On the Scalability of Computing Triplet and Quartet Distances

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Introduction

- Trees are used in many branches of science.
- Phylogenetic trees are especially used in biology and bioinformatics.
- We want to measure how different two such trees are.

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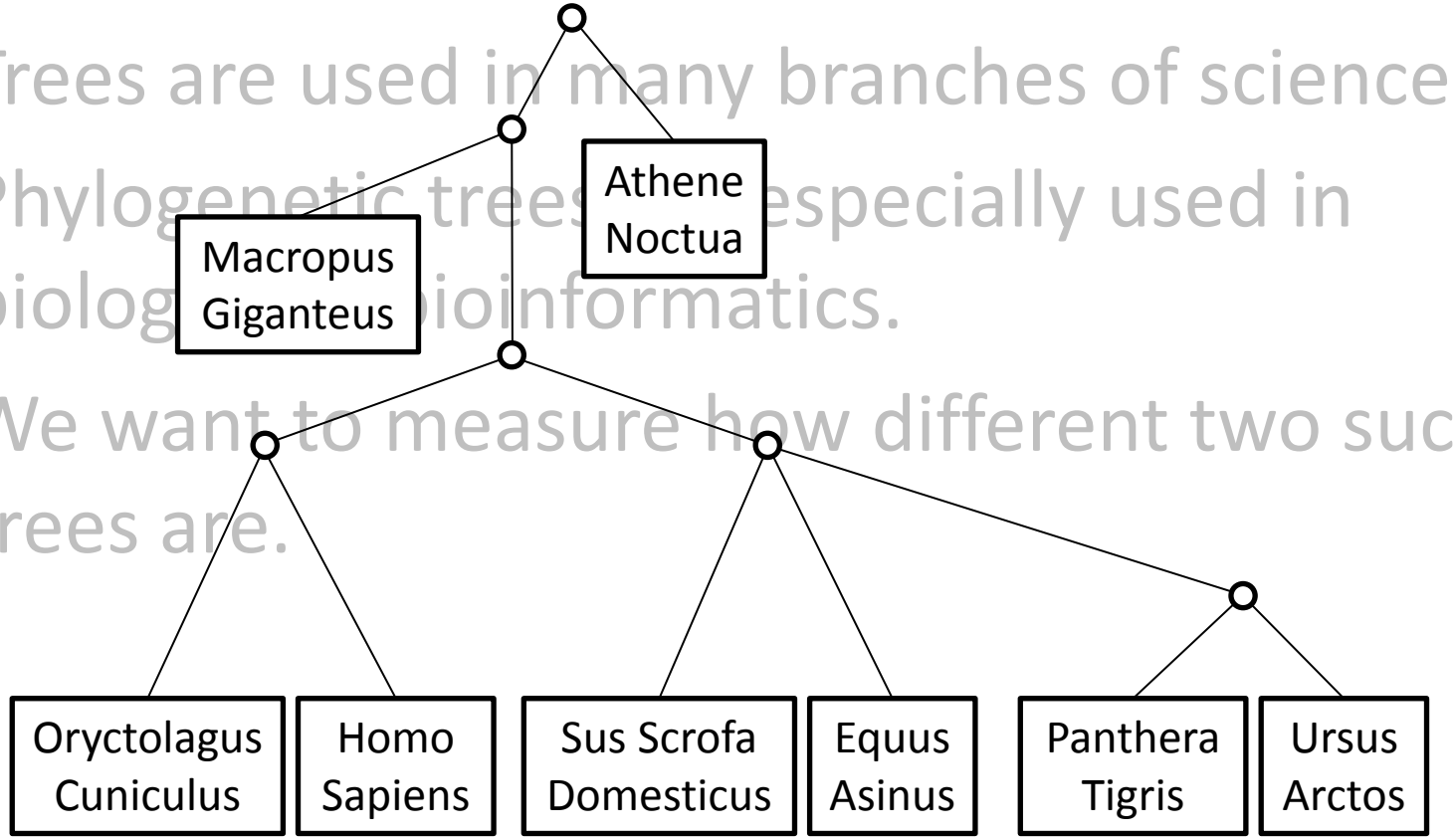
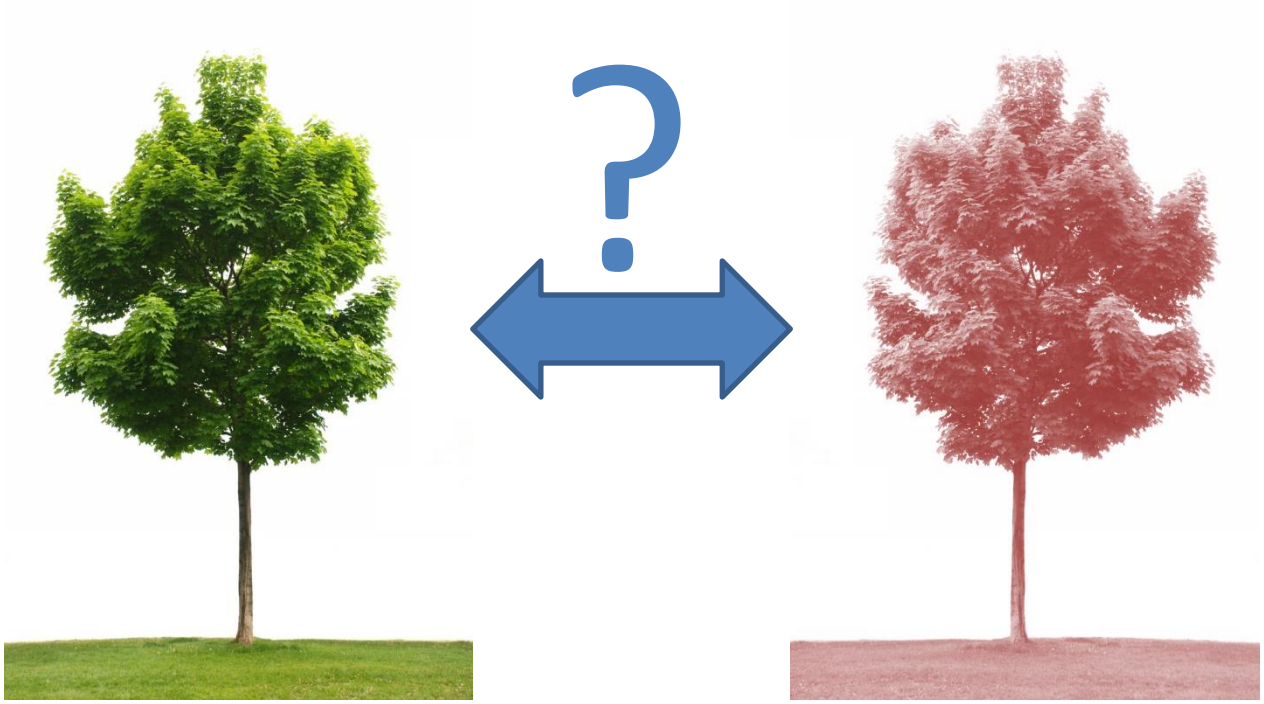


