

MENDEL: A DISTRIBUTED STORAGE SYSTEM FOR EFFICIENT SIMILARITY SEARCHES AND SEQUENCE ALIGNMENT

Outline

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- Motivation
- Overview
- Vantage-Point Tree
- System Architecture
- Results
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Motivation

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- Due to exponential growth of biological datasets, current similarity search tools are becoming less sufficient
 - ▣ BLAST, BLAT, YASS, FASTA, etc...
 - ▣ Algorithm centric, different heuristics on similar algorithm with different trade-offs
- Similarity between sequences, or lack thereof, can explain relationships between them
 - ▣ In some cases can provide important clues about common evolutionary roots of organisms



Basic Idea

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- Inverted index
 - ▣ Map content to its location in the database
 - Rather than indexing what each location contains
 - ▣ Allows for efficient searches at the cost of additional processing for insertions
- DHTs provide extremely fast lookups for distributed datasets



Basic Idea

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- Searching DNA sequences for subsequences is a challenging problem
 - ▣ Must consider partial matches, insertions/deletions (indels), repeated regions, etc..
- Sliding window over DNA sequence indexing on each substring
 - ▣ Sliding window can identify indels
- Store data with in a DHT with a nearest neighbor data structure
 - ▣ Nearest neighbor structure finds partial matches



Challenges

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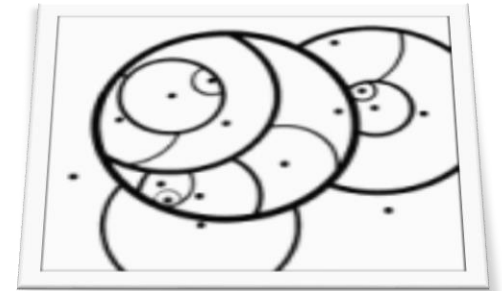
- How to locate matches for a non-exact match query in a DHT?
- How to balance content load on storage nodes?



Vantage Point Tree

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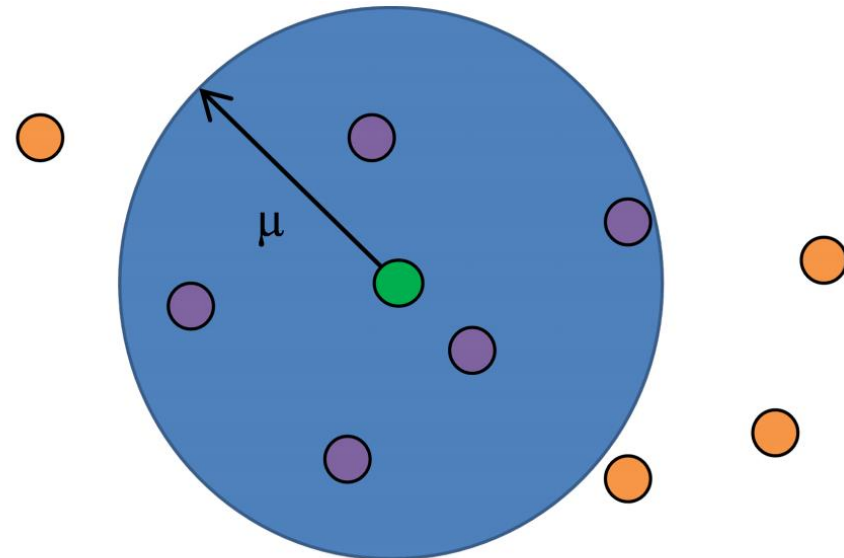
- Developed by Peter Yianilos and Jeffrey Uhlmann independently
- Data structure used for nearest neighbor searches in metric space
- Recursively partition data points into two divisions
 - ▣ Points that are within a threshold distance of the vantage point
 - ▣ Points that are outside the same threshold



Vantage-Point Tree

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- Each node in a vp-tree maintains four values:
 - Input value
 - Radius, μ
 - Left child
 - Right child

