Scalable Visual Comparison of Biological Trees and Sequences

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Outline

Stirring up controversy

Comparing big phylogenetic trees

- TreeJuxtaposer
  - phylogeny background
  - structural difference computation
  - guaranteed visibility

Browsing huge trees

- TJC, TJC-Q

Comparing many large gene sequences

- SequenceJuxtaposer

Collaborators

TreeJuxtaposer joint work with

- Francois Guimbretiere, Maryland
- Serdar Tasiran, Compaq SRC
- Li Zhang, Compaq SRC
- Yunhong Zhou, Compaq SRC
- James Slack, UBC

TJC, TJC-Q joint work with

- Dale Beerman, Virginia
- Greg Humphreys, Virginia

SequenceJuxtaposer joint work with

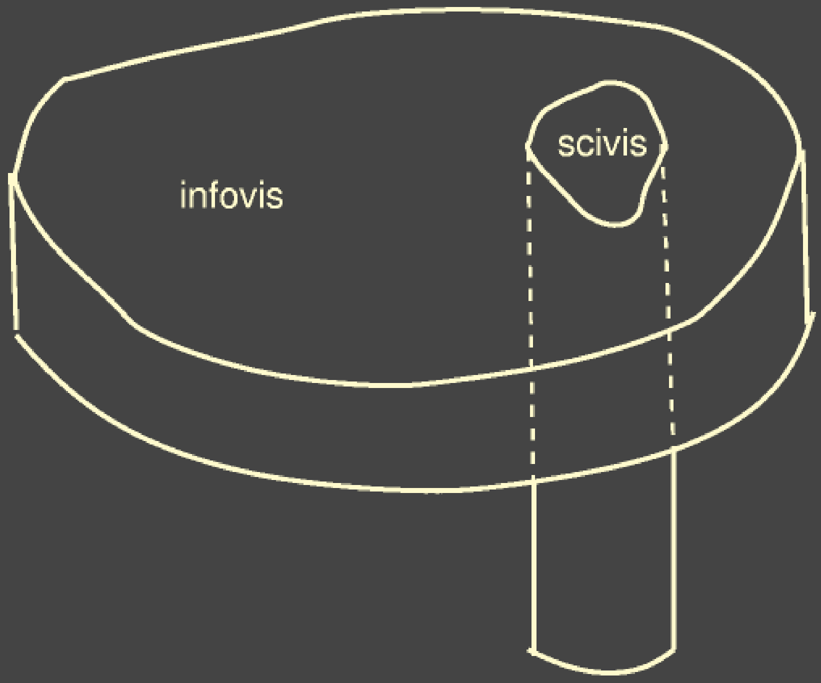
- James Slack, UBC
- Kristian Hildebrand, UBC
- Katherine St. John, CUNY/Lehman

Funding: NSF/DEB-0121682

Stirring up controversy

definitions and scope, infovis vs. scivis:

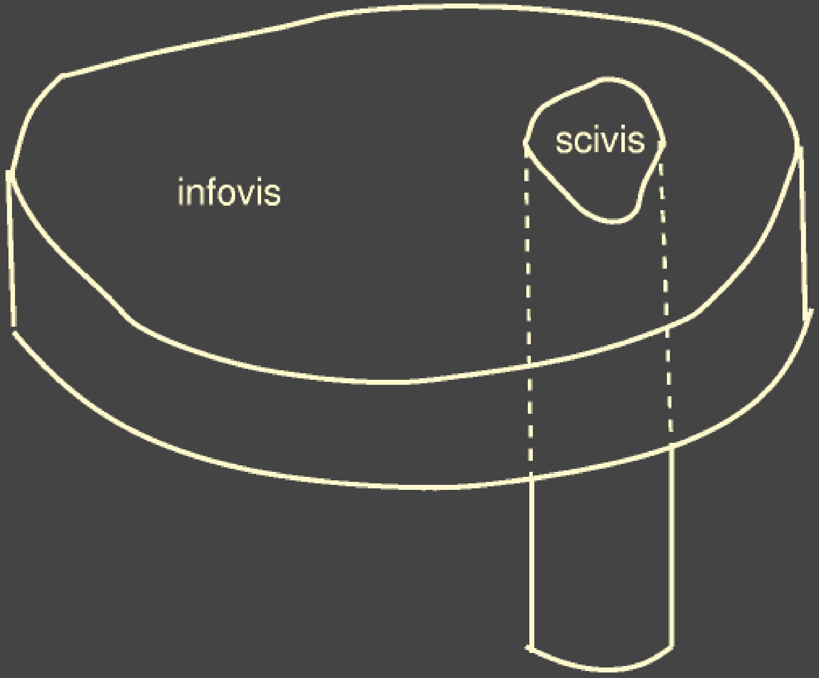
- spatialization chosen not given



Stirring up controversy

definitions and scope, infovis vs. scivis:

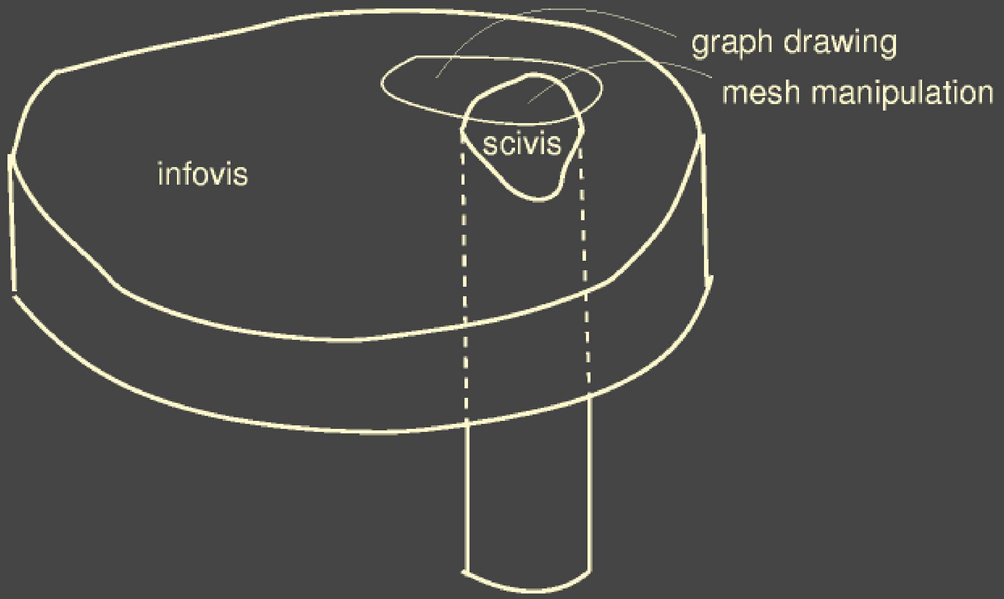
- spatialization chosen not given
- big parameter space, justify design decisions
- wider scope, mostly more shallowly explored



Stirring up controversy

definitions and scope, infovis vs. scivis:

- spatialization chosen not given
- big parameter space, justify design decisions
- wider scope, mostly more shallowly explored
- many algorithms and techniques span the border



Navigation

intimate relationship with spatial layout choices

- constrained
- nonliteral

Focus+Context

- overview and detail integrated into single view
- show features in context
- help users maintain their orientation

distortion-based navigation

- preserve topological order
- nonlinearly compress/expand geometry

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Tree comparison

active area: hierarchy browsing

- previous work: browsing
- comparison still open problem

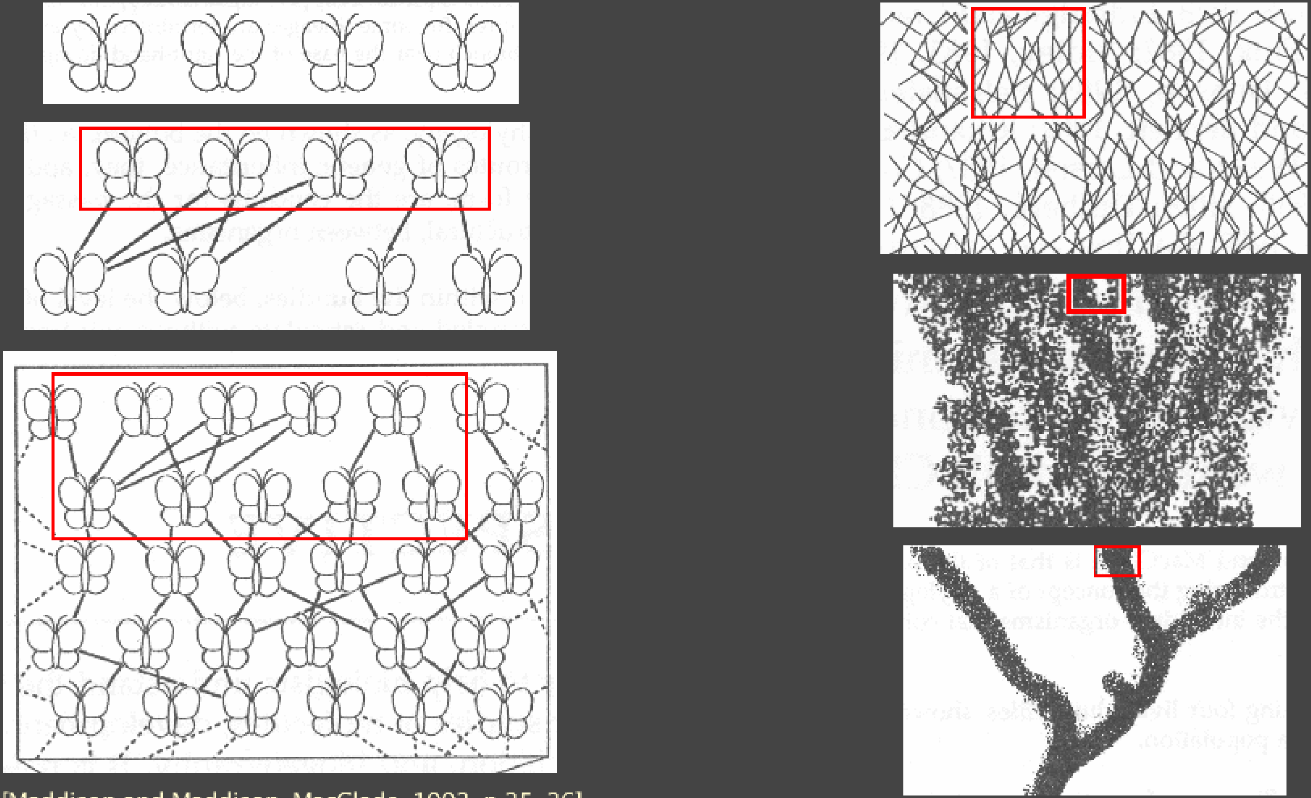
bioinformatics applicationn

- phylogenetic trees reconstructed from DNA

Phylogeny background

tree describing evolutionary relationships

- leaves (taxa): species, genes, disease strains

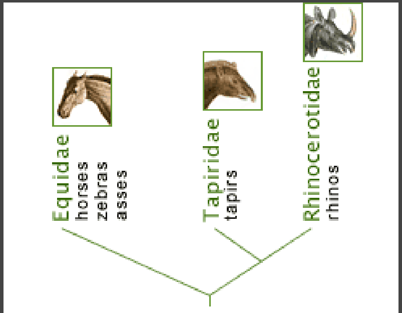


[Maddison and Maddison, MacClade, 1992, p 25-26]

