Data Structures and Algorithms

Cardinality and Similarity Sketches

CS 225

April 29, 2022

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Learning Objectives

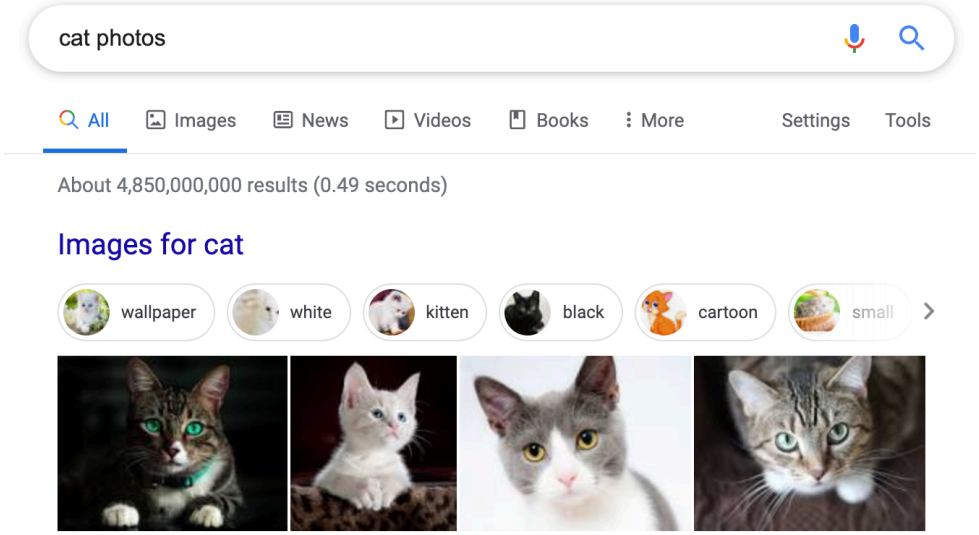
Introduce the concept of cardinality and cardinality estimation

See how hashing is an effective tool for approximation

Demonstrate the Minhash and HyperLogLog sketches

Cardinality

How many *distinct* (unique) values there are in a dataset



Google Index Estimate: >60 billion webpages

Google Universe Estimate (2013): >130 trillion webpages

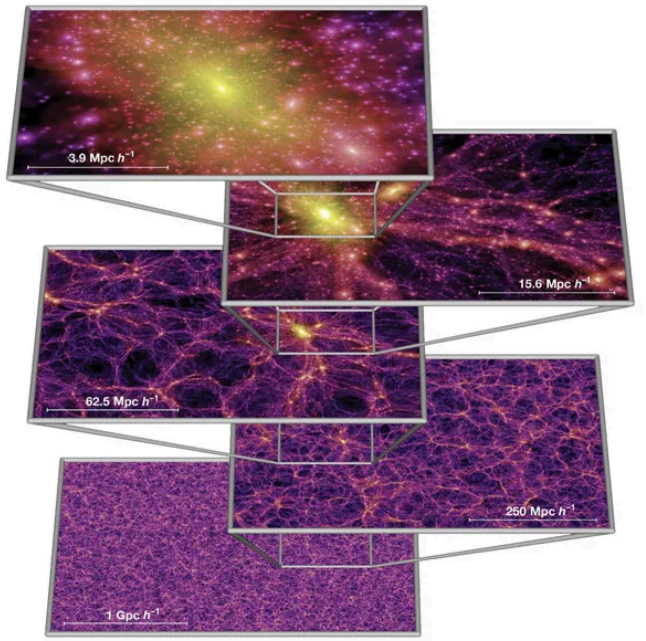
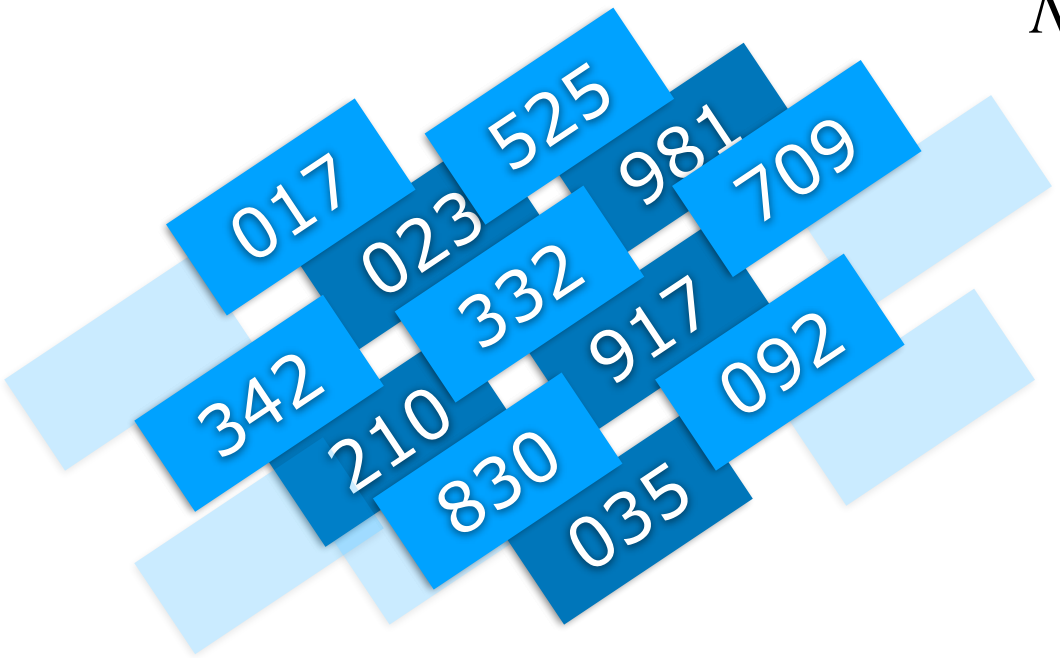