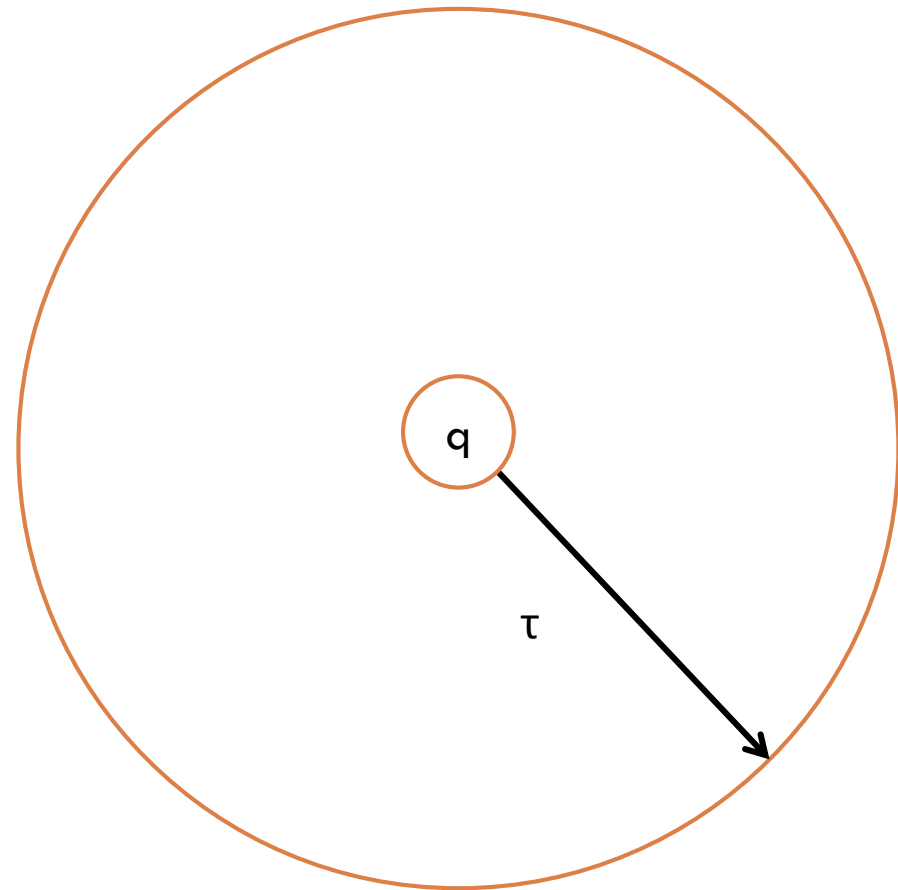


- Parent (vantage point)
- Left child
- Right child

Searching vp-trees

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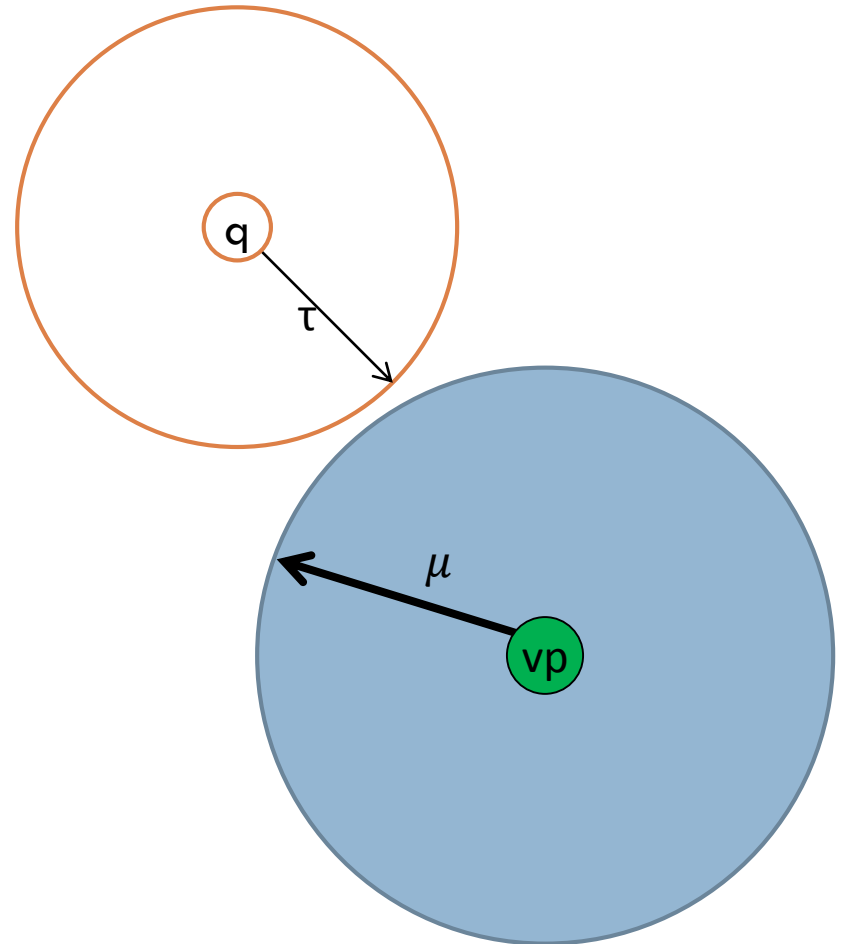
- Let query be q
- Let radius of q be τ
- k nearest neighbors are contained within τ
- $\tau = \min(\text{dist}(q \rightarrow v, \tau))$
- 3 cases
 - τ lies completely within μ