Distances

- Natural in some cases.
- Between trees?



Triplets and Quartets

Triplets

- Used in **rooted** trees.
- Sub-trees consisting of **three** leaves.
- $\binom{n}{3}$ in a tree with n leaves.
- With 2,000 leaves, 1,331,334,000 triplets.
- Naïve algorithm runs in at least $\Omega(n^3)$.
- Number of *disagreeing* triplets.

Quartets

- Used in **unrooted** trees.
- Sub-trees consisting of **four** leaves.
- $\binom{n}{4}$ in a tree with n leaves.
- With 2,000 leaves, 664,668,499,500 quartets.
- Naïve algorithm runs in at least $\Omega(n^4)$.
- Number of *disagreeing* quartets.

Goal

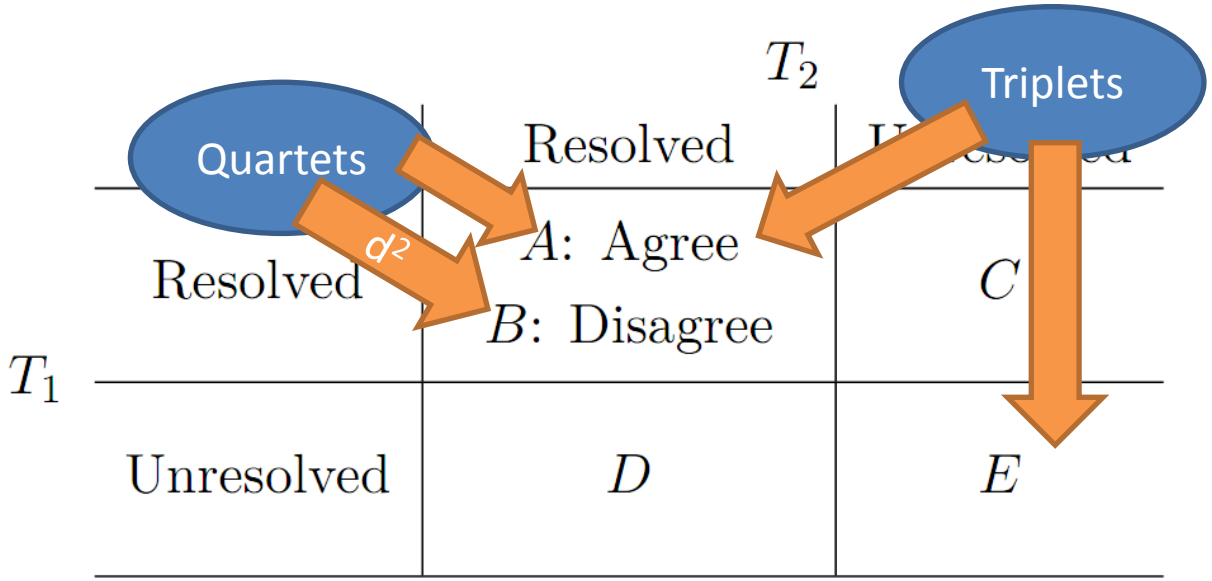
- Comparison of two trees ($\mathbf{T_1}$ and $\mathbf{T_2}$) with the same set of leaf-labels.
  - Numerical value of the **difference** of the two trees.
  - Number of different triplets (quartets) in the two input trees.
- A tree has a distance of 0 to itself.