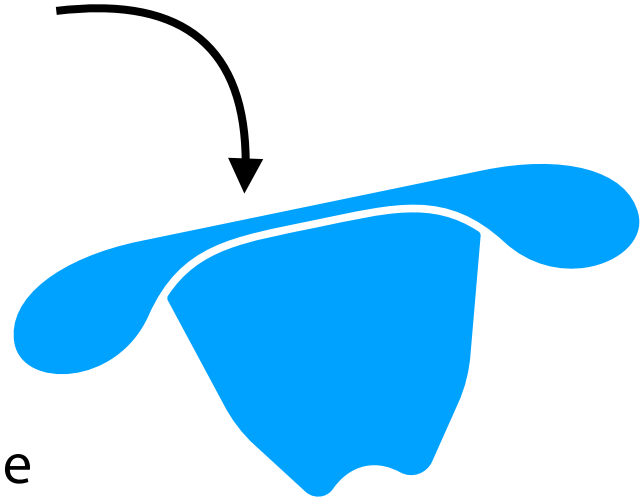
Image: https://doi.org/10.1038/nature03597

Cardinality

I take cards labeled 1--1,000 and choose a random subset of size N to hide in my hat



We want to estimate N



We can see **one representative** from the cards in the hat; which to pick?

Minimum, median, maximum? Something else?

Cardinality

What if **minimum** was 500? ...10? ... 4?

If minimum is 95, what's our estimate for N?

Cardinality

What if **minimum** was 500? ...10? ... 4?

If minimum is 95, what's our estimate for N?

Conceptually: If we scatter N points randomly across the interval, we end up with $N + 1$ parts, each about $1000/(N + 1)$ long

Assuming our first 'partition' is about average:

$$95 \approx 1000/(N + 1)$$

$$N + 1 \approx 10.5$$

$$N \approx 9.5$$

Cardinality

Now imagine we have a SUHA hash (let h_{64} be a 64-bit hash)

$$\frac{h_{64}(x)}{2^{64}-1}$$

The randomness in the hash function turns any dataset-cardinality problem into the “hat problem”

Cardinality

Let $M = \min(X_1, X_2, \ldots, X_N)$, where each X_i is an independent uniform draw between [0, 1]

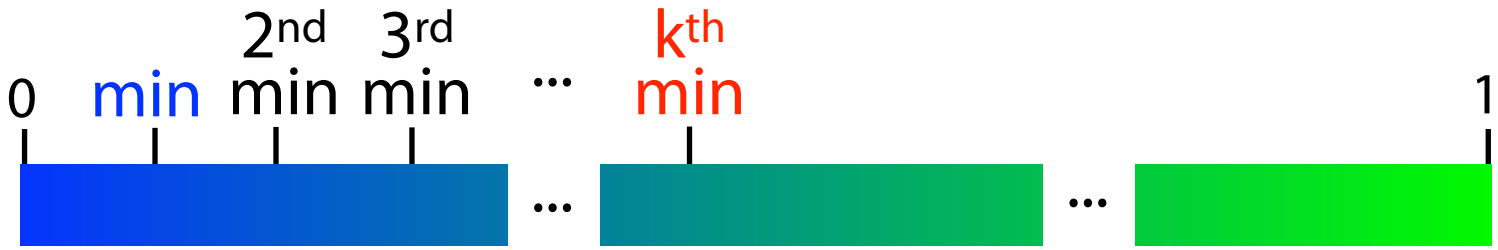
Claim: $\mathbf{E}[M] = \frac{1}{N+1}$

Cardinality

Attempt 1	0.455	0.220	0.951	0.236	0.979
Attempt 2	0.968	0.234	0.835	0.642	0.349
Attempt 3	0.774	0.484	0.309	0.526	0.143

Cardinality

Can the k^{th}-smallest hash value estimate the cardinality better than the minimum?



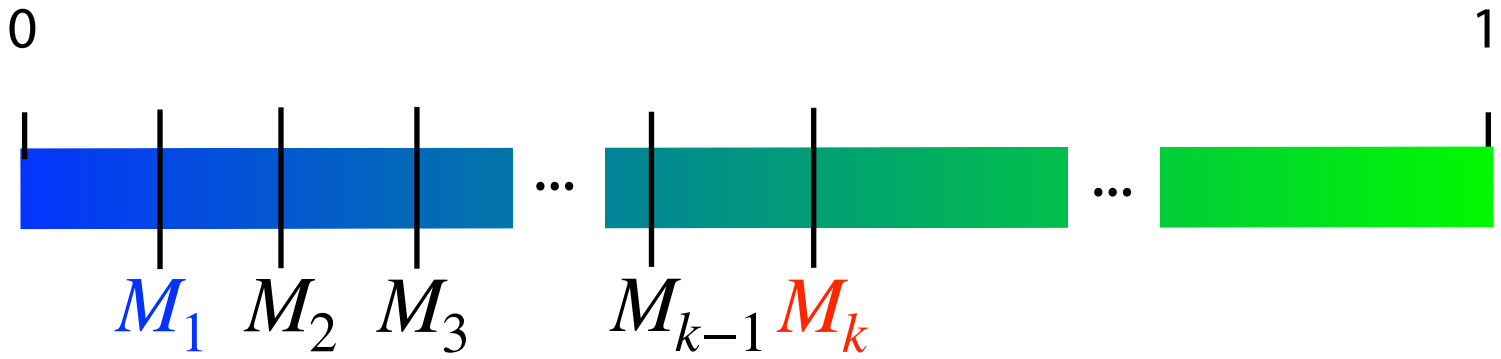
Cardinality

Can the k^{th}-smallest hash value estimate the cardinality better than the minimum?