Phylogenetic reconstruction

know leaves, infer interior nodes

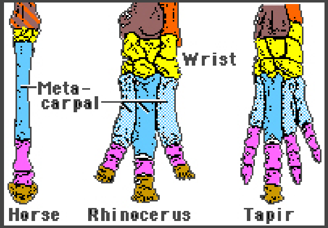
- similarity:
  parallel evolution or common ancestor?
- siblings unordered



[research.amnh.org/programs/genomelab]

old: morphology

- observable similarities



[gwis2.circ.gwu.edu/~atkins]

new: molecular

- DNA sequences – nucleotides
- protein sequences – amino acids

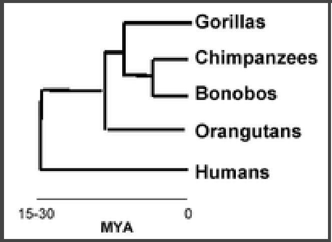
```
horse: ...CCTGAACCG...
tapir: ...ACTCTACCG...
rhino: ...GCTCTACCG...
```

Phylogeny uses

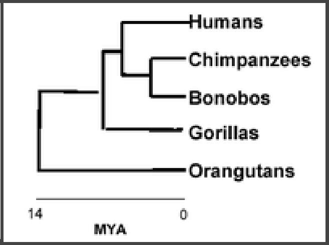
establish relationships

- understand species evolution

old: morphology



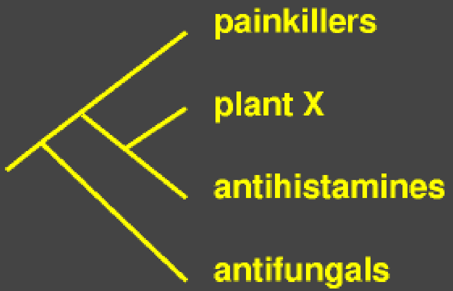
new: molecular



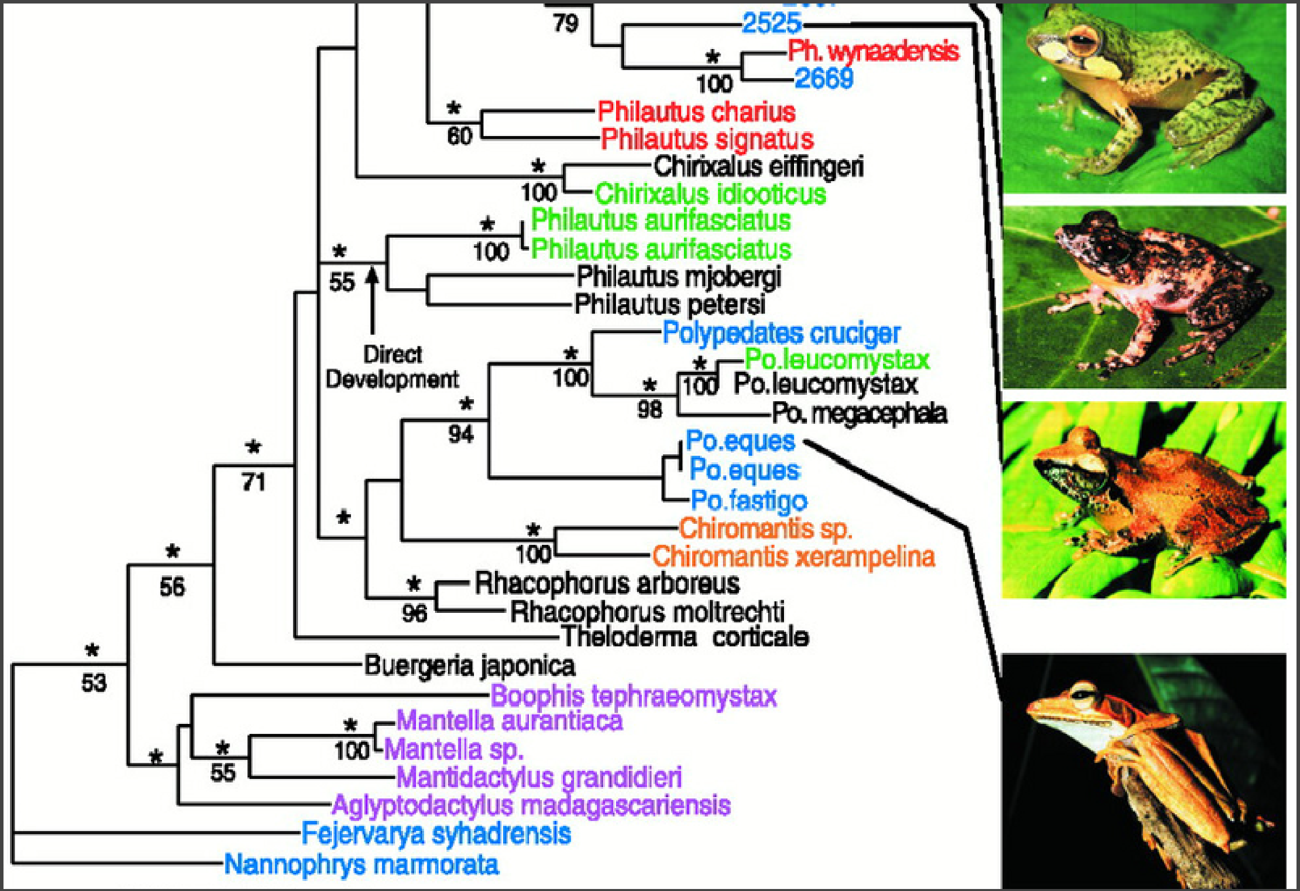
- track diseases
  genes evolve 1M x faster

predict characteristics

- design drugs
- reveal gene function

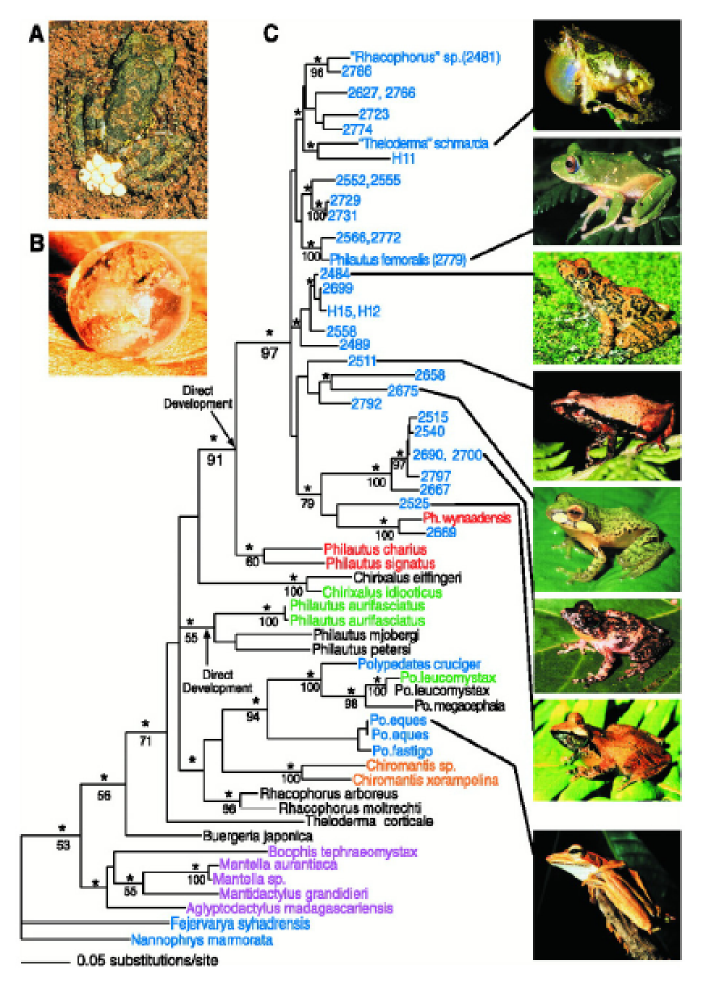


Phylogenetic/Evolutionary tree



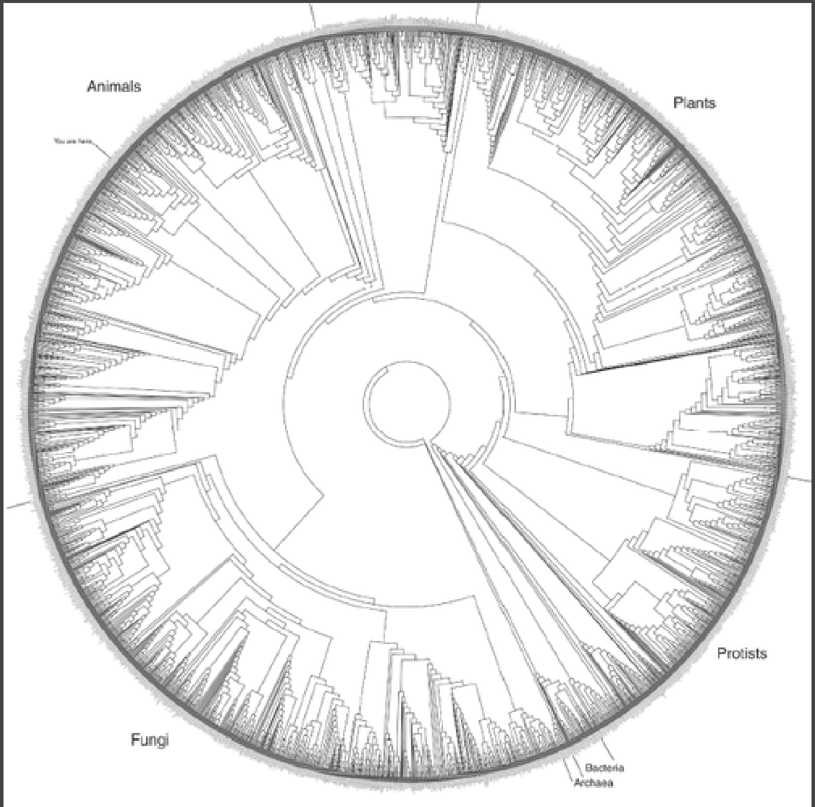
[M Meegaskumbura et al., Science, 298:379 (2002)]