Brodal *et al.* [SODA13]

		T_2	
		Resolved	Unresolved
T_1	Resolved	A: Agree B: Disagree	C
	Unresolved	D	E

- For binary trees C, D and E are all zero ☺

Brodal *et al.* [SODA13]



- For binary trees C, D and E are all zero ☺

Brodal *et al.* [SODA13]

	Binary	Arbitrary degree
Triplets	$O(n \lg n)$ Up to $4d+2$ counters in each HDT node	
Quartets	$O(n \lg n)$ $2d^2 + 79d + 22$ counters	$O(\max(d_1, d_2)\, n \lg n)$ $2d^2 + 79d + 22$ counters

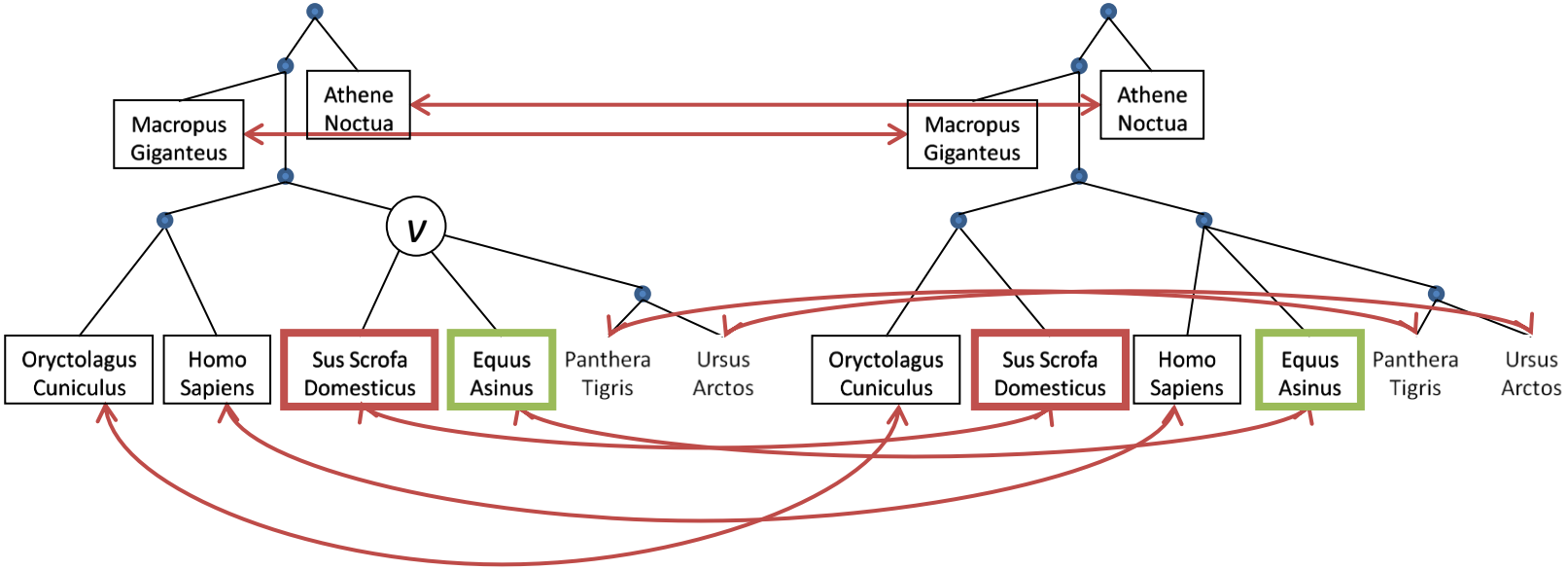
- A lot of counters ☹. Is this even feasible?
- Why the *d* factor on arbitrary degree quartets?
  - d^2 counters