$$\mathbf{E}[M_1] = \frac{1}{N+1} \qquad \mathbf{E}[M_k] = \frac{k}{N+1}$$

Cardinality

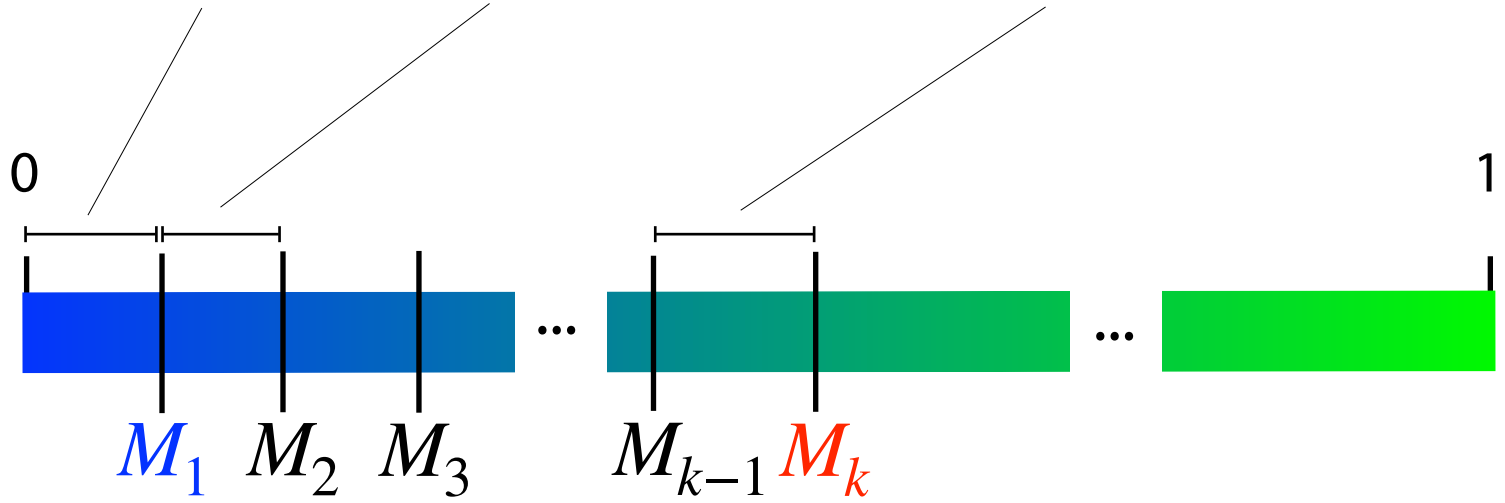
$$\frac{1}{N+1} = \frac{\mathbf{E}[M_k]}{k}$$



Cardinality

$$\frac{1}{N+1} = \frac{\mathbf{E}[M_k]}{k}$$

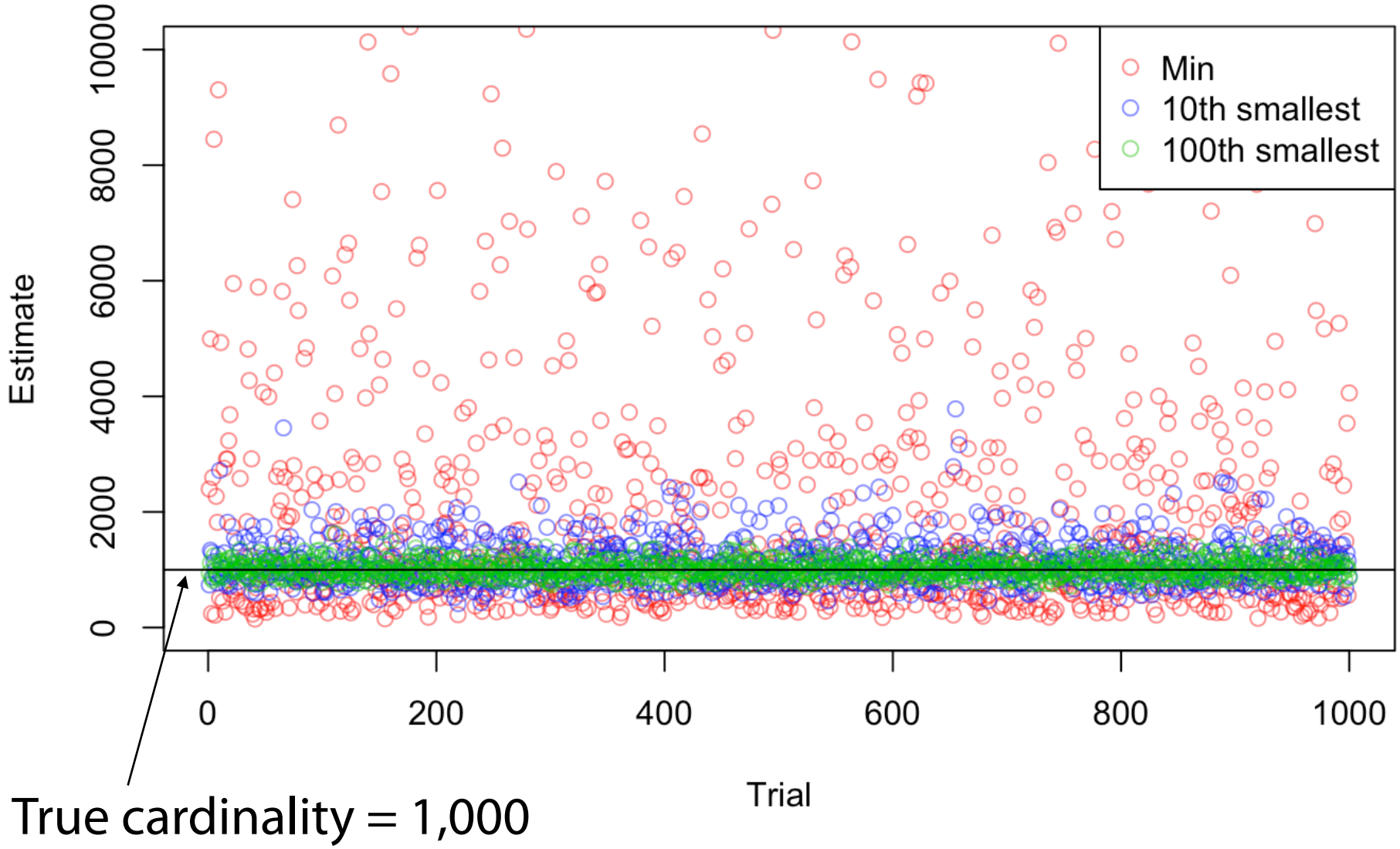
$$= \left[\mathbf{E}[M_1] + (\mathbf{E}[M_2] - \mathbf{E}[M_1]) + \ldots + (\mathbf{E}[M_k] - \mathbf{E}[M_{k-1}])\right] \cdot \frac{1}{k}$$