Common tree size now



[M.Meegaskumbura et al., Science, 298:379 (2002)]

Tree of Life: 10M species

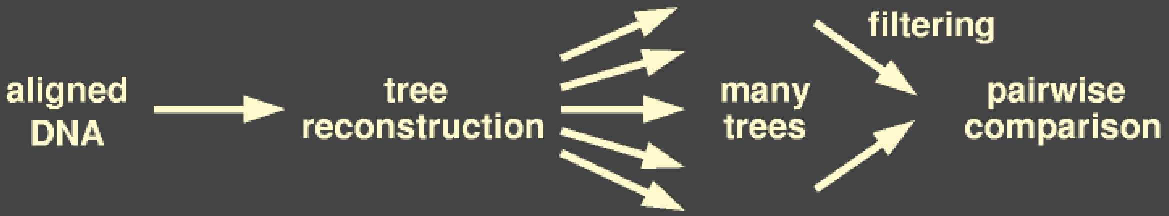


[David Hillis, Science, 300:1687, 2003]

Phylogenetic reconstruction

multiple trees

- reconstruction algorithm returns many possibilities
- different biological assumptions or data



aligned DNA

tree reconstruction

many trees

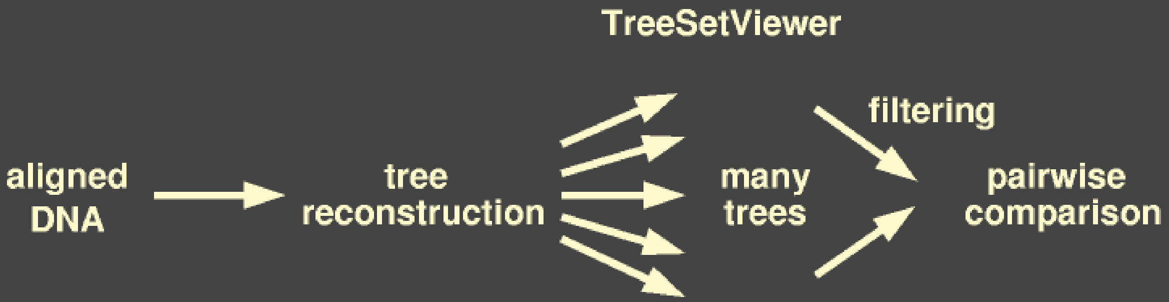
filtering

pairwise comparison

Phylogenetic reconstruction

multiple trees

- reconstruction algorithm returns many possibilities
- different biological assumptions or data



TreeSetViewer

aligned DNA

tree reconstruction

many trees

filtering

pairwise comparison

visually filtering large sets of trees

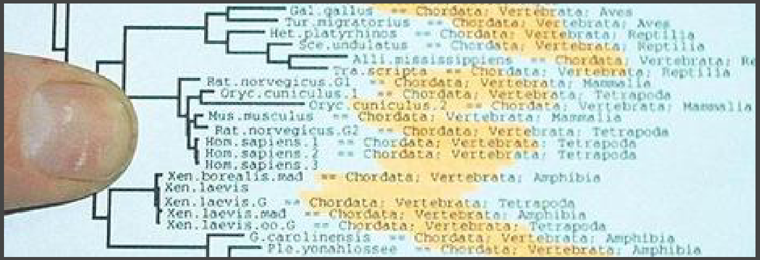
- TreeSet Viewer, MDS approach
  [Amenta and Klingner, InfoVis 2002]

visual pairwise comparison

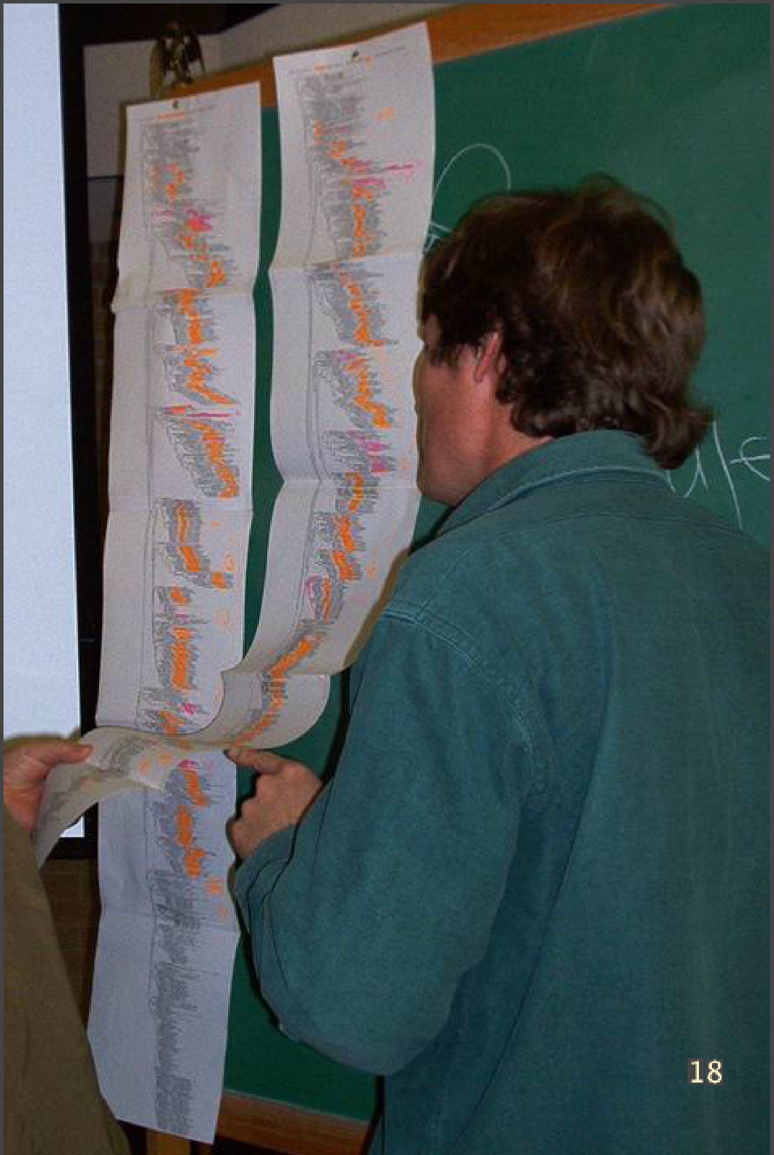
- open problem

Paper comparison

focus


Gal.gallus == Chordata; Vertebrata; Aves
Tur.migratorius == Chordata; Vertebrata; Aves
Het.platyrhinos == Chordata; Vertebrata; Reptilia
Sce.undulatus == Chordata; Vertebrata; Reptilia
Alli.mississippiens == Chordata; Vertebrata; Re
Tra.scripta == Chordata; Vertebrata; Reptilia
Rat.norvegicus.G1 == Chordata; Vertebrata; Mammalia
Oryc.cuniculus.1 == Chordata; Vertebrata; Tetrapoda
Oryc.cuniculus.2 == Chordata; Vertebrata; Mammalia
Mus.musculus == Chordata; Vertebrata; Mammalia
Rat.norvegicus.G2 == Chordata; Vertebrata; Tetrapoda
Hom.sapiens.1 == Chordata; Vertebrata; Tetrapoda
Hom.sapiens.2 == Chordata; Vertebrata; Tetrapoda
Hom.sapiens.3
Xen.borealis.mad == Chordata; Vertebrata; Amphibia
Xen.laevis
Xen.laevis.G == Chordata; Vertebrata; Tetrapoda
Xen.laevis.mad == Chordata; Vertebrata; Amphibia
Xen.laevis.oo.G == Chordata; Vertebrata; Tetrapoda
G.carolinensis == Chordata; Vertebrata; Amphibia
Ple.yonahlossee == Chordata; Vertebrata; Amphibia

context



Will Fischer, UT-Austin, May 2003

TreeJuxtaposer video

platforms shown

- java 1.4, GL4Java 2.7 bindings for OpenGL

Windows

- 2.4 GHz P3, nVidia Quadro4 700XGL
- 1.1GB java heap
- window sizes 1280x1024, 3800x2400

Linux

- 3.1 GHz P4, nVidia GeForce FX 5800 Ultra
- 1.7GB java heap
- window size 800x600

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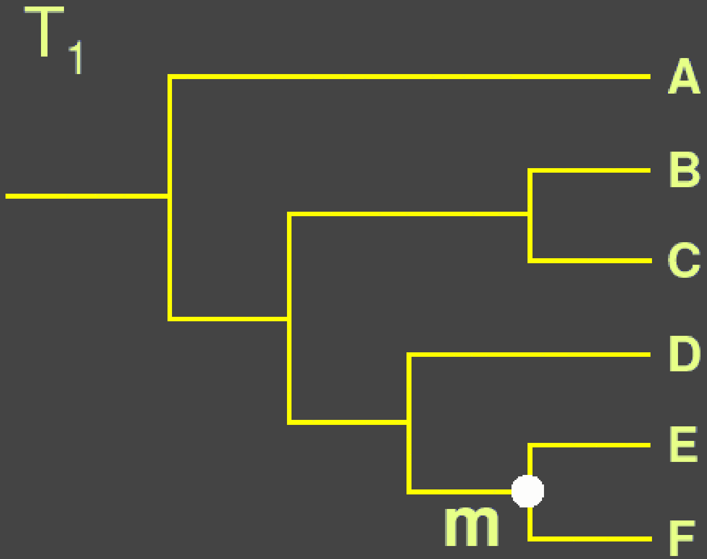
- SequenceJuxtaposer