Overview

- Basic idea
  - Each triplet (quartet) is anchored somewhere in $\mathbf{T_1}$.
  - Run through $\mathbf{T_1}$, and for each triplet (quartet), check if they are anchored the same way in $\mathbf{T_2}$.
- The algorithm consists of **four** parts
  1. Coloring
  2. Counting
  3. Hierarchical Decomposition Tree (HDT)
  4. Extraction and contraction

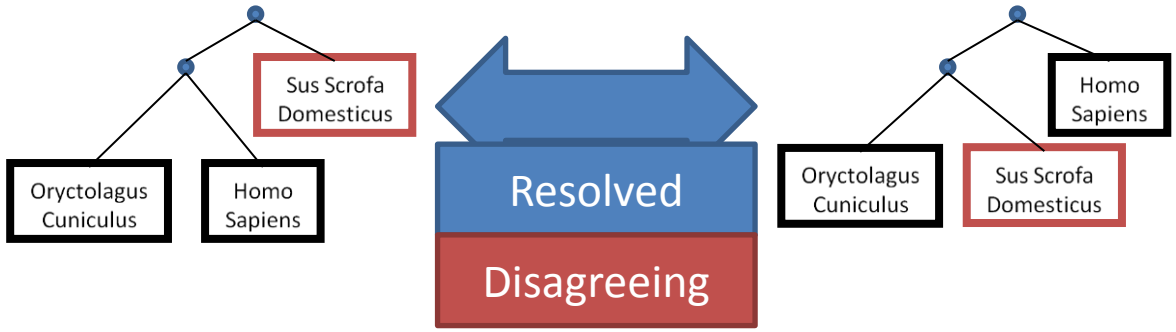
1. Coloring

- Consists of two steps
  1. Leaf-linking O(n)
  2. Recursive coloring O(n lg n)



2. Counting

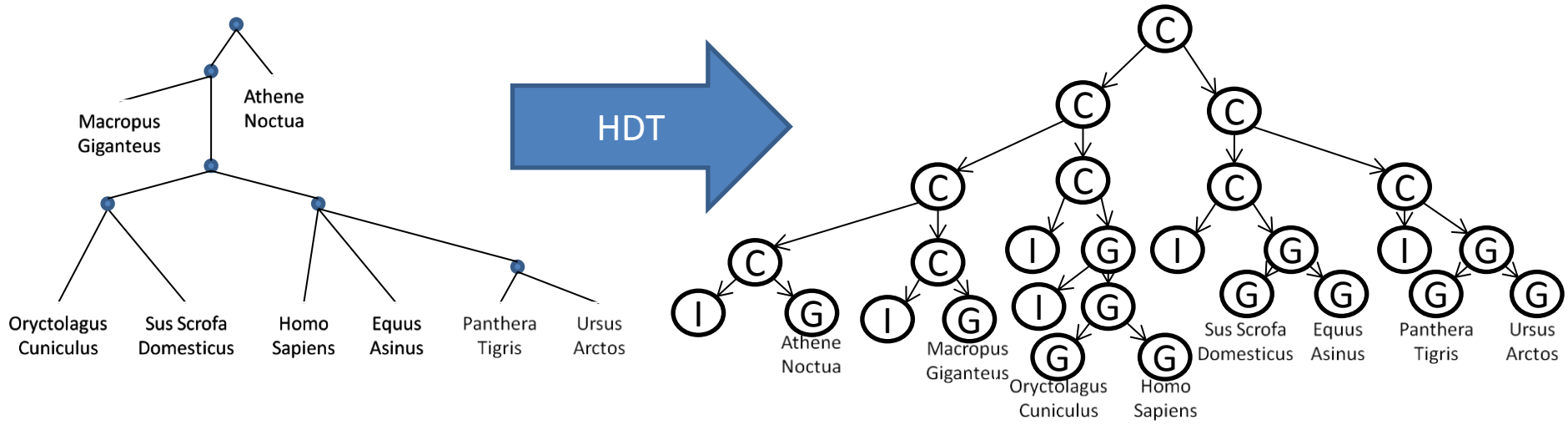
- Using the coloring of $\mathbf{T_1}$ and $\mathbf{T_2}$ we count the number of similar triplets (quartets).



- No reason to look at all triplets (would be much too slow)
  - Instead, look at inner nodes.
- In each inner node, we can keep track of the number of different triplets (quartets), rooted at the given node.
- Using counting and coloring, the triplet distance can be calculated in $O(n^2)$.

