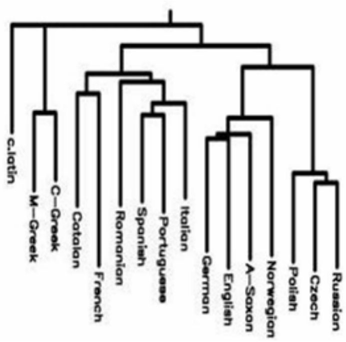
CS216: Program and Data Representation
University of Virginia Computer Science
Spring 2006 David Evans

Lecture 1: Introduction

Menu

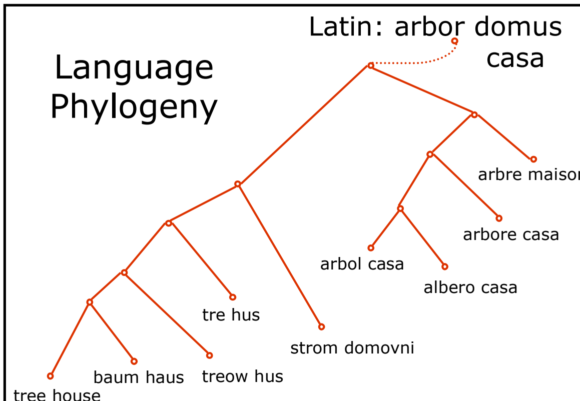
- Motivating Problem
- Course Structure, Expectations, Goals
- Analyzing Algorithms

Phylogeny

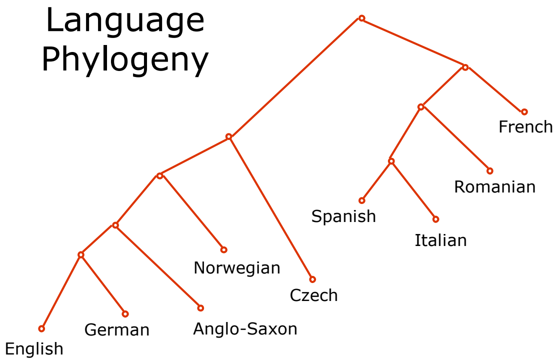


from http://www.shef.ac.uk/language/quantling/

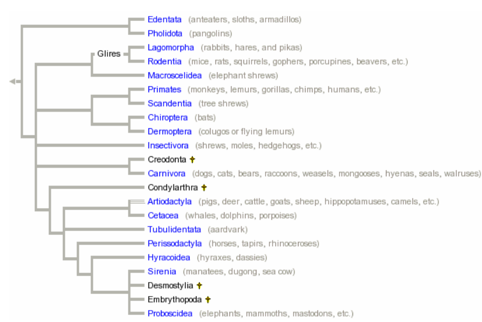
Language Phylogeny



Language Phylogeny



Tree of Life



From http://tolweb.org/

Finding a Phylogeny

- Speculate on history based on current evidence
  - Not guaranteed to be correct
- Find the "most likely" history
  - Parsimony: find the evolutionary tree that explains the observations with the fewest possible changes

Measuring Changes

- Natural Languages
  - Grammatical Rules
  - Lexicon
  - Hard to quantify how similar two languages are
- Species
  - Genomes (only recently)
  - Easy to quantify: genome differences are measurable

How Species Evolve

- Point Mutations (Substitution): one base is replaced with another

UV Ray

...CAT...

...CTT...

With only point mutations, easy to tell how close two genomes are, just count the different bases

How Species Evolve 2

- Insertions: one or more bases are inserted

  ...GCATG... ...GCA**CA**TG...

- Deletions: one or more bases are removed

  ...GCATCATG... ...GCATG...

Caused by copying errors (enzymes slipping, etc.)