Previous work

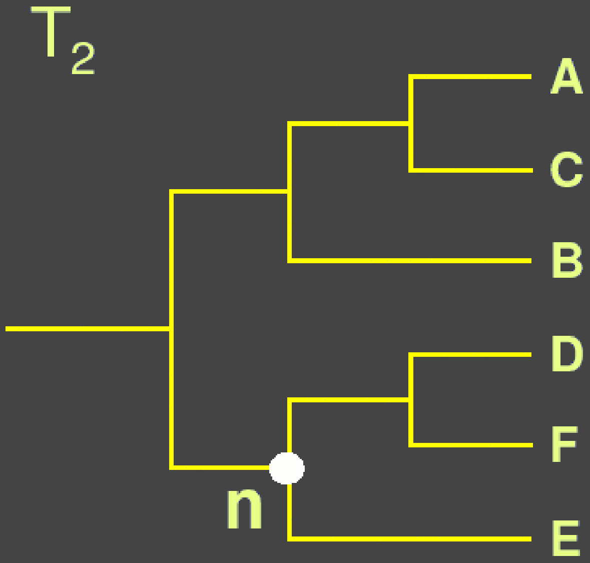
tree comparison

- RF distance [Robinson and Foulds 81]
- perfect node matching [Day 85]
- creation/deletion [Chi and Card 99]
- leaves only [Graham and Kennedy 01]

Similarity score



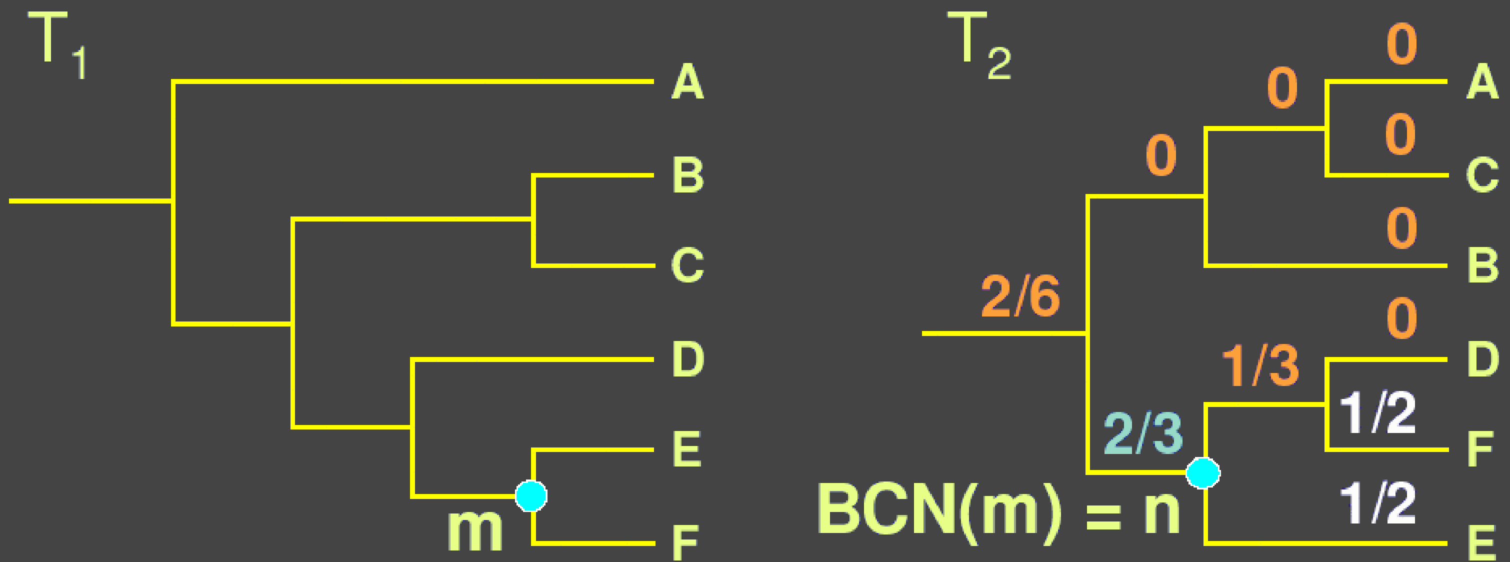
$L(\mathrm{m}) = \{\mathrm{E,F}\}$



$L(\mathrm{n}) = \{\mathrm{D,E,F}\}$

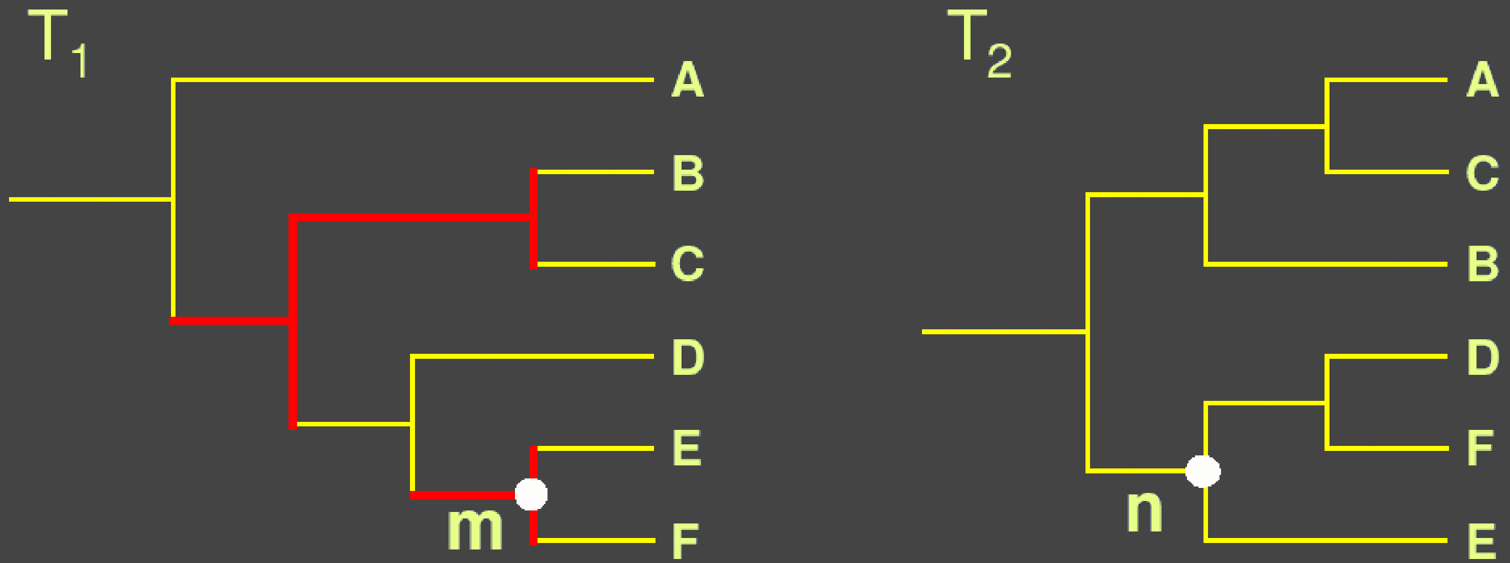
$$S(\mathrm{m,n}) = \frac{|L(\mathrm{m}) \cap L(\mathrm{n})|}{|L(\mathrm{m}) \cup L(\mathrm{n})|} = \frac{|\{\mathrm{E,F}\}|}{|\{\mathrm{D,E,F}\}|} = \frac{2}{3}$$

Best corresponding node



- $\text{BCN}(m) = \text{argmax}_{v \in T_2}(S(m, v))$
  - computable in O(n $\log^2$ n)
  - linked highlighting

Marking structural differences



- Nodes for which $S(v, \mathrm{BCN}(v)) \neq 1$

Structural difference algorithm

powerful and totally automatic

matches intuition

- UT-Austin biology lab
- other biologists
- other domains

leads users to important locations

efficient algorithms: 7s for 2 x 140K nodes

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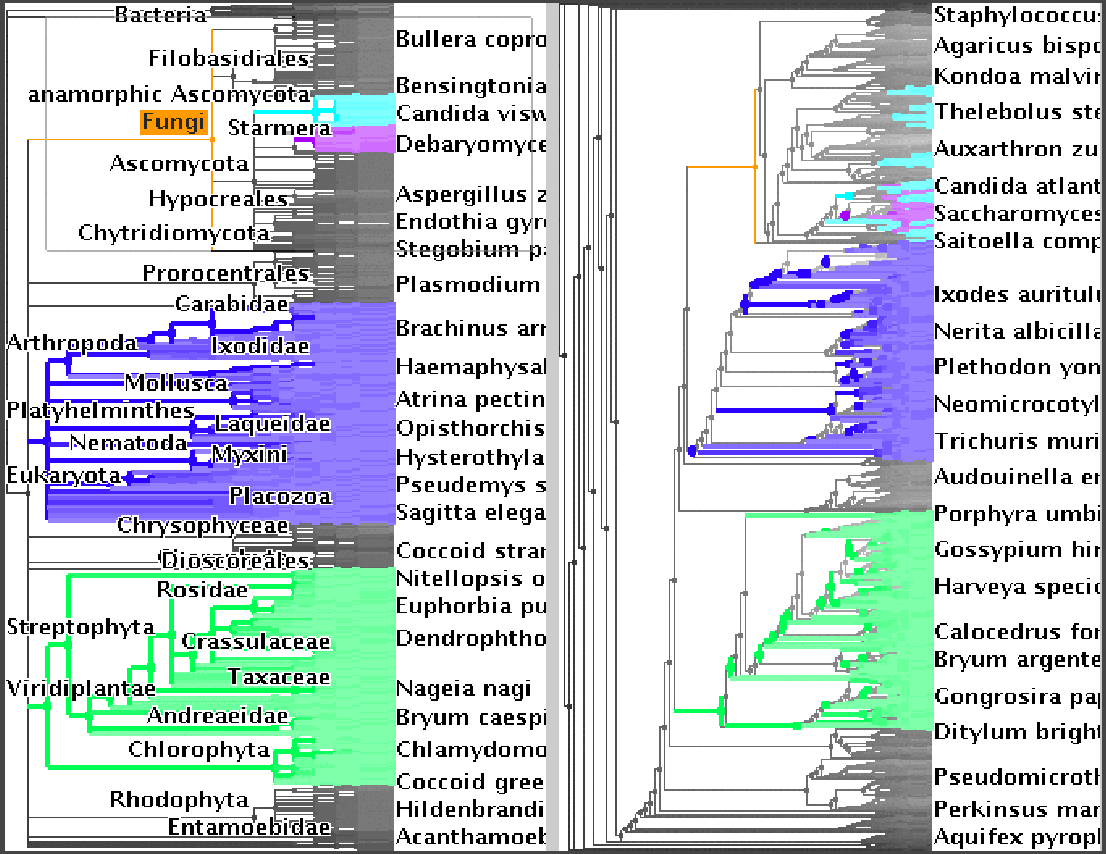
Guaranteed mark visibility