3. Hierarchical Decomposition Tree (HDT)

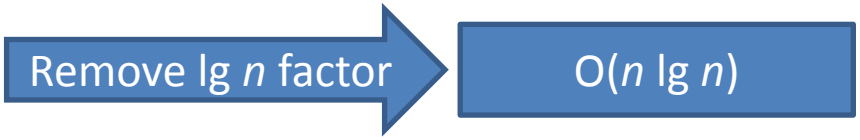
- Problem: $\mathbf{T_2}$ is unbalanced.
- Solution: Hierarchical Decomposition Trees.



Built in linear time | Locally balanced | Triplet distance in $O(n \lg^2 n)$

4. Extraction and Contraction

- Ensuring that the HDT is small, we can cut off that lg *n* factor.
- If the HDT is too large, remove the irrelevant parts.



Optimizations

1. [SODA13] hints at constructing HDTs early.
   Problem: HDTs take up a lot of memory.
   Solution: Postpone HDT construction.
   Result: **25-50%** reduction in memory usage.
   4-10% reduction in runtime.
2. Utilizing the standard C++ vector data structure.
   Problem: Relatively slow (for our needs).
   Solution: A purpose-built linked list implementation.
   Result: **6-9%** reduction in runtime on binary trees.
3. Allocating memory whenever needed.
   Problem: (Relatively) slow to allocate memory.
   Solution: Allocation in large blocks.
   Result: **18-25%** improvement in the runtime.
   10-20% increase in memory usage on large input.

25% improvement in runtime

45% reduction in memory usage

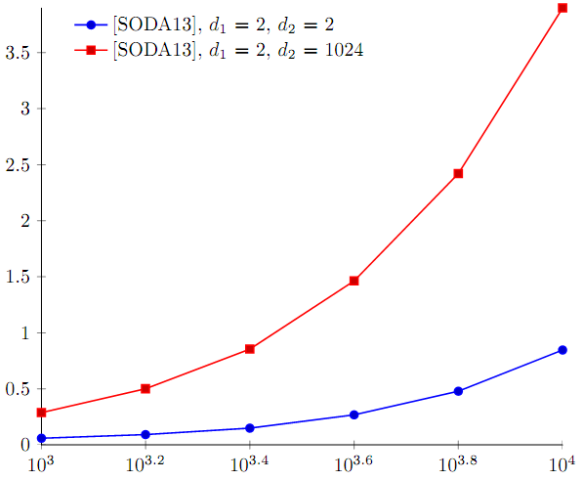
Limitations

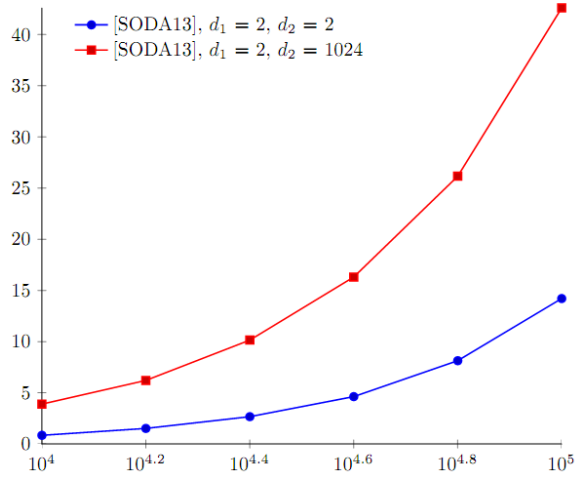
Two primary limitations in our implementation:

- **Integer representation**
  - $\binom{n}{3}$ and $\binom{n}{4}$ are in the order of n^3 and n^4.
  - With signed 64-bit integers, quartet distance of only 55,000 leaves.
  - *Solution:* Signed 128-bit integers for n^4 counters.
    - Quartet distance of up to 2,000,000 leaves.
- **Recursion depth**
  - OS imposed limitation in recursion stack depth.
  - Input, consisting of a very long chain, will fail.
  - Windows: Height ~4,000.
  - Linux: Height ~48,000.
  - *Solution:* Purpose built stack implementation*.

*Not done in the implementation

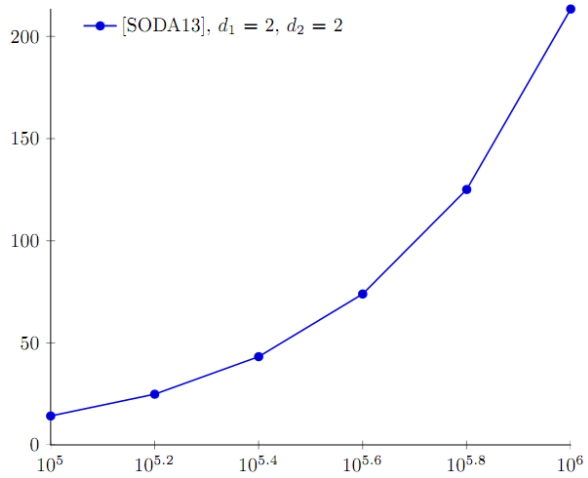
Results: [SODA13]





It works, and it is fast!