Measuring Genome Similarity

- Insertions and Deletions this hard

```
ACATCATCATCAT

CATCATCATCATC
```

are more "similar" than

```
ACATCATCATCAT
 | |   |   |
TCGTTCGCGAAAA
```


Sequence Alignment

- Align sequences by inserting gaps:

```
ACATCATCATCAT
 ||||||||||||
-CATCATCATCAT
```

- Find best alignment inserting gaps given:
  - value of matching bases (point mutations) = c
  - cost of a gap (insertion/deletion) = g

We use $c = 10$, $g = 2$: goodness $= 12 * c - g = 118$

Brute Force Alignment

To find the best alignment of sequences *U* and *V* with correct value *c* and gap penalty *g*:

if *U* or *V* is empty

U, V is the best alignment

otherwise,

[next slide]

Brute Force Alignment: Otherwise…

Try three possibilities:

U[1:] means *U* with the first element removed

1. First elements of *U* and *V* are aligned: score of best alignments of *U*[1:] and *V*[1:] + *c* if *U*[0] == *V*[0]
2. First element of *U* is aligned with a gap in *V* score of best alignments of *U*[1:] and *V* + *g*
3. First element of *V* is aligned with a gap in *U* score of best alignments of *U* and *V*[1:] + *g*

Pick the choice with the highest score

Course Structure, Expectations, Goals

Staff

- Me: David Evans (Call me “Dave” or “Coach”)
  - Office Hours posted on course website
  - Always available by email, if I don’t reply in 24 hours, send again and complain
- Assistant Coaches: Erika Chin, David Faulkner, Erin Golub, Sam Guarnieri, Katherine Jogerst, and Pitchaya (“Yam”) Sitthi-Amorn
  - Will lead Monday and Tuesday sections
  - Available in Small Hall lab at posted times ***(only)***

Meetings

- Lectures: 2 per week
  - Will include material not in the book
  - Most lectures will use slides and notes
- Section meetings: 1 per week
  - You must sign up for one of the sections
  - Classroom work, group exercises, review, quizzes, …
- Staffed time in Small Hall
  - Take advantage of help from the ACs and your classmates

Problem Sets

- 8 total, 1-2½ weeks each
- Work on them when and where you want (but take advantage of staffed lab time in Small Hall)
- Usually will work with partners
- Mix of programming and analysis
- Main way most will learn
- Turn in on paper at beginning of class (first is due Wednesday)

My Teaching Philosophy: Drinking from a Firehose

It may hurt a little bit, and a lot of water will go by you, but you won't go away thirsty!

Expectations: Programming Background

- You understand basic programming:
  - Can write a program longer than a screenful
  - Can understand multi-file programs
  - Familiar with common control structures, procedures, recursive definitions
- You don't freak out when you are expected to learn a new language on your own

Expectations: Math and Logic Background

- You remember some things from CS202 (or will learn/re-learn them when you need them):
  - Arithmetic, logarithms, sets, graphs
  - Symbolic logic, implication
  - Proof techniques (induction, contradiction)
- The textbook is quite mathematical – you may need to read things more than once

Course Goals

Course Goal 1

Learn to write delightful programs.

correct, readable, elegant, economical, efficient, scalable, maintainable, secure, dependable

Course Goal 2

Be able to ***predict*** how decisions about data representation will impact properties of an implementation.

running time, memory use, ease of implementation, scalability, …

Course Goal 3

Understand how a program executes at levels of abstraction ranging from a high-level programming language to machine memory.

We will talk about what this means in Monday's class.

Is this a "good" solution?

if *U* or *V* is empty
  U, V is the best alignment
otherwise,
  Try three possibilities:
  1. First elements of *U* and *V* are aligned:
     score of best alignments of *U*[1:] and *V*[1:] + *c*   if *U*[0] == *V*[0]
  2. First element of *U* is aligned with a gap in *V*
     score of best alignments of *U*[1:] and *V* + *g*
  3. First element of *V* is aligned with a gap in *U*
     score of best alignments of *U* and *V*[1:] + *g*
  Pick the choice with the highest score

Algorithm Properties

- Implementable – can be readily expressed as a program
- Termination – always finishes
- Correctness – always gives the correct answer
- Efficient – uses resources wisely