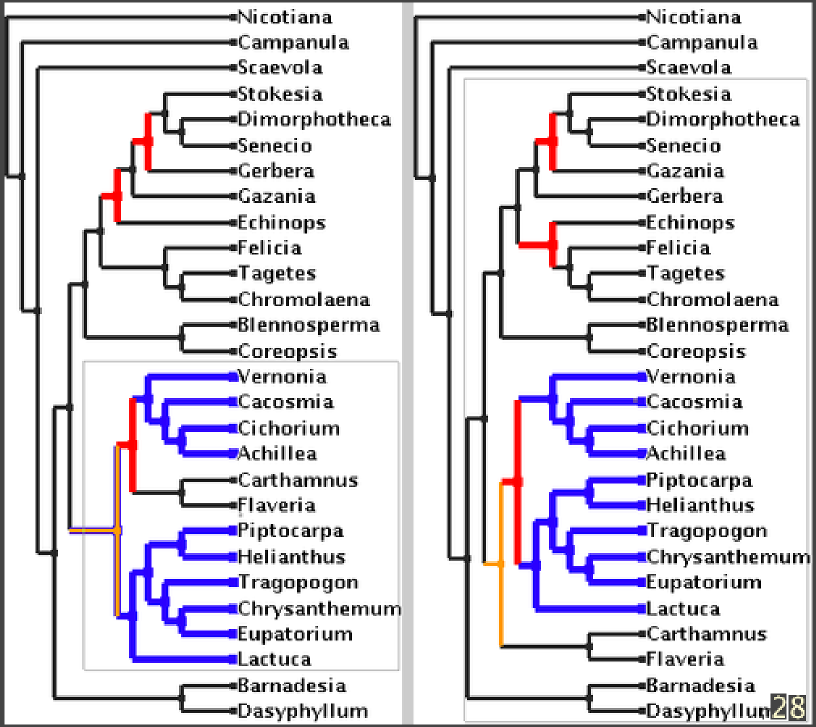
Marks (Features)

regions of interest shown with color highlight

- structural difference
- search results
- user-specified

purpose

- guide navigation
- provide landmarks
- contiguity check for subtrees



How can a mark disappear?

moving outside viewport

- choose global Focus+Context navigation
  - "tacked-down" borders

Focus+Context previous work

combine overview and detail into single view

Focus+Context

- large tree browsing
    - Cone Trees [Robertson et al 91]
    - Hyperbolic Trees [Lamping et al 95, Munzner 97]
    - Space Tree [Plaisant et al 03]
    - DOI Tree [Card and Nation 02]
- global
    - Document Lens [Robertson and Mackinlay 93]
    - Rubber Sheets [Sarker et al 93]

our contribution

- scalability, guaranteed visibility

How can a mark disappear?

moving outside viewport

- choose global Focus+Context navigation
  - "tacked-down" borders

occlusion

- choose 2D++ layout

culling at subpixel sizes

- develop efficient check for marks when culling
- cost depending on visible, not total, node count

Mark checking when culling

does region of space enclose mark on this tree?

- precompute range beneath subtree
- correllate objects to spatial extent with quadtree

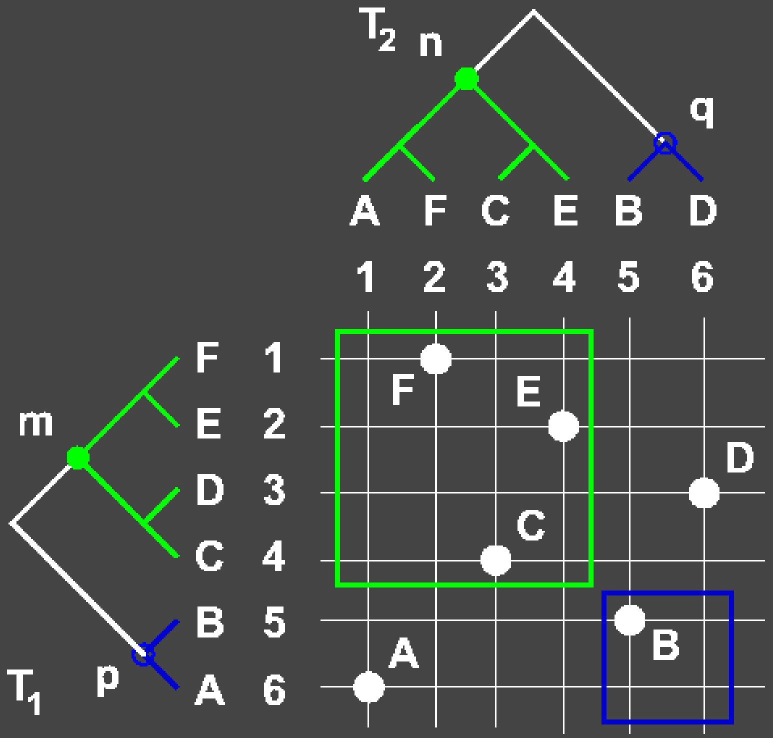
does region of space enclose linked mark from other tree?

- up to O(n) to look up best match for each node
- solution: intersect node ranges between trees
  - reduces to point in polygon test
  - O(n log n) preprocess, O(log^2 n) lookup

Intersecting ranges between trees

point in polygon

- tuple of indices in N-dim range



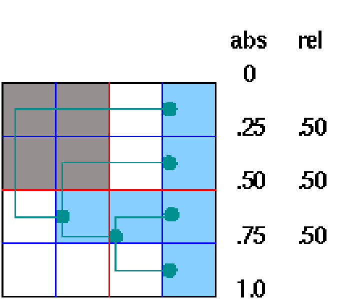
Focus+Context quadtrees

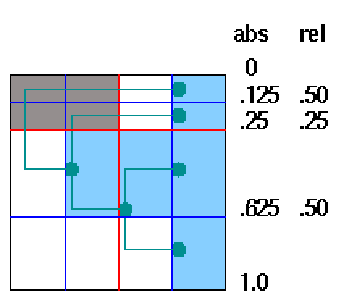
quadtree cells also "painted on rubber sheet"

- geometry at fixed offset from cell boundary
- opposite of kinetic data structures
- must update boundary position when stretch/shrink

hierarchical position encoding

- absolute location for boundary
  lookup: O(1), update: O(n)
- relative distance between parent cell boundaries
  lookup: O(log n), update: O(log n)





Guaranteed visibility

infrastructure needed for efficient computation

relief from exhaustive exploration

- missed marks lead to false conclusions
- hard to determine completion
- tedious, error-prone

compelling reason for Focus+Context

- controversy: does distortion help or hurt?
- strong rationale for comparison

TreeJuxtaposer contributions

first interactive tree comparison system

- automatic structural difference computation
- guaranteed visibility of landmark areas

scalable to large datasets

- 250,000 to 500,000 total nodes
- all preprecessing subquadratic
- all realtime rendering sublinear

