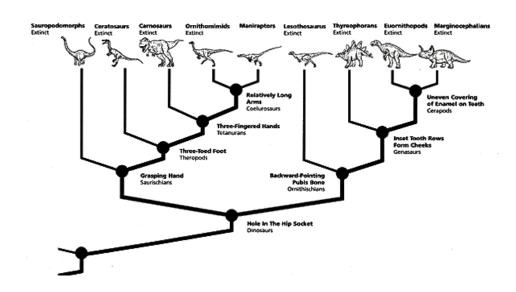
Introduction to Phylogeny

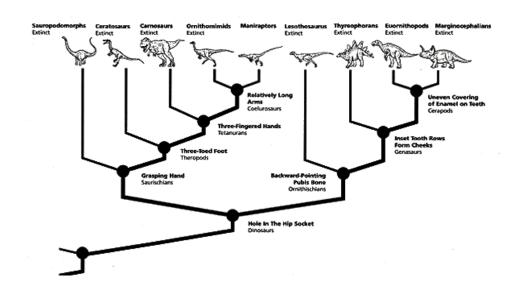
Lecture Notes for 9 October 2003
CMP 464/788: Introduction to Computational Biology
Prof. St. John
Lehman College
City University of New York

Goal: Reconstruct the Evolutionary History



(www.amnh.org/education/teacherguides/dinosaurs)

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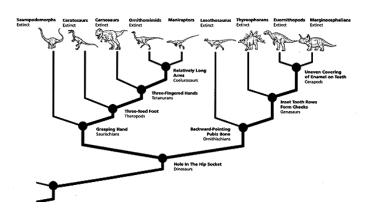
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The evolutionary process not only determines relationships among taxa, but allows prediction of structural, physiological, and biochemical properties.

Process for Reconstruction: Input Data

Start with information about the taxa. For example:

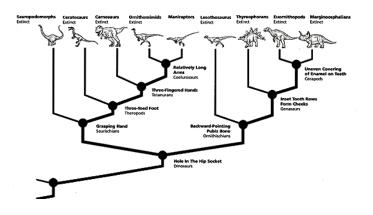
Morphological Characters



Process for Reconstruction: Input Data

Start with information about the taxa. For example:

Morphological Characters



Biomolecular Sequences

- A GTTAGAAGGCGGCCAGCGAC...
- B CATTTGTCCTAACTTGACGG...
- C CAAGAGGCCACTGCAGAATC...
- D CCGACTTCCAACCTCATGCG...
- E ATGGGGCACGATGGATATCG...
- F TACAAATACGCGCAAGTTCG...

Input Data

- A GTTAGAAGGC...
- B CATTTGTCCT...
- C CAAGAGGCCA...
- D CCGACTTCCA...
- E ATGGGGCACG...
- F TACAAATACG...

Input Data

Reconstruction Algorithms

```
A GTTAGAAGGC...

B CATTTGTCCT...

C CAAGAGGCCA...

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E ATGGGGCACG...

F TACAAATACG...
```

Maximum Parsimony Maximum Likelihood Distance Methods: NJ, Quartet-Based, Fast Convering, :

Input Data

Reconstruction Algorithms

Output Tree

A GTTAGAAGGC...

B CATTTGTCCT...

C CAAGAGGCCA...

D CCGACTTCCA...

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- drug discovery: used to determine structural and biochemical properties of potential drugs
- determining origins of HIV infection
- origin of other virus and bacteria strains

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 - This is not feasible for more than 20 taxa.

Approximation Algorithms

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Approximation Algorithms

- Since calculating the exact answer is hard, algorithms that estimate the answer have been developed.
 - Heuristics for maximum parsimony and maximum likelihood estimation
 (use clever ways to limit the number of trees checked, while still sampling much of "tree-space")
 - Polynomial-time methods, based on the distance between taxa

• These methods calculate the distance between taxa:

	В	D	А	С	F	E
В	0	0.496505	0.496505	0.444519	0.375798	0.268166
D	0.496505	0	0.496505	0.375798	0.275673	0.279728
A	0.496505	0.496505	0	0.362124	0.323812	0.496505
C	0.444519	0.375798	0.362124	0	0.496505	0.496505
F	0.375798	0.275673	0.323812	0.496505	0	0.496505
E	0.268166	0.279728	0.496505	0.496505	0.496505	0

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 One way to calculate distance is to take differences divided by the length (the normalized Hamming distance).

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- Many of these methods have good performance empirically, and some can be proven to have nice accuracy properties.

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- In biological applications, the true, historical tree is almost never known, which makes assessing the quality of phylogenetic reconstruction methods problematic. (an exception: Hillis '92 created an evolutionary tree in the laboratory)
- Simulation is used instead to evaluate methods, given a model of evolution.

1. Construct a

"model" tree.

Construct a
 "Evolve"
 sequences down the tree.

- A GTTAGAAGGCGGCCA...
- B CATTTGTCCTAACTT...
- C CAAGAGGCCACTGCA...
- D CCGACTTCCAACCTC...
- E ATGGGGCACGATGGA...
- F TACAAATACGCGCAA...

 Construct a "model" tree.

2. "Evolve" sequences down the tree.

3. Reconstruct the tree using method.

- A GTTAGAAGGCGGCCA...
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4. Evaluate the accuracy of the constructed tree.