 - τ lies completely outside μ
 - τ and μ intersect
- Stop recursing when leaves are reached



Searching vp-trees

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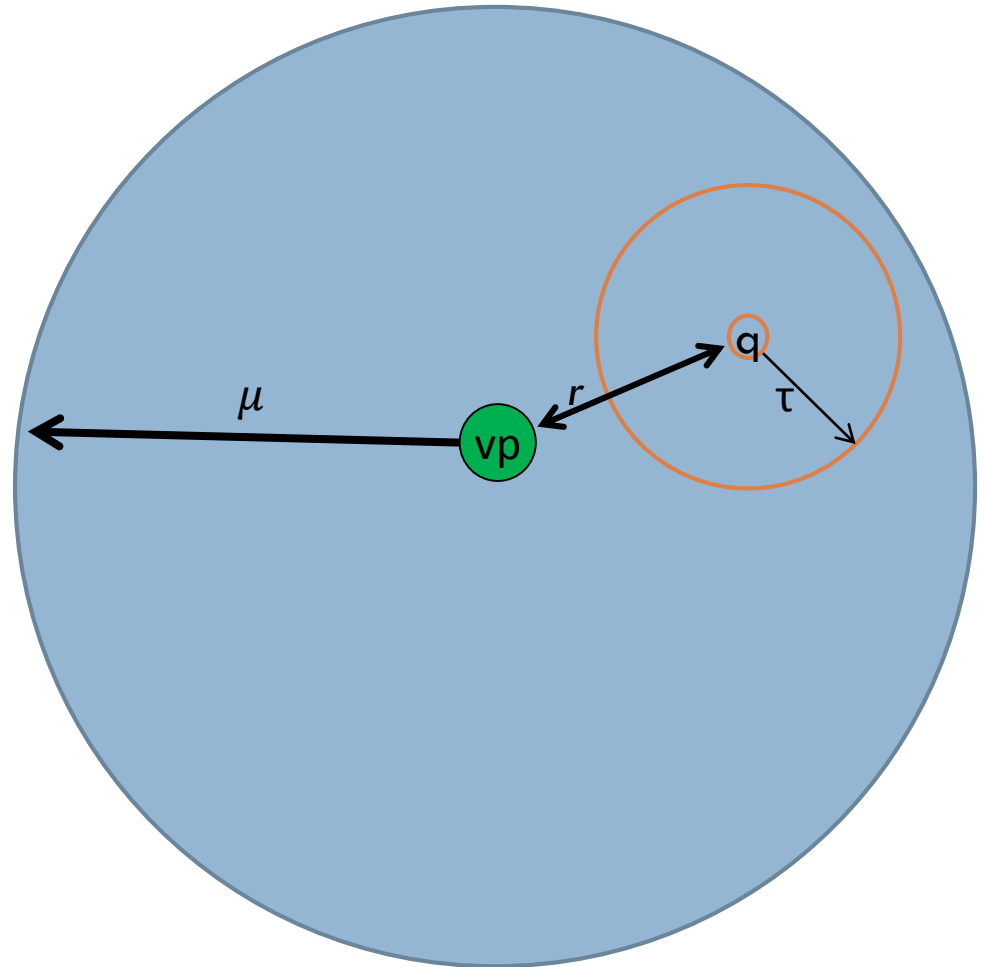
- Case 1: τ completely outside of μ
 - Don't need to search left subtree
- $\tau = \min(\text{dist}(q \rightarrow vp), \tau)$
 - Recurse on right subtree