techniques broadly applicable

- not limited to biological trees

overall winner: InfoVis Contest 2003

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Scaling up

TreeJuxtaposer limits

- memory footprint
- rendering CPU bound, want graphics bound

goal: browse huge trees

- concentrate on browsing

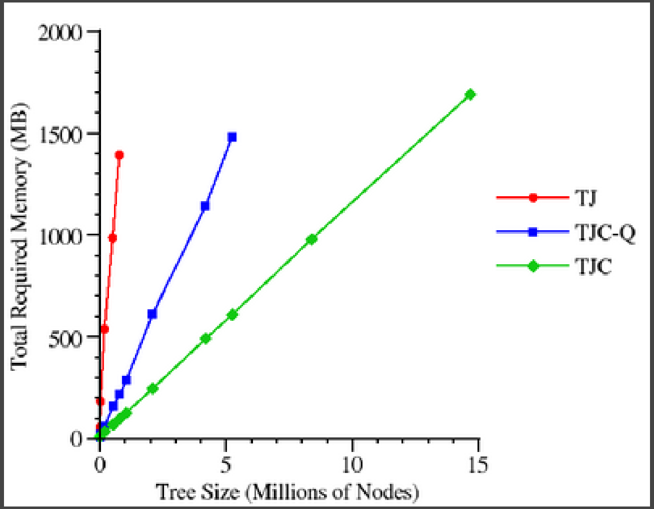
TJC-Q: 5M nodes

- commodity platforms

TJC: 15M nodes

- leading-edge graphics hardware

Memory footprint reduction



TJ Focus+Context quadtrees

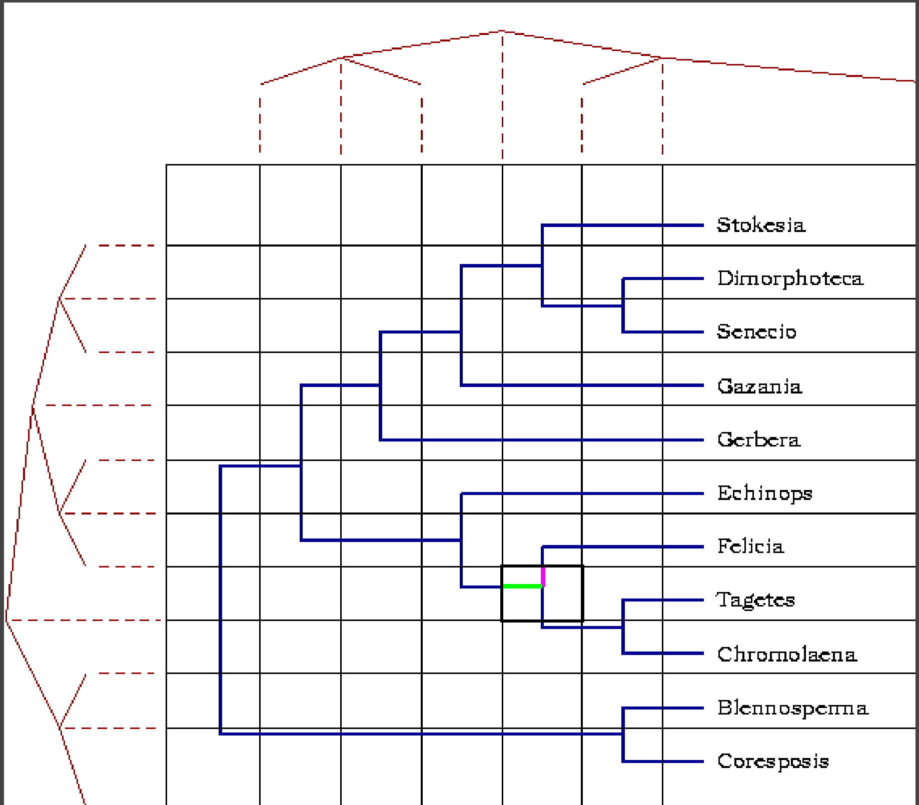
- navigating, culling, drawing, picking

new data structures and algorithms instead

Quadtree: navigating

navigating with stretch/shrink

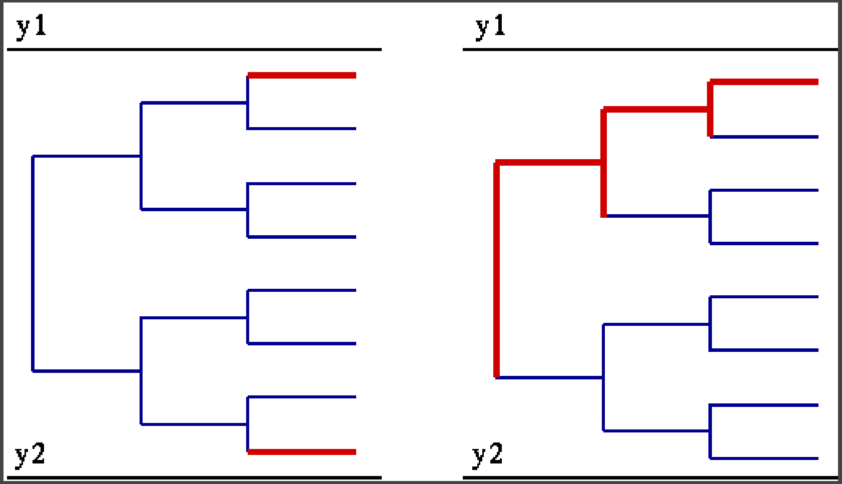
- TJ: quadtree
- new: lightweight grid data structure



Quadtree: culling and drawing

culling subpixel objects

- TJ: quadtree cell size test
- new: leaf overlap test



drawing

- TJ: progressive in order of importance
- new: from root

  new alg fast enough to ignore order

Quadtree: picking

TJ: picking with spatial subdivision

TJC: multiple render target buffer

- encode object ID into offscreen buffer
- supported in hardware on latest ATI cards

TJC-Q: low-memory quadtrees

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Accordion drawing

not just for trees!

general scalable visualization infrastructure

- "rubber sheet" navigation
- guaranteed visibility of marked areas

implementation: modular package

- layer below TreeJuxtaposer

SequenceJuxtaposer

accordion drawing for DNA/RNA

previous work: web-based sequence browsers

- Ensembl, UCSC Genome Browser, NCBI MapViewer
- heavily used, huge server-side databases

- zoom or pan in jumps
- can't see context

fluid Focus+Context navigation

guaranteed visibility

- establish when these features useful
- proof of concept prototype, eventually merge

SJ in action

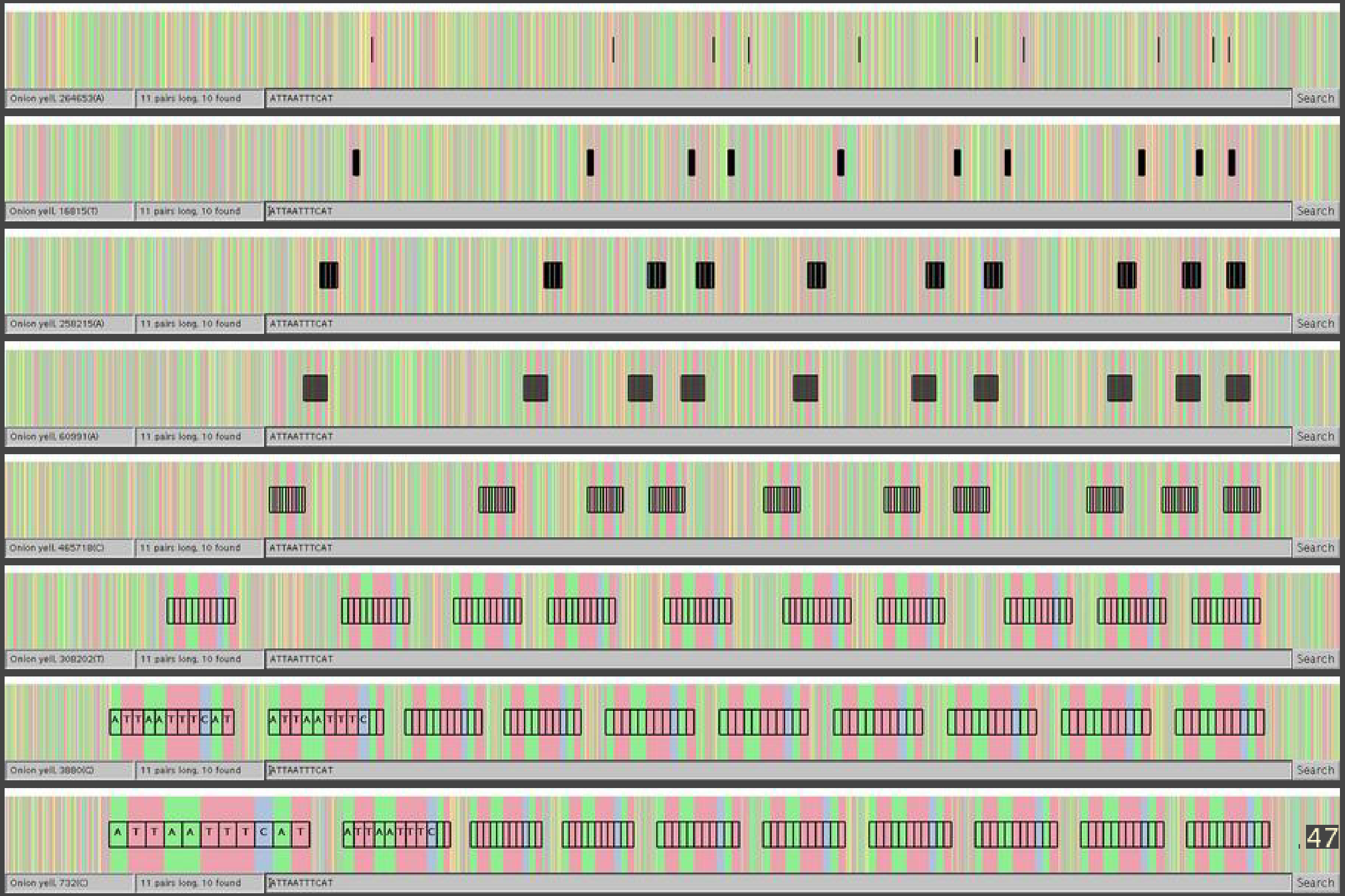
shown on publicly available data

- onion yellows phytoplasma: whole genome
  860 Kbp
- Murphy: 22 genes
  44 mammals x 17000 bp each = 748 Kbp
- Treezilla: single gene
  500 plants x 1428 bp each = 714 Kbp

scales to 1.7 Mbp with 1.7GB heap

[videos]

Expanding search results



Onion yell. 264653(A) | 11 pairs long, 10 found | ATTAATTTCAT

Onion yell. 16815(T) | 11 pairs long, 10 found | ATTAATTTCAT

Onion yell. 258215(A) | 11 pairs long, 10 found | ATTAATTTCAT

Onion yell. 60991(A) | 11 pairs long, 10 found | ATTAATTTCAT

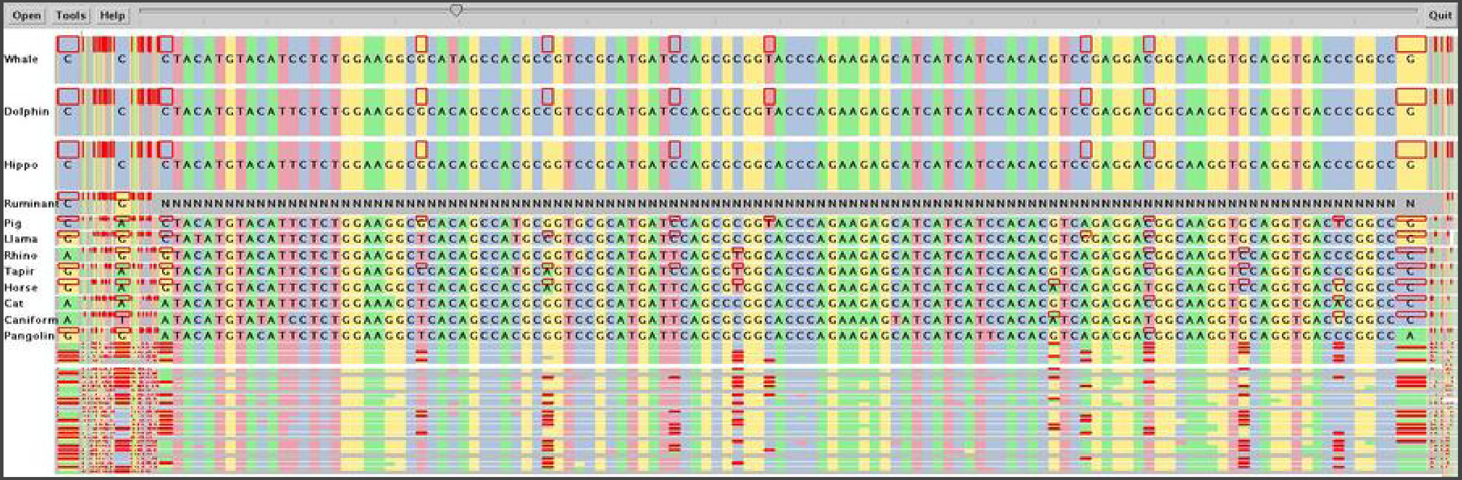
Onion yell. 465718(C) | 11 pairs long, 10 found | ATTAATTTCAT