☺

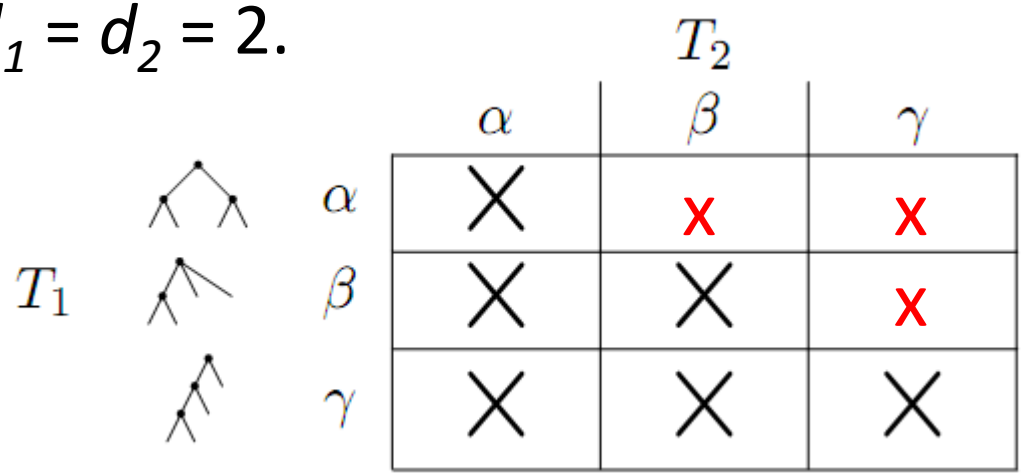


Leaves	Time (s)
1,000	.29
10,000	3.90
100,000	42.60
1,000,000	N/A

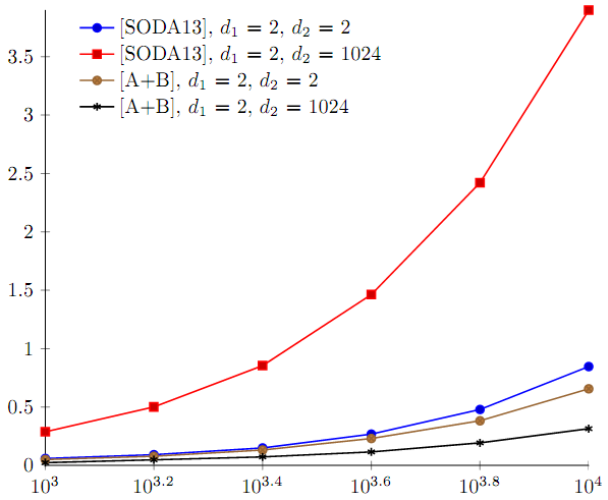
Improvements

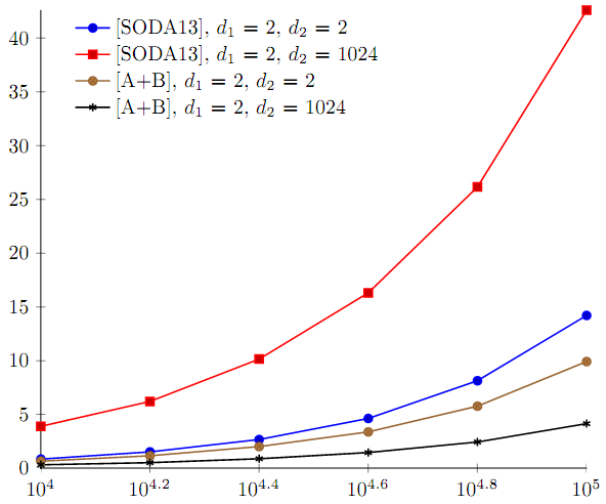
- Why min (d_1, d_2)?
  - d-counters given by first input tree
  - [SODA13]: Calculates 6 out of 9 cases.
  - [SODA13]: $d_1 = 2$, $d_2 = 1024$ is much slower than $d_1 = d_2 = 2$.