k^{th} minimum value (KMV)

Averages k estimates for $\frac{1}{N+1}$

Cardinality



Cardinality

Given any dataset and a SUHA hash function, we can estimate the number of unique items by tracking the minimum hash values.

Hash

0.135	0.220	0.236	0.36	0.41

Applied Cardinalities

Cardinalities

$|A|$

$|B|$

$|A \cup B|$

$|A \cap B|$

Set similarities

$$O = \frac{|A \cap B|}{min(|A|, |B|)}$$

$$J = \frac{|A \cap B|}{|A \cup B|}$$

Real-world Meaning

```
AGGCCACAGTGTATTATGACTG
|||||||||||  |||||||||
AGGCCACAGTGAGTTATGACTG

AAAAAAAAAAAGATGT-AAGTA
|||||||||||||||| |||||
AAAAAAAAAAAGATGTAAAGTA

GAGG--TCAGATTCACAGCCAC
||||  ||||||||||||||||
GAGGGGTCAGATTCACAGCCAC
```

Set Operations

$A = \{1, 2, 3, 4\}$ $B = \{3, 4, 5, 6, 7\}$

Union $A \cup B$

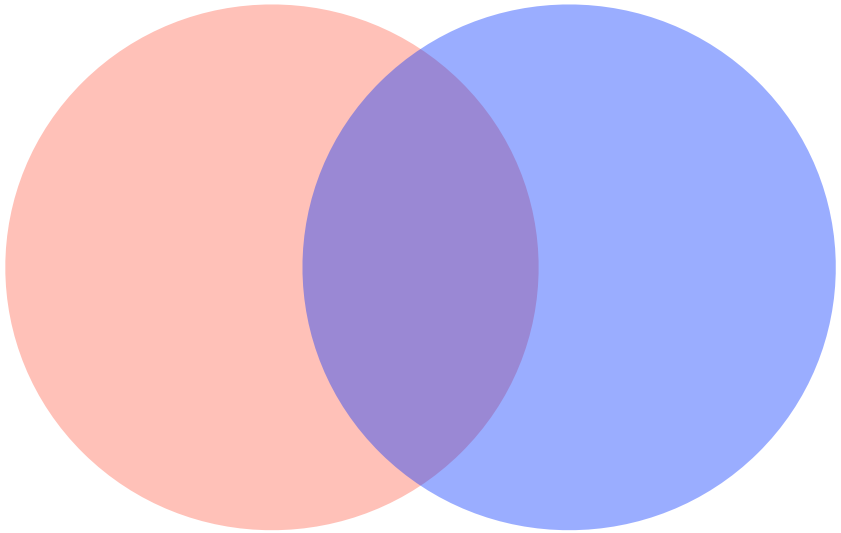
Intersection $A \cap B$

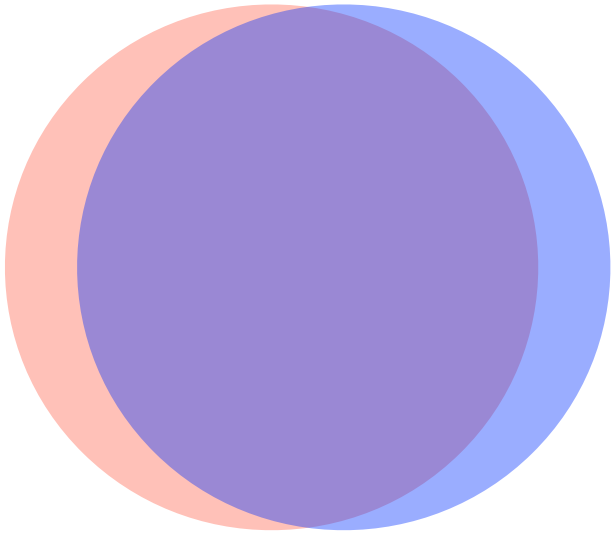
Difference A / B

Symmetric difference $A \triangle B$

Set Similarity

How can we describe how ***similar*** two sets are?