Searching vp-trees

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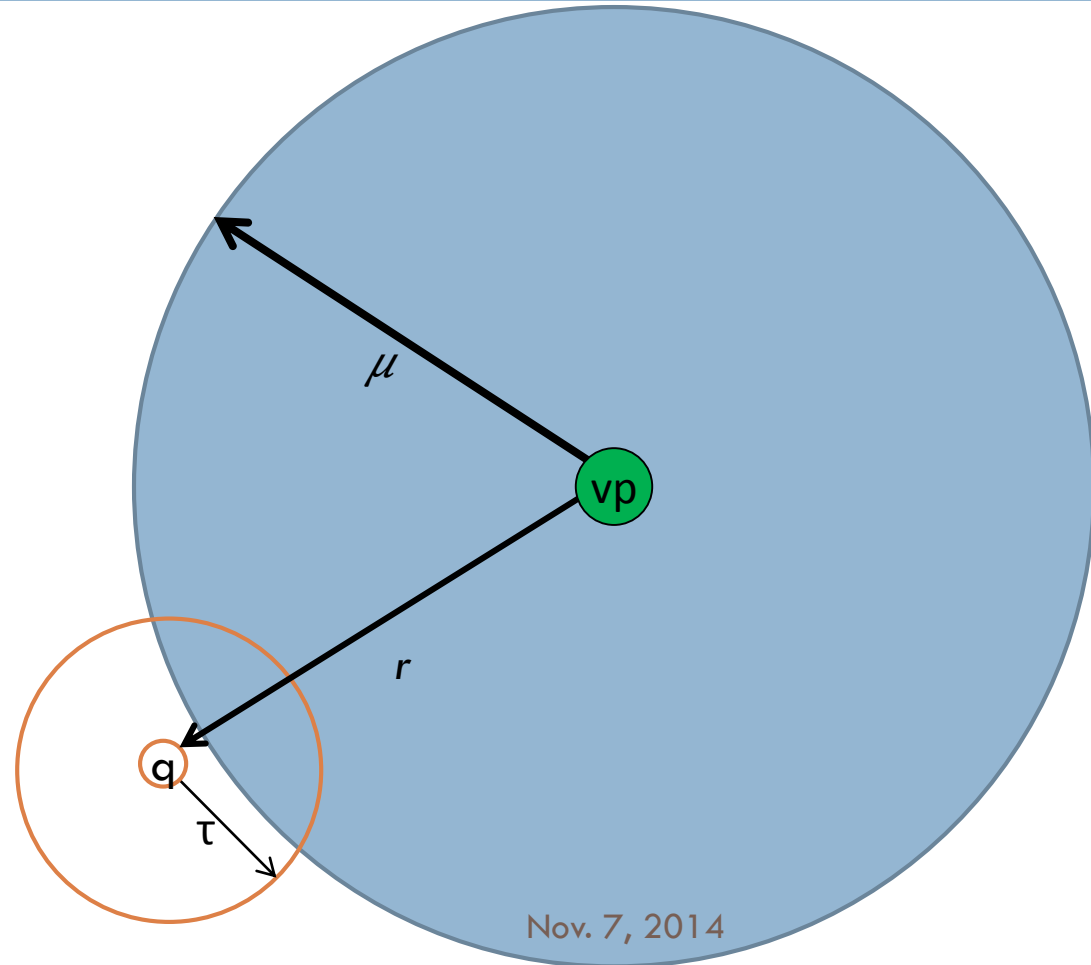
- Case 2: τ completely inside μ
 - Don't need to search right subtree
- $\tau = \min(r, \tau)$
 - Recurse on left subtree