Note: Chapter 2 of text has a similar list but separates "Implementable" into Effectiveness and Program Complexity

Is it Implementable?

```
def bestAlignment (U, V, c, g):
   if len(U) == 0 or len(V) == 0: return U, V
   else:
      (U0, V0) = bestAlignment (U[1:], V[1:], c, g)
      scoreNoGap = goodnessScore (U0, V0, c, g)
      if U[0] == V[0]: scoreNoGap += c

      # try inserting a gap in U (no match for V[0])
      (U1, V1) = bestAlignment (U, V[1:], c, g)
      scoreGapU = goodnessScore (U1, V1, c, g) - g
      # try inserting a gap in V (no match for U[0])
      (U2, V2) = bestAlignment (U[1:], V, c, g)
      scoreGapV = goodnessScore (U2, V2, c, g) - g
      …
```


Is it Implementable?

```
def bestAlignment (U, V, c, g):
   if len(U) == 0 or len(V) == 0: return U, V
   else:
      (U0, V0) = bestAlignment (U[1:], V[1:], c, g)
      scoreNoGap = goodnessScore (U0, V0, c, g)
      if U[0] == V[0]: scoreNoGap += c
      # try inserting a gap in U (no match for V[0])
      (U1, V1) = bestAlignment (U, V[1:], c, g)
      scoreGapU = goodnessScore (U1, V1, c, g) - g
      # try inserting a gap in V (no match for U[0])
      (U2, V2) = bestAlignment (U[1:], V, c, g)
      scoreGapV = goodnessScore (U2, V2, c, g) - g
      if scoreNoGap >= scoreGapU and scoreNoGap >= scoreGapV:
            return U[0] + U0, V[0] + V0
        elif scoreGapU >= scoreGapV:
            return GAP + U1, V[0] + V1
        else: return U[0] + U2, GAP + V2
```


Algorithm Properties

✓ Implementable – can be readily expressed as a program
- **Termination – always finishes**
- Correctness – always gives the correct answer
- Efficient – uses resources wisely

Termination?

if *U* or *V* is empty
  U, V is the best alignment
otherwise,
  Try three possibilities:
  1. First elements of *U* and *V* are aligned:
     score of best alignments of *U*[1:] and *V*[1:]
       + *c*   if *U*[0] == *V*[0]
  2. First element of *U* is aligned with a gap in *V*
     score of best alignments of *U*[1:] and *V* + *g*
  3. First element of *V* is aligned with a gap in *U*
     score of best alignments of *U* and *V*[1:] + *g*
  Pick the choice with the highest score

if *U* or *V* is empty
  U, V is the best alignment
otherwise,
  Try three possibilities:
  1. First elements of *U* and *V* are aligned:
     score of best alignments of ***U*[1:]** and ***V*[1:]**
       + *c*   if *U*[0] == *V*[0]
  2. First element of *U* is aligned with a gap in *V*
     score of best alignments of ***U*[1:]** and *V* + *g*
  3. First element of *V* is aligned with a gap in *U*
     score of best alignments of *U* and ***V*[1:]** + *g*
  Pick the choice with the highest score

Every attempt, at least one element is removed (and none added). Initial length is finite, so must terminate.

Algorithm Properties

✓Implementable – can be readily expressed as a program
✓Termination – always finishes
- Correctness – always gives the correct answer
  - Very informally: it tries all possibilities and picks the best one
- **Efficient** – uses resources wisely

Efficiency?

- What resources do we care about?
  - Programmer Time
  - **Running Time**
  - **Space Use**

Measuring Resource Use

- Space
  - Fundamental unit: bit
- Running Time
  - No fundamental unit
    - Number of steps?
    - How much can you do in one step?
    - How long does a step take?
- How does it scale with the size of the input

Answering for this algorithm is a PS1 question

Charge

- Registration Survey
  - Linked from course web site
  - Submit by Friday 5pm
- Text: Read chapters 1-3
- PS1: Out now, due in 1 week
  - Start now – the section time is not for doing PSs
- Monday: Levels of Abstraction, Order Notation