Set Similarity

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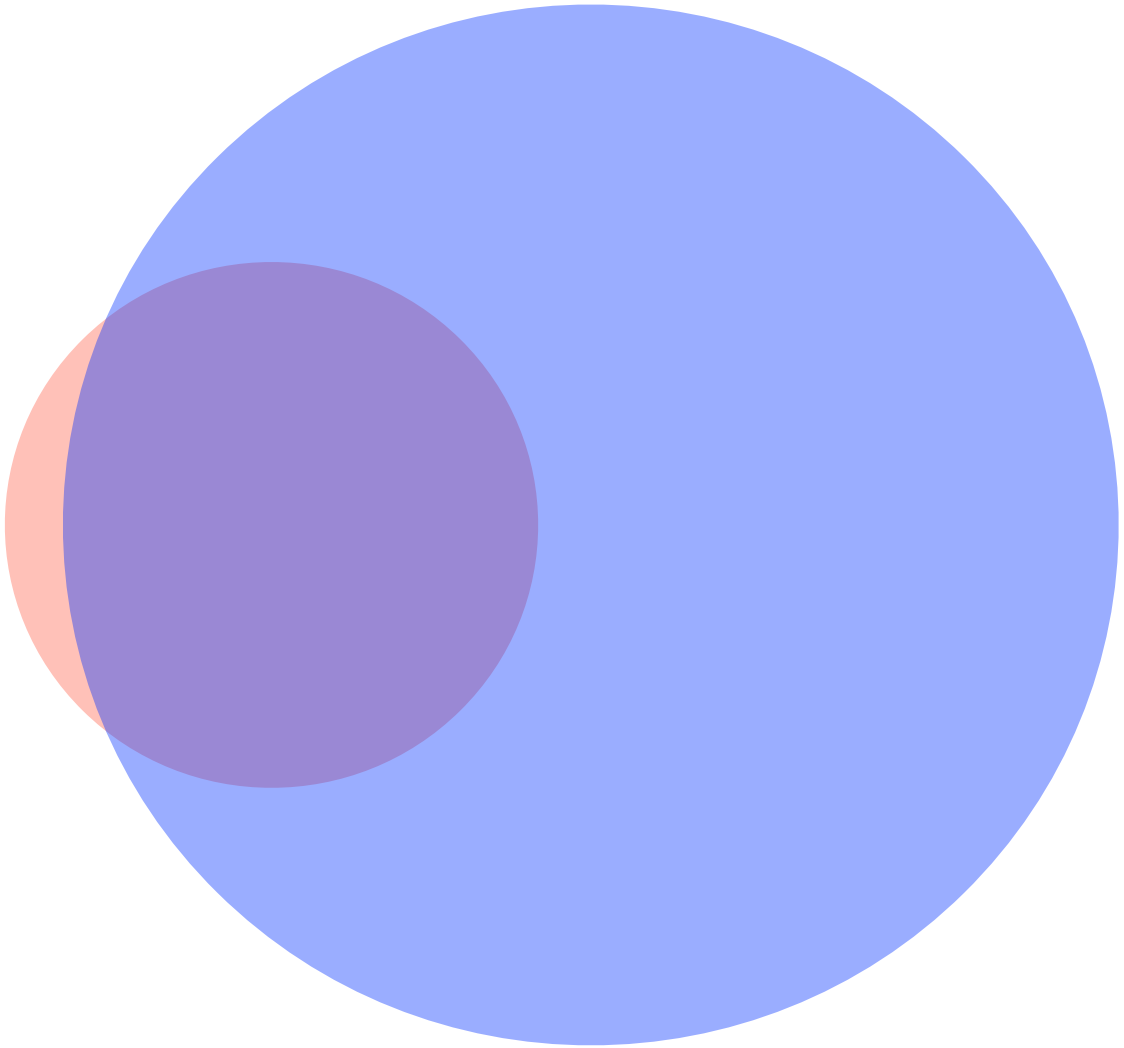
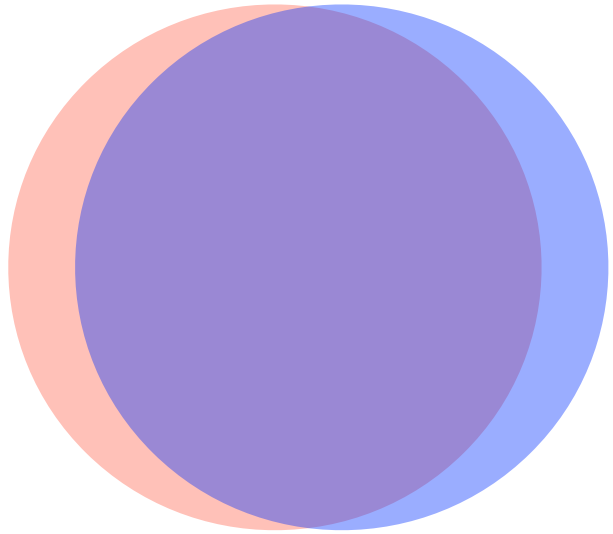
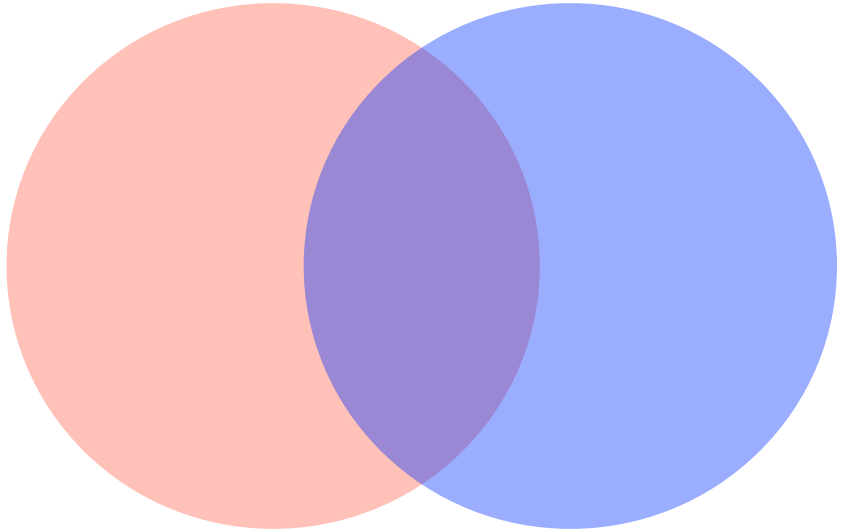




Set Similarity

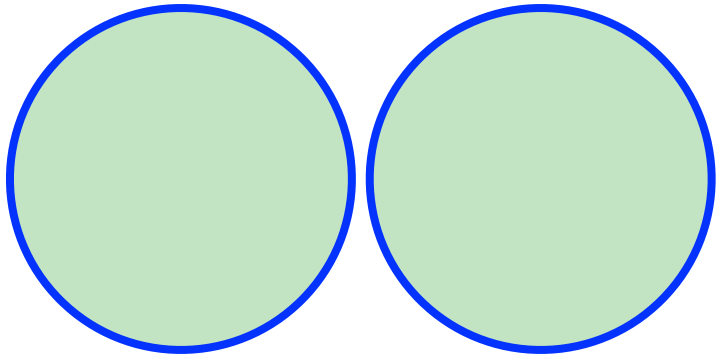
To measure **similarity** of A & B, we need both a measure of how similar the sets are but also the total size of both sets.