Searching vp-trees

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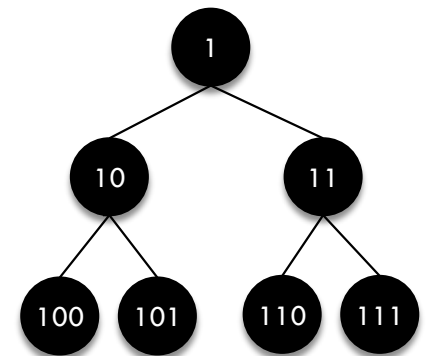
- Case 3: worst case intersect
 - Must search both trees
- $\tau = \min(r, \tau)$
 - Recurse on both subtrees



Vantage-point prefix tree

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- Global vp-tree as an index is not scalable
 - ▣ Utilize vp-tree as a similarity based hashing function
- Alter vp-tree node to contain a prefix
$$prefix_{left} = prefix_{parent} \ll 1$$
$$prefix_{right} = (prefix_{parent} \ll 1) + 1$$
- Use as a group hash by assigning groups to subtrees
 - ▣ Requires a balanced vpp-tree



System Architecture

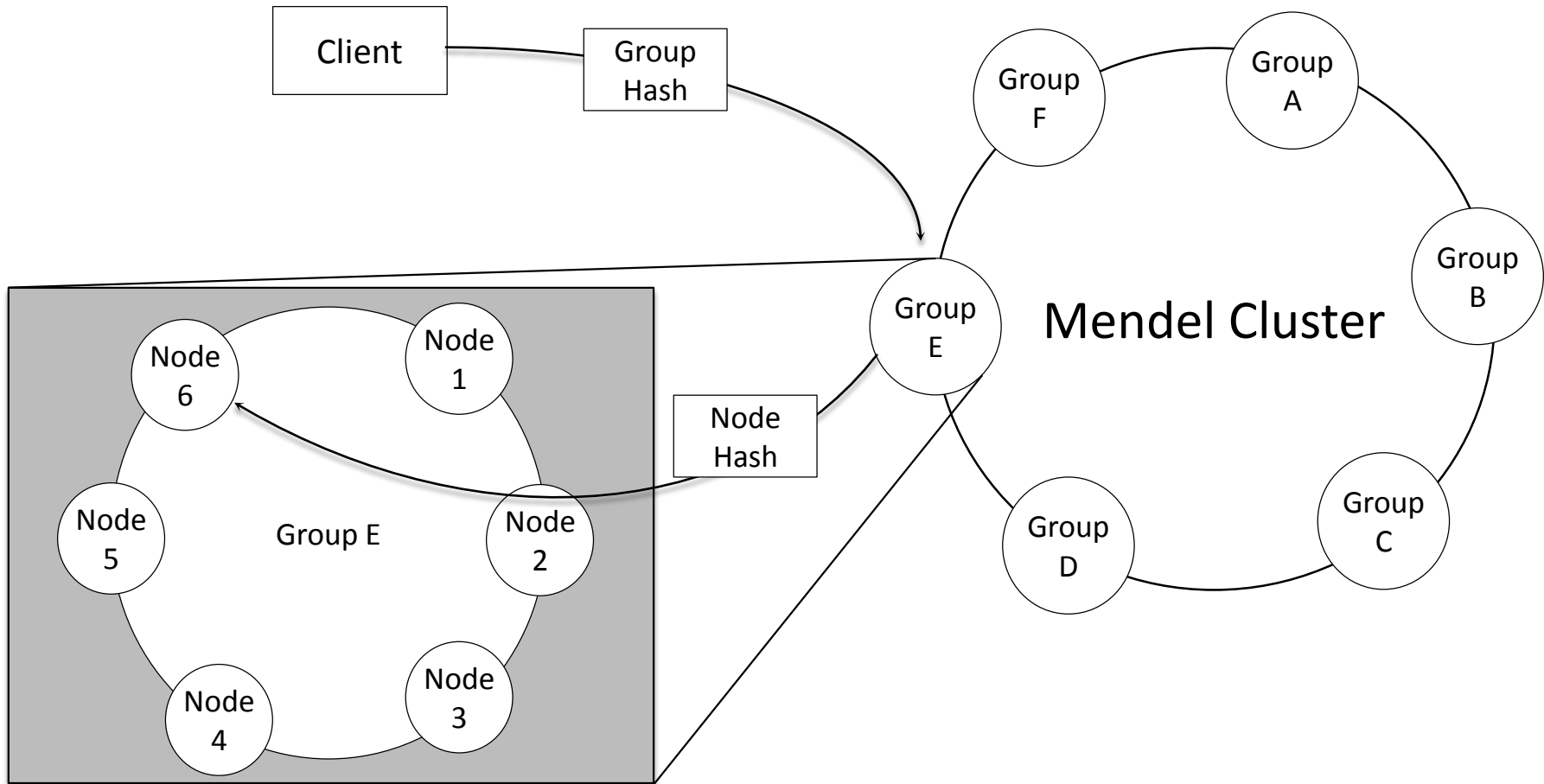
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- Zero-hop distributed hash table
 - ▣ Such as Apache Cassandra and Amazon Dynamo
- Hierarchical, two-tier hashing scheme
- Each node belongs to a group
 - ▣ Groups are placed on the hashing ring
 - ▣ Two rounds of hashing required to place or retrieve data
 - Hashed to a group using the vpp-tree
 - Second hash among group nodes



System Architecture

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Indexing Data

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- 100bp sliding window over each contig
 - ▣ Each 100bp subsequence is individually indexed
- Passed through the vpp-tree to determine storage grouping
- Within the group, the subsequence is distributed using a SHA-1 hash to a storage node
- The subsequence block is maintained in a vp-tree local to its storage node



Query Evaluation

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- Query is “hashed” in the vpp-prefix tree to find all subtrees that *may* have matching subsequences
- Each node in the selected group(s) performs a lookup in their vp-tree
 - ▣ Results are aggregated and filtered
- Results are send back to the client



Results

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- ▣ Three benchmarks to test indexing speed, data distribution, and query speed
- ▣ Sourced real world data from the Genome Assembly Golden-standard Evaluation (GAGE)
 - Four genomes ranging from 2 Mbp to 3 Gbp
- ▣ Benchmark 1: index each of the genomes into the system and measure the time to complete