Add $5d^2 + 18d + 7$ counters
Total $7d^2 + 97d + 29$ counters
Remove need for swapping
$O(\min(d_1, d_2)\, n \lg n)$

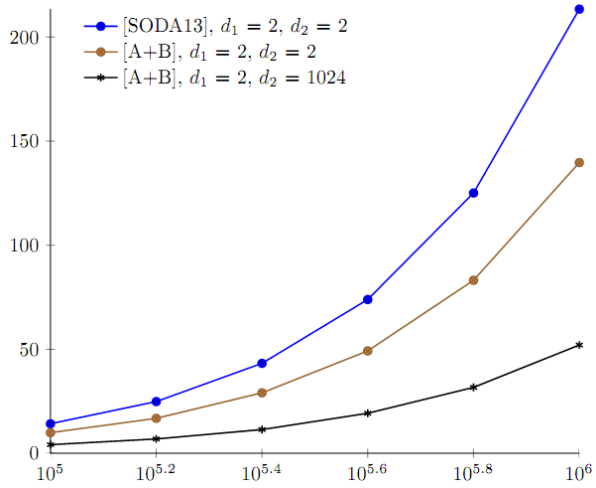


Results: Improved





Faster in alle cases ☺



Leaves	Time (s)
1,000	.02
10,000	.31
100,000	4.14
1,000,000	52.05

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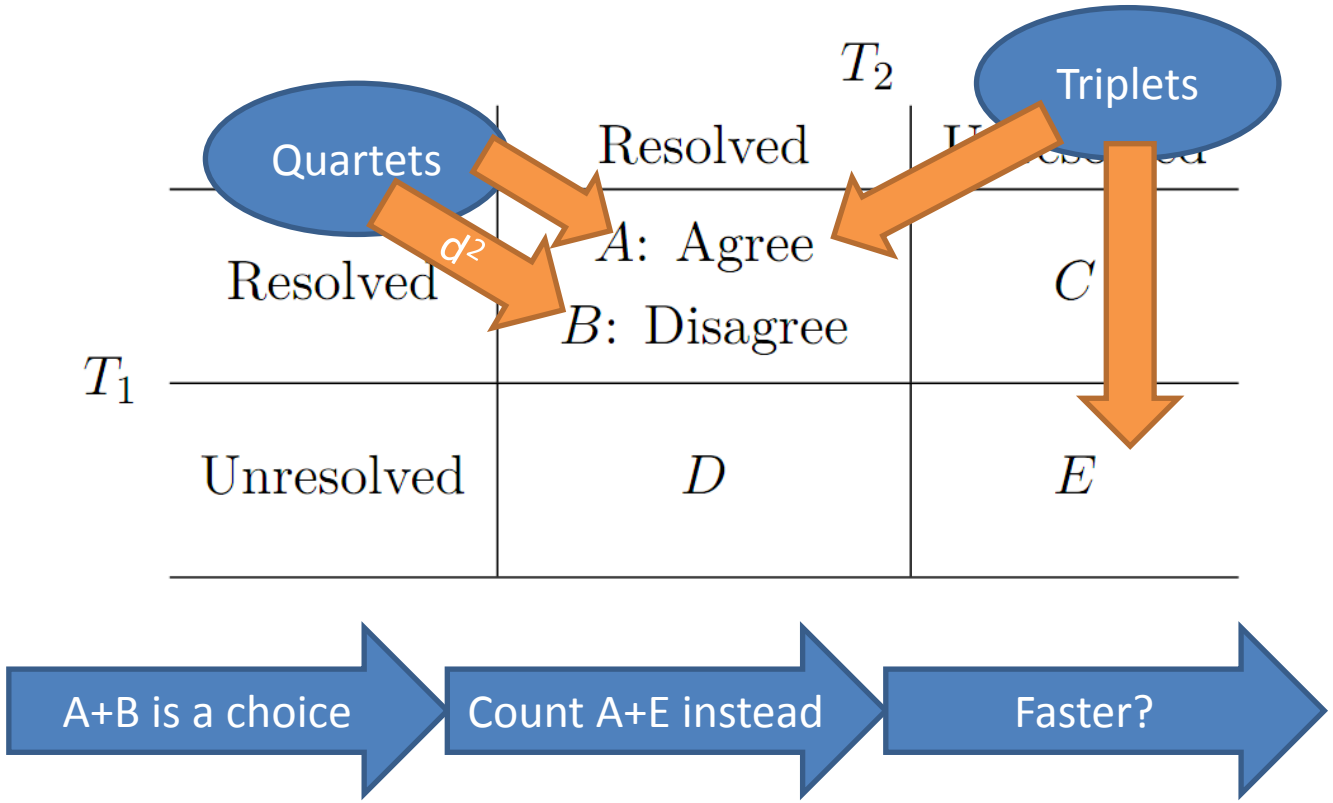
More improvements