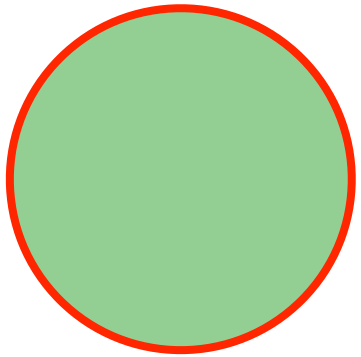
$$J = \frac{|A \cap B|}{|A \cup B|}$$

J is the ***Jaccard coefficient***

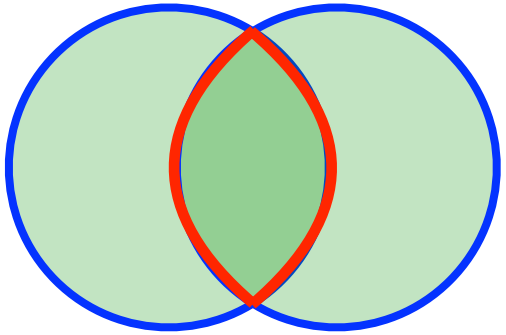
Set Similarity



$$\frac{|A \cap B|}{|A \cup B|} = 0$$



$$\frac{|A \cap B|}{|A \cup B|} = 1$$



$$0 < \frac{|A \cap B|}{|A \cup B|} < 1$$

Set Similarity

$$A = \{1, 2, 3, 4\} \qquad B = \{3, 4, 5, 6, 7\}$$

$$J = \frac{|A \cap B|}{|A \cup B|} =$$

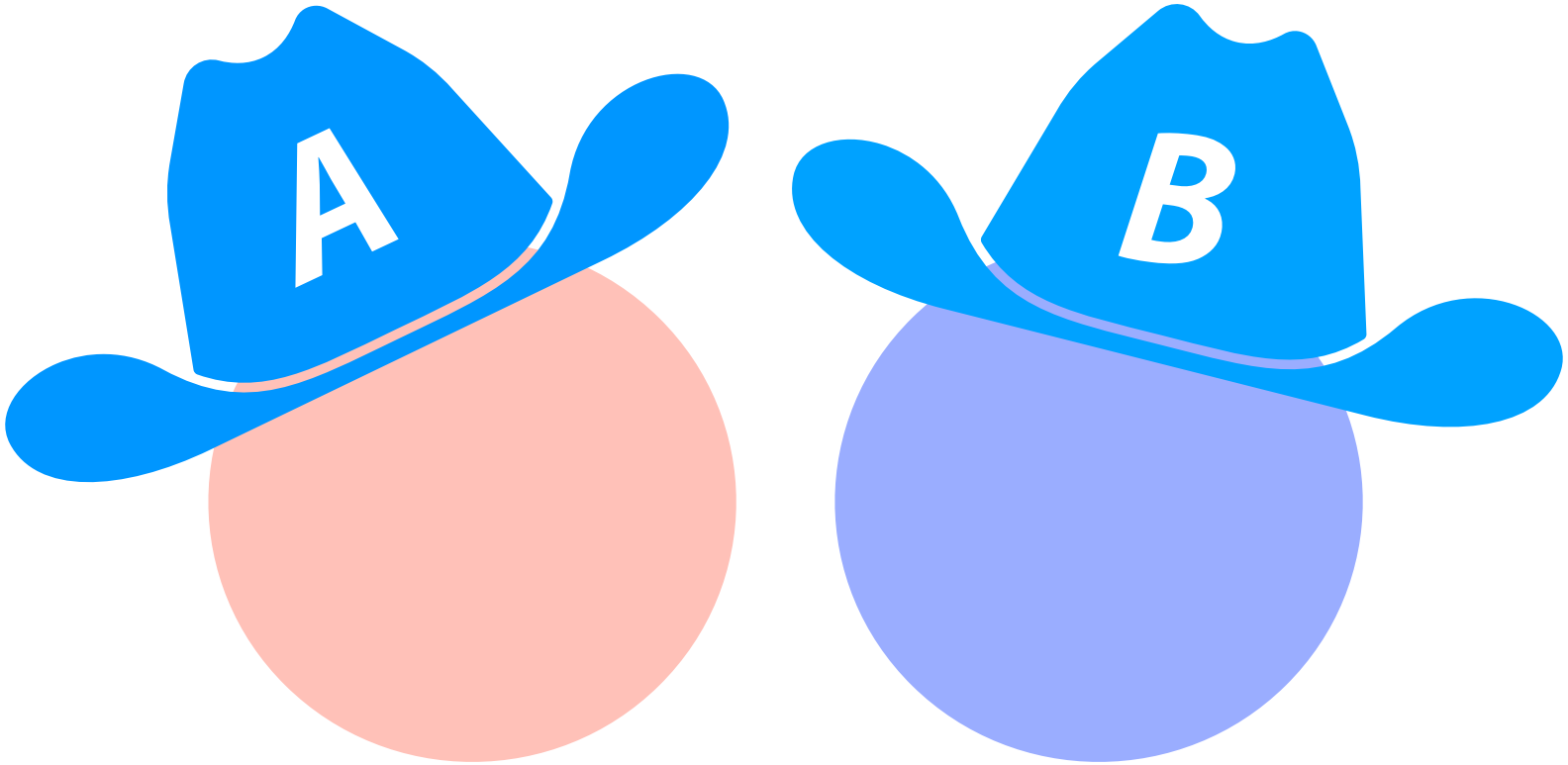
Set Similarity

$$A = \{1, 2, 3, 4\} \qquad B = \{3, 4, 5, 6, 7\}$$

$$J = \frac{|A \cap B|}{|A \cup B|} = \frac{|\{3,4\}|}{|\{1,2,3,4,5,6,7\}|} = \frac{2}{7}$$

Similarity Sketches

But what do we do when we only have a sketch?



