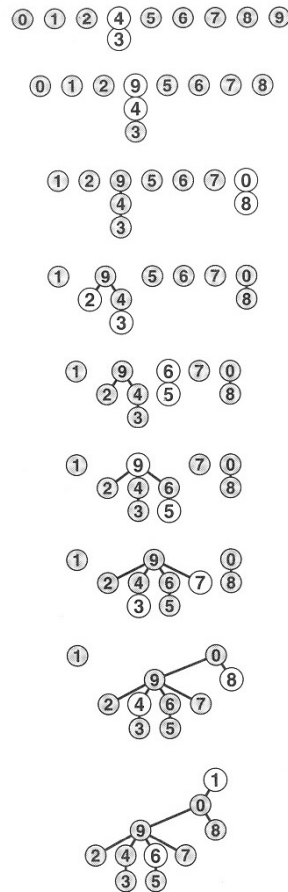
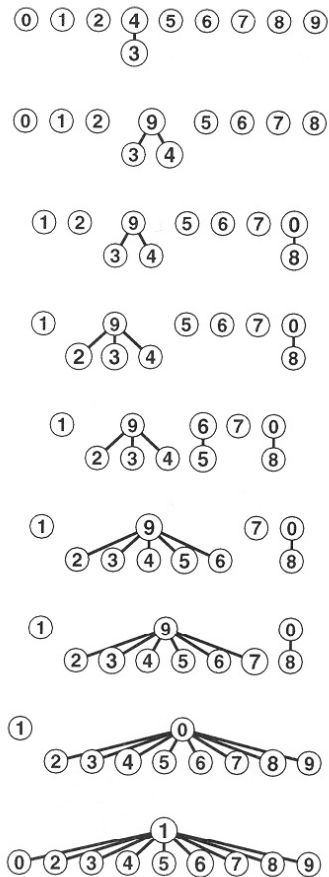
## Efficiency of Weighted Quick Union

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- Guarantees that pointer chains are no more than  $\log_2 N$  elements long
- Overall, requires about  $M \log_2 N$  operations
- Suitable for very large data sets with millions of objects and connections

# Pictorial Comparison

## Quick Union Quick Find Weighted



## Empirical Timings in Seconds

<b>Nodes (Connections)</b>	<b>Quick Find</b>	<b>Quick Union</b>	<b>Weighted Quick Union</b>
50,000 (50,000)	6	1	<1
100,000 (100,000)	12	4	<1
200,000 (200,000)	25	15	<1

## Summary

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- Considered 3 alternative solutions to the “connectivity problem”
  - Are any connections in a set redundant?
  - Are all objects in a set connected?
- Compared some of the computational cost for the different methods



## Reading Material

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- Read Chapter 1 of Sedgewick
- [www.sph.umich.edu/csg/abecasis/class/](http://www.sph.umich.edu/csg/abecasis/class/)