Onion yell. 308202(T) | 11 pairs long, 10 found | ATTAATTTCAT

Onion yell. 3880(C) | 11 pairs long, 10 found | ATTAATTTCAT

Onion yell. 732(C) | 11 pairs long, 10 found | ATTAATTTCAT

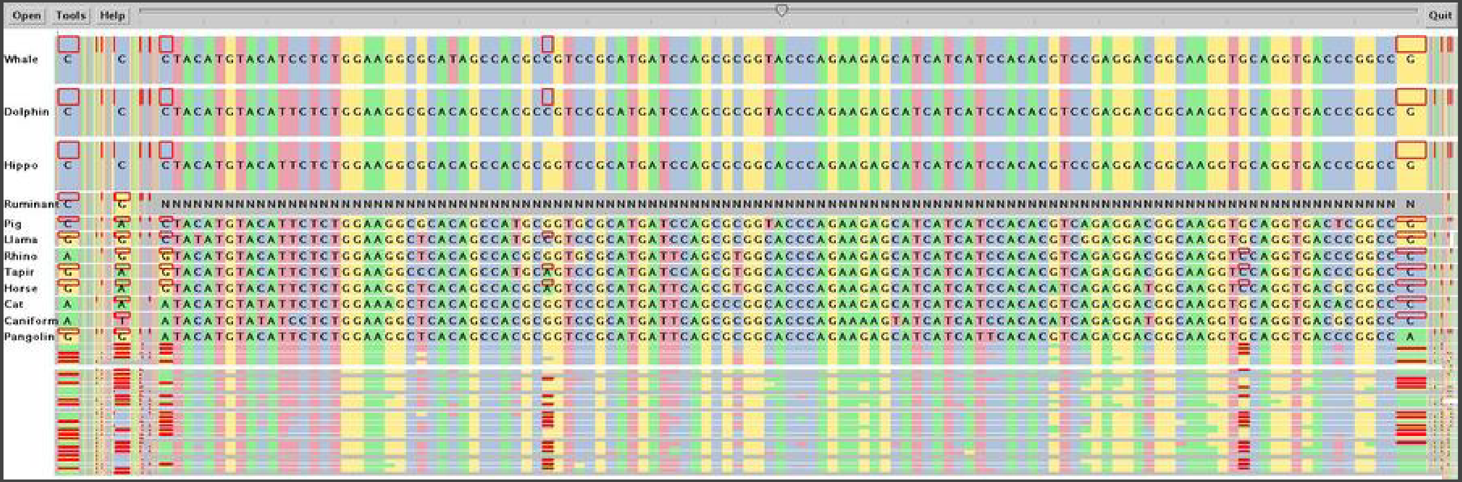
Changing difference thresholds



25%

inspecting 1 of 22 genes

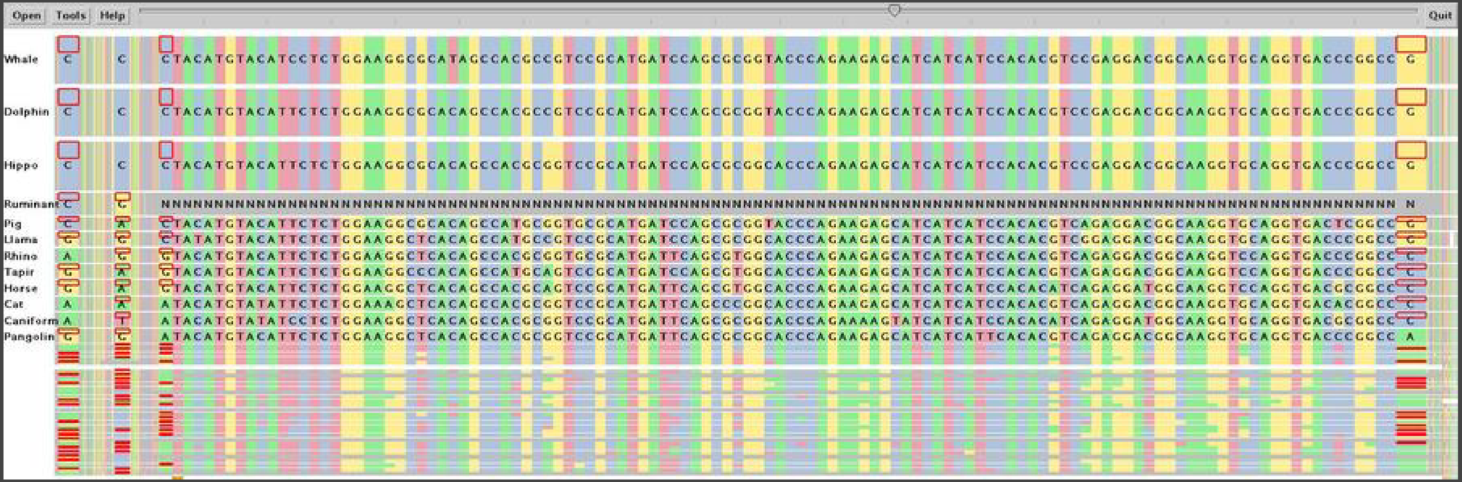
Changing difference thresholds



```
Whale     C   C   CTACATGTACATCCTCTGGAAGGCGCATAGCCACGCCGTCCGCATGATCCAGCGCGGTACCCAGAAGAGCATCATCATCCACACGTCCGAGGACGGCAAGGTGCAGGTGACCCGGCC G
Dolphin   C   C   CTACATGTACATTCTCTGGAAGGCGCACAGCCACGCCGTCCGCATGATCCAGCGCGGTACCCAGAAGAGCATCATCATCCACACGTCCGAGGACGGCAAGGTGCAGGTGACCCGGCC G
Hippo     C   C   CTACATGTACATTCTCTGGAAGGCGCACAGCCACGCGGTCCGCATGATCCAGCGCGGCACCCAGAAGAGCATCATCATCCACACGTCCGAGGACGGCAAGGTGCAGGTGACCCGGCC G
Ruminant  C   G   NNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNN N
Pig       C   A   CTACATGTACATTCTCTGGAAGGCGCACAGCCATGCGGTGCGCATGATCCAGCGCGGTACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTGCAGGTGACTCGGCC G
Llama     G   G   CTATATGTACATTCTCTGGAAGGCTCACAGCCATGCCGTCCGCATGATCCAGCGCGGCACCCAGAAGAGCATCATCATCCACACGTCGGAGGACGGCAAGGTGCAGGTGACCCGGCC G
Rhino     A   G   GTACATGTACATTCTCTGGAAGGCTCACAGCCACGCGGTGCGCATGATTCAGCGTGGCACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTCCAGGTGACCCGGCC C
Tapir     G   A   GTACATGTACATTCTCTGGAAGGCCCACAGCCATGCAGTCCGCATGATCCAGCGTGGCACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTCCAGGTGACCCGGCC C
Horse     G   A   GTACATGTACATTCTCTGGAAGGCTCACAGCCACGCAGTCCGCATGATTCAGCGTGGCACCCAGAAGAGCATCATCATCCACACATCAGAGGATGGCAAGGTCCAGGTGACGCGGCC C
Cat       A   A   ATACATGTATATTCTCTGGAAAGCTCACAGCCACGCGGTCCGCATGATTCAGCCCGGCACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTGCAGGTGACACGGCC C
Caniform  A   T   ATACATGTATATCCTCTGGAAGGCTCACAGCCACGCGGTCCGCATGATTCAGCGCGGCACCCAGAAAAGTATCATCATCCACACATCAGAGGATGGCAAGGTGCAGGTGACGCGGCC C
Pangolin  G   G   ATACATGTACATTCTCTGGAAGGCTCACAGCCACGCGGTCCGCATGATTCAGCGCGGCACCCAGAAGAGCATCATCATTCACACGTCAGAGGACGGCAAGGTGCAGGTGACCCGGCC A
```