Similarity Sketches

Imagine we 'sketched' two datasets by hashing all objects…

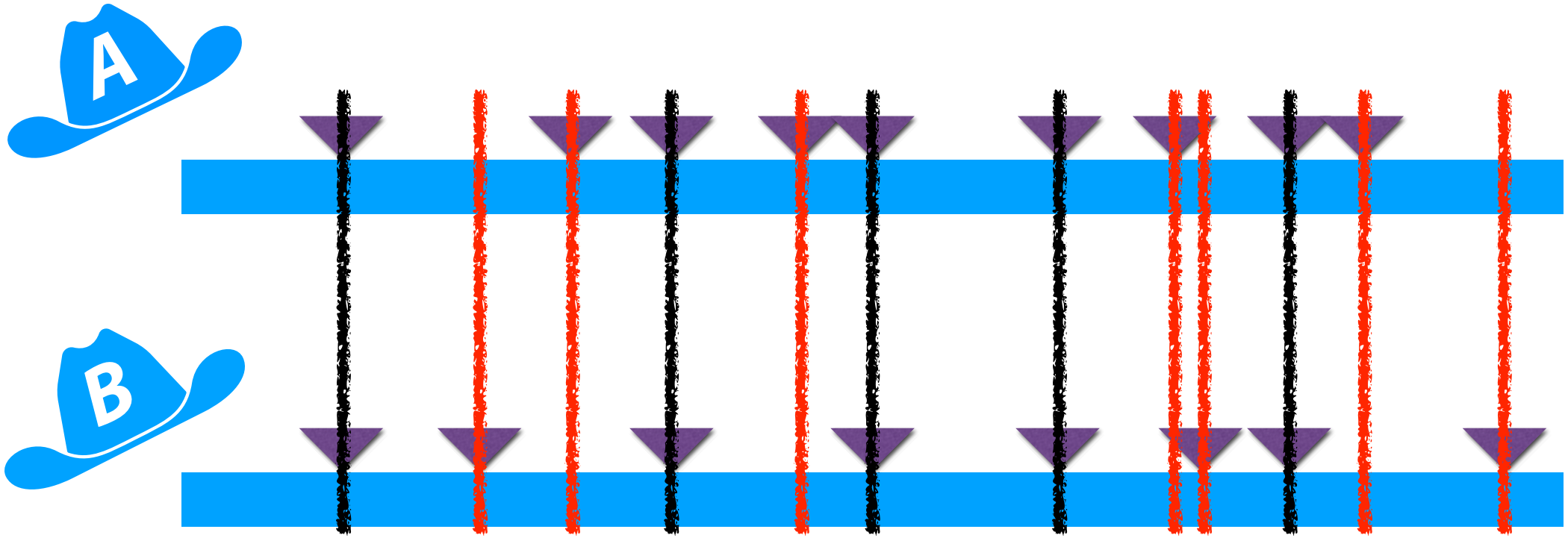
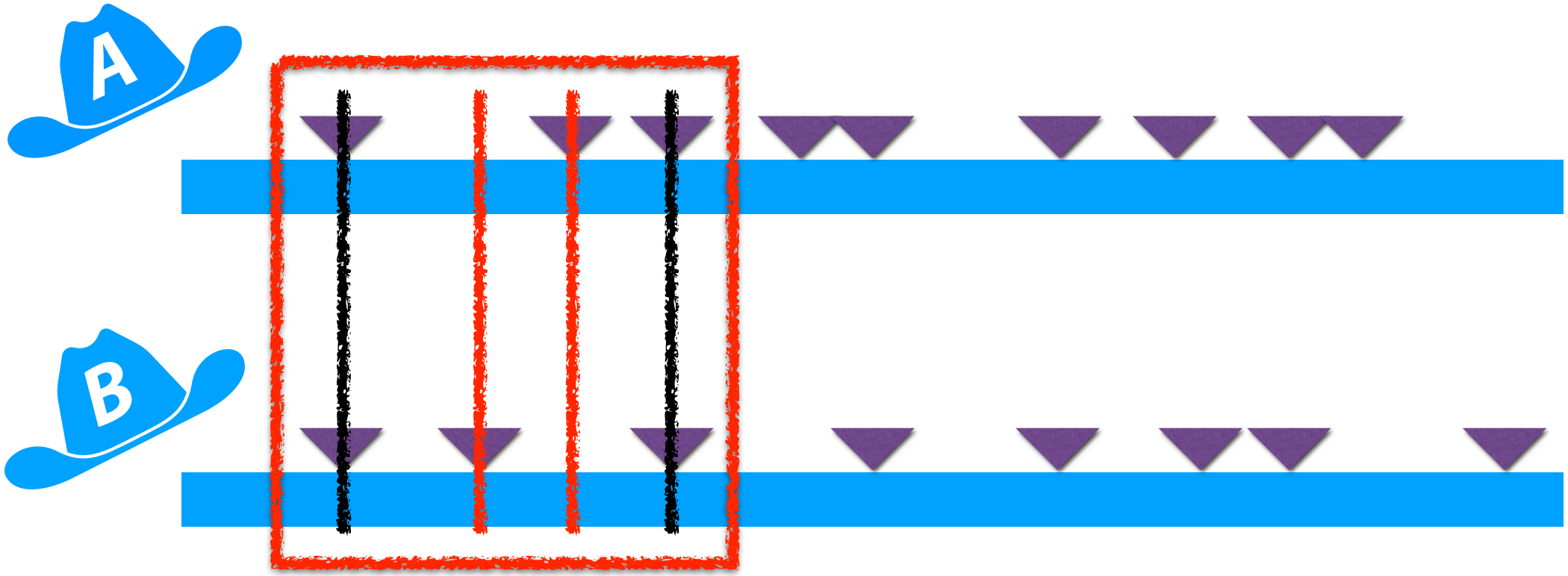


Image inspired by: Ondov B, Starrett G, Sappington A, Kostic A, Koren S, Buck CB, Phillippy AM. **Mash Screen: high-throughput sequence containment estimation for genome discovery**. *Genome Biol* 20, 232 (2019)

Similarity Sketches

Claim: Under SUHA, set similarity can be estimated by sketch similarity!