Results

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TABLE I
INDEXING TIMES

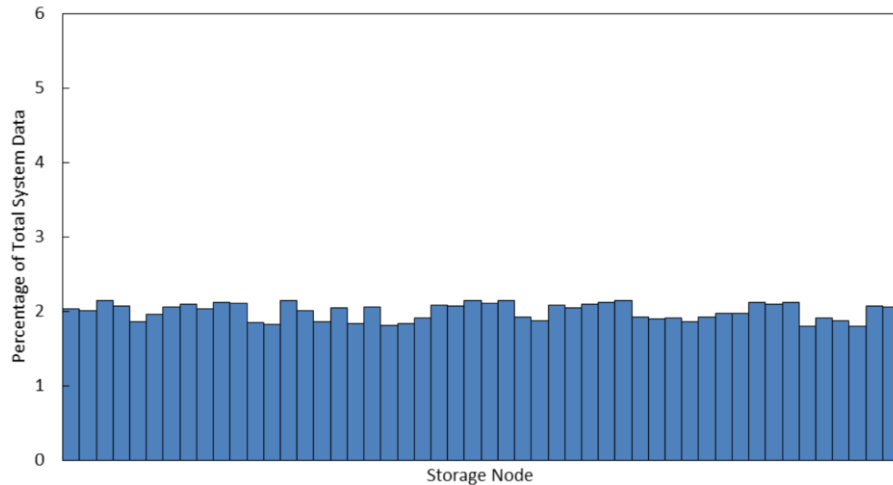
Genome	Base Pairs	Blocks	Index Time
<i>S. aureus</i>	2.8 Mbp	28,261	1.80 s
<i>R. sphaeroides</i>	4.6 Mbp	45,984	2.61 s
<i>H. sapiens</i> C. 14	88 Mbp	882,468	21.83 s
<i>B. impatiens</i>	250 Mbp	2,491,627	88.14 s

Results

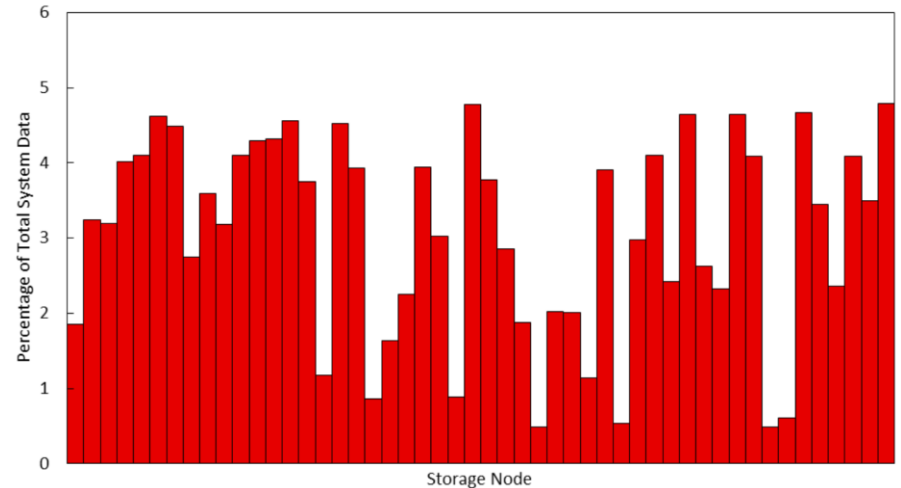
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- Benchmark 2: Data distribution
 - After all datasets have been indexed count files per node
 - Compare versus flat SHA-1 hash

Data Distribution (SHA-1 Hash)



Data Distribution (Similarity Hash)



Results

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- Benchmark 3: Issue a series of queries; measure response time and number of results
 - ▣ Exact match query whose target exists in the database
 - ▣ Exact match query whose target has a few errors to its match
 - ▣ Similarity query whose target exists in the database
 - ▣ Similarity whose target has a few errors to its match
 - ▣ Similarity whose target is randomly generated



Results

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TABLE II
RETRIEVAL TIMES

Query	Number of results	Time (ms)
Exact Match, exists	1	403
Exact Match, erroneous	0	346
Similarity, exists	8	409
Similarity, erroneous	8	476
Similarity, random	10	480

Conclusion & Future Work

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- The hashing scheme needs to be refined substantially in order to level the out the dispersion of the data
 - ▣ Data input one-by-one
 - ▣ Choosing initial vantage point (root)
- Currently queries must match the window they were indexed with
 - ▣ Sliding window over queries



Questions?

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□ Thanks!