50%

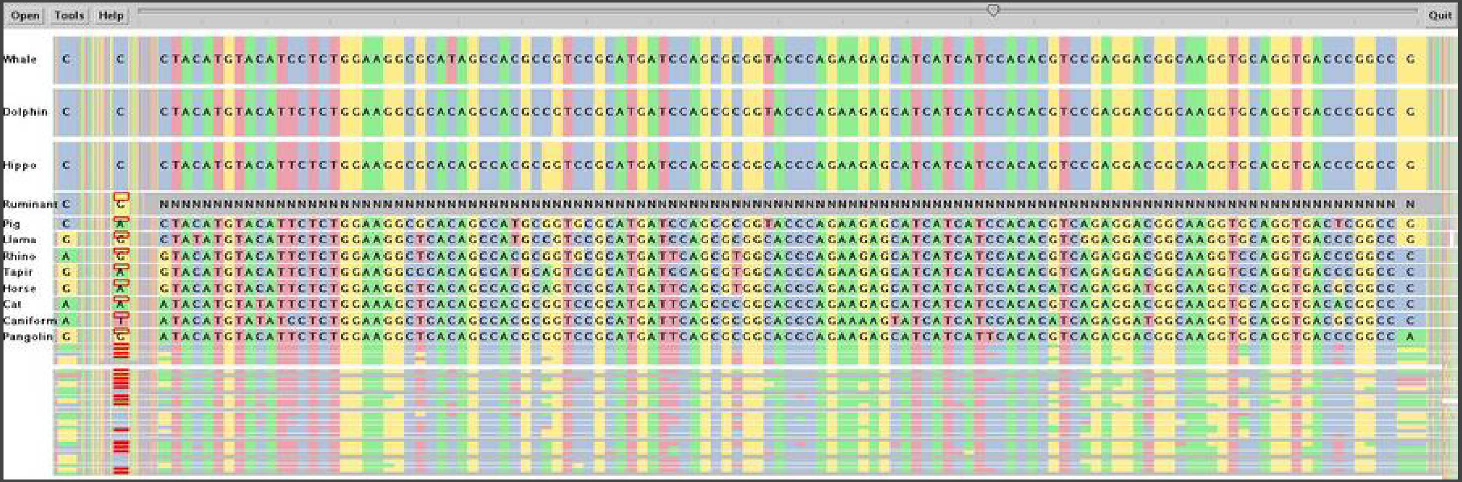
Changing difference thresholds



```
Whale     C  C  CTACATGTACATCCTCTGGAAGGCGCATAGCCACGCCGTCCGCATGATCCAGCGCGGTACCCAGAAGAGCATCATCATCCACACGTCCGAGGACGGCAAGGTGCAGGTGACCCGGCC  G
Dolphin   C  C  CTACATGTACATTCTCTGGAAGGCGCACAGCCACGCCGTCCGCATGATCCAGCGCGGTACCCAGAAGAGCATCATCATCCACACGTCCGAGGACGGCAAGGTGCAGGTGACCCGGCC  G
Hippo     C  C  CTACATGTACATTCTCTGGAAGGCGCACAGCCACGCGGTCCGCATGATCCAGCGCGGCACCCAGAAGAGCATCATCATCCACACGTCCGAGGACGGCAAGGTGCAGGTGACCCGGCC  G
Ruminant  C  G  NNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNN  N
Pig       C  A  CTACATGTACATTCTCTGGAAGGCGCACAGCCATGCGGTGCGCATGATCCAGCGCGGTACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTGCAGGTGACTCGGCC  G
Llama     G  G  CTATATGTACATTCTCTGGAAGGCTCACAGCCATGCCCGTCCGCATGATCCAGCGCGGCACCCAGAAGAGCATCATCATCCACACGTCGGAGGACGGCAAGGTGCAGGTGACCCGGCC  G
Rhino     A  G  GTACATGTACATTCTCTGGAAGGCTCACAGCCACGCGGTGCGCATGATTCAGCGTGGCACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTCCAGGTGACCCGGCC  C
Tapir     G  A  GTACATGTACATTCTCTGGAAGGCCCACAGCCATGCAGTCCGCATGATCCAGCGTGGCACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTCCAGGTGACCCGGCC  C
Horse     G  A  GTACATGTACATTCTCTGGAAGGCTCACAGCCACGCAGTCCGCATGATTCAGCGTGGCACCCAGAAGAGCATCATCATCCACACATCAGAGGATGGCAAGGTCCAGGTGACGCCGGCC  C
Cat       A  A  ATACATGTATATTCTCTGGAAAGCTCACAGCCACGCGGTCCGCATGATTCAGCCCGGCACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTGCAGGTGACACCGGCC  C
Caniform  A  T  ATACATGTATATCCTCTGGAAGGCTCACAGCCACGCGGTCCGCATGATTCAGCGCGGCACCCAGAAAAGTATCATCATCCACACATCAGAGGATGGCAAGGTGCAGGTGACGCCGGCC  C
Pangolin  G  G  ATACATGTACATTCTCTGGAAGGCTCACAGCCACGCGGTCCGCATGATTCAGCGCGGCACCCAGAAGAGCATCATCATTCACACGTCAGAGGACGGCAAGGTGCAGGTGACCCGGCC  A
```

60%

Changing difference thresholds



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Whale     C  C  CTACATGTACATCCTCTGGAAGGCGCATAGCCACGCCGTCCGCATGATCCAGCGCGGTACCCAGAAGAGCATCATCATCCACACGTCCGAGGACGGCAAGGTGCAGGTGACCCGGCC  G
Dolphin   C  C  CTACATGTACATTCTCTGGAAGGCGCACAGCCACGCCGTCCGCATGATCCAGCGCGGTACCCAGAAGAGCATCATCATCCACACGTCCGAGGACGGCAAGGTGCAGGTGACCCGGCC  G
Hippo     C  C  CTACATGTACATTCTCTGGAAGGCGCACAGCCACGCGGTCCGCATGATCCAGCGCGGCACCCAGAAGAGCATCATCATCCACACGTCCGAGGACGGCAAGGTGCAGGTGACCCGGCC  G
Ruminant  C  G  NNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNN  N
Pig       C  A  CTACATGTACATTCTCTGGAAGGCGCACAGCCATGCGGTGCGCATGATCCAGCGCGGTACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTGCAGGTGACTCGGCC  G
Llama     G  G  CTATATGTACATTCTCTGGAAGGCTCACAGCCATGCCGTCCGCATGATCCAGCGCGGCACCCAGAAGAGCATCATCATCCACACGTCGGAGGACGGCAAGGTGCAGGTGACCCGGCC  G
Rhino     A  G  GTACATGTACATTCTCTGGAAGGCTCACAGCCACGCGGTGCGCATGATTCAGCGTGGCACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTCCAGGTGACCCGGCC  C
Tapir     G  A  GTACATGTACATTCTCTGGAAGGCCCACAGCCATGCAGTCCGCATGATCCAGCGTGGCACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTCCAGGTGACCCGGCC  C
Horse     G  A  GTACATGTACATTCTCTGGAAGGCTCACAGCCACGCAGTCCGCATGATTCAGCGTGGCACCCAGAAGAGCATCATCATCCACACATCAGAGGATGGCAAGGTCCAGGTGACGCGGCC  C
Cat       A  A  ATACATGTATATTCTCTGGAAAGCTCACAGCCACGCGGTCCGCATGATTCAGCCCGGCACCCAGAAGAGCATCATCATCCACACGTCAGAGGACGGCAAGGTGCAGGTGACACGGCC  C
Caniform  A  T  ATACATGTATATCCTCTGGAAGGCTCACAGCCACGCGGTCCGCATGATTCAGCGCGGCACCCAGAAAAGTATCATCATCCACACATCAGAGGATGGCAAGGTGCAGGTGACGCGGCC  C
Pangolin  G  G  ATACATGTACATTCTCTGGAAGGCTCACAGCCACGCGGTCCGCATGATTCAGCGCGGCACCCAGAAGAGCATCATCATTCACACGTCAGAGGACGGCAAGGTGCAGGTGACCCGGCC  A
```

67%

sequences in phylogenetic order

- phylogenetic signal visible

Work in progress

trees with weighted edges

protein sequences

linking tree and sequence navigation

accordion drawing for sets

- data mining: transaction processing

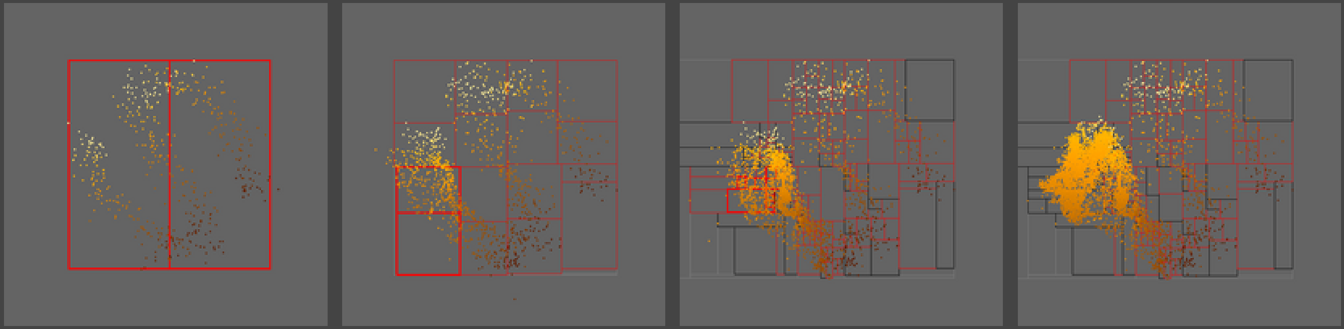
open-source release

- olduvai.sourceforge.net

Other projects in progress

dimensionality reduction

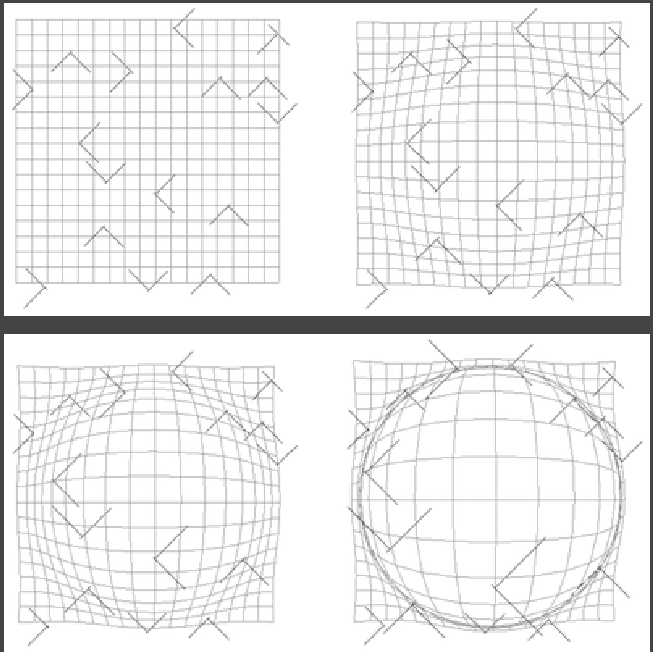
- steerable MDS (multidimensional scaling)
- with Matt Williams



Other projects in progress

perception experiments

- quantifying cost of Focus+Context fisheye distortions
- no-cost and low-cost regions for visual search task
- with Keith Lau, Ron Rensink



More information

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papers, slides, images, movies

software: olduvai.sourceforge.net