More improvements

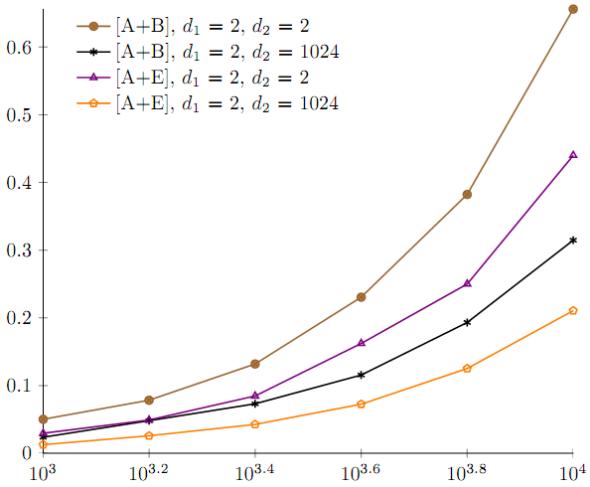
To count B

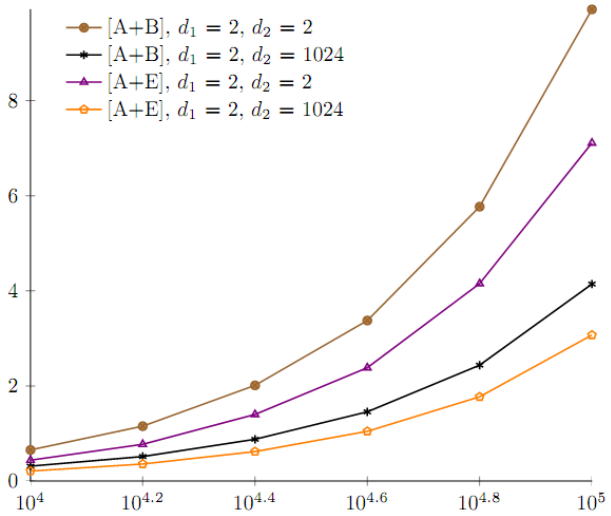
- 14 cases
- 92 sums
- $5d^2 + 48d + 8$ counters
- $O(\min(d_1, d_2)\, n \lg n)$

To Count E

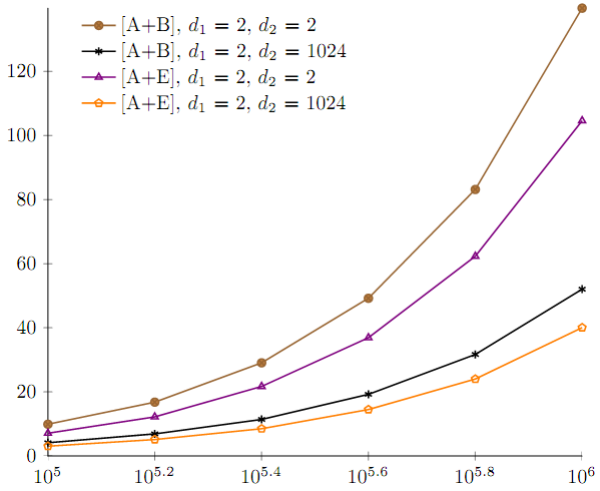
- 5 cases
- 21 sums
- $1d^2 + 12d + 12$ counters
- $O(\min(d_1, d_2)\, n \lg n)$

Results: More improvements





Fastest in the field ☺



Leaves	Time (s)
1,000	.01
10,000	.21
100,000	3.07
1,000,000	40.06

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Overview

	Binary	**Arbitrary degree** $d_1 = d_2 = 256$
Triplets	[SODA13]: O(n lg n) [SODA13]: ~34 seconds	[SODA13]: O(n lg n) [SODA13]: ~7 seconds
Quartets	[SODA13]: O(n lg n) [SODA13]: ~125 seconds [ALENEX14] v1: ~83 seconds [ALENEX14] v2: ~62 seconds	[SODA13]: O(max(d_1, d_2) n lg n) [ALENEX14]: O(min(d_1, d_2) n lg n) [SODA13]: ~139 seconds [ALENEX14] v1: ~112 seconds [ALENEX14] v2: ~45 seconds

Balanced tree, 630.000 leaves

Conclusion

- [SODA13] is both practical and implementable.
- We have
  - Performed a thorough study of the alternative choices not studied in [SODA13].
  - Theoretically, and practically, found good choices for the parameters.
  - Shown that [SODA13], and derivatives, successfully scales up to trees with millions of nodes.
- Open problem
  - Current algorithm makes heavy use of random accesses, and doesn't scale to external memory.
  - Current algorithm is single-threaded.