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Similarity Sketches

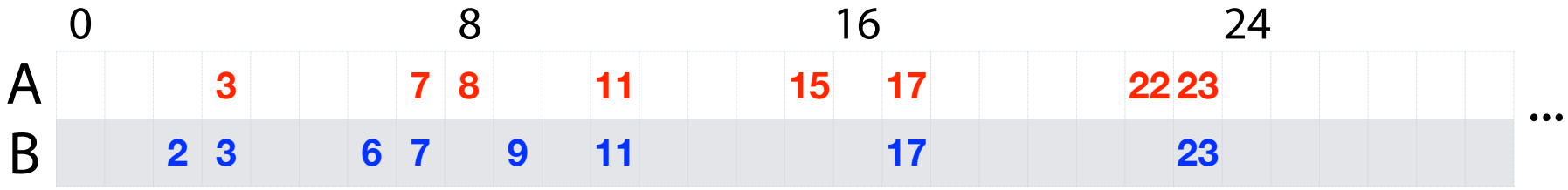
Say we find the 8 minimum hashes (bottom-8) for items in set A and B

Sketch A

3	15
7	17
8	22
11	23

Sketch B

2	9
3	11
6	17
7	23



Similarity Sketches

To get similarity, we want to estimate $|A \cup B|$ and $|A \cap B|$ …

Sketch A

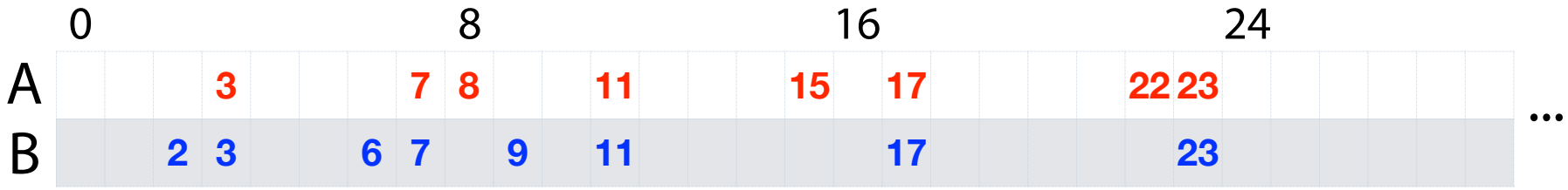
3	15
7	17
8	22
11	23

$\cup$

Sketch B

2	9
3	11
6	17
7	23

$=$



Similarity Sketches

To get similarity, we want to estimate $|A \cup B|$ and $|A \cap B|$ …

Sketch A

3	15
7	17
8	22
11	23

$\cup$

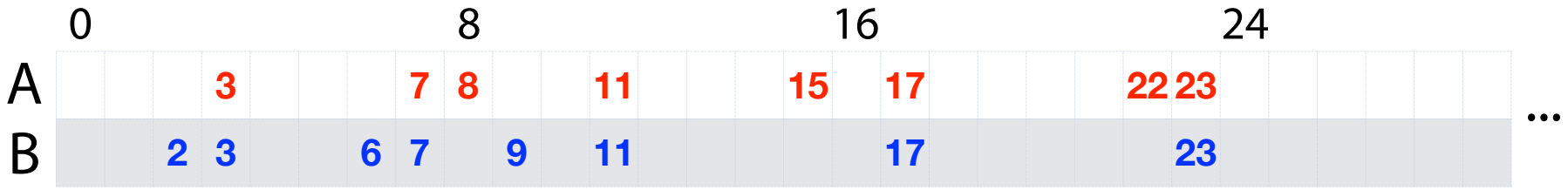
Sketch B

2	9
3	11
6	17
7	23

$=$

$|A \cup B|$

2	8
3	9
6	11
7	15



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To get similarity, we want to estimate $|A \cup B|$ and $|A \cap B|$ …

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$\cap$

Sketch B

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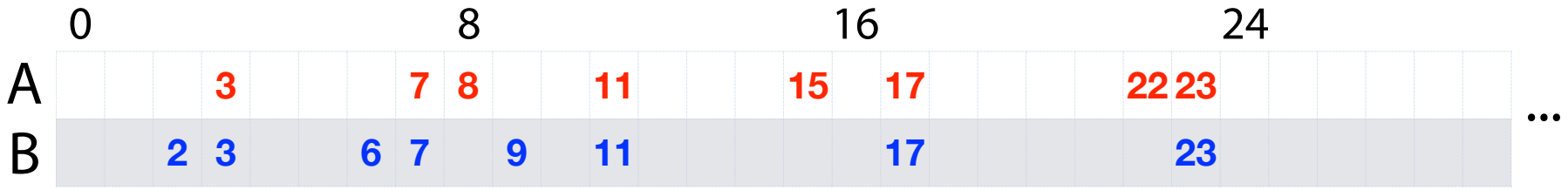
$=$



Similarity Sketches

Claim: Can approximate the intersection of our sketches as our datasets!

Sketch A

3	15
7	17
8	22
11	23

Sketch B

2	9
3	11
6	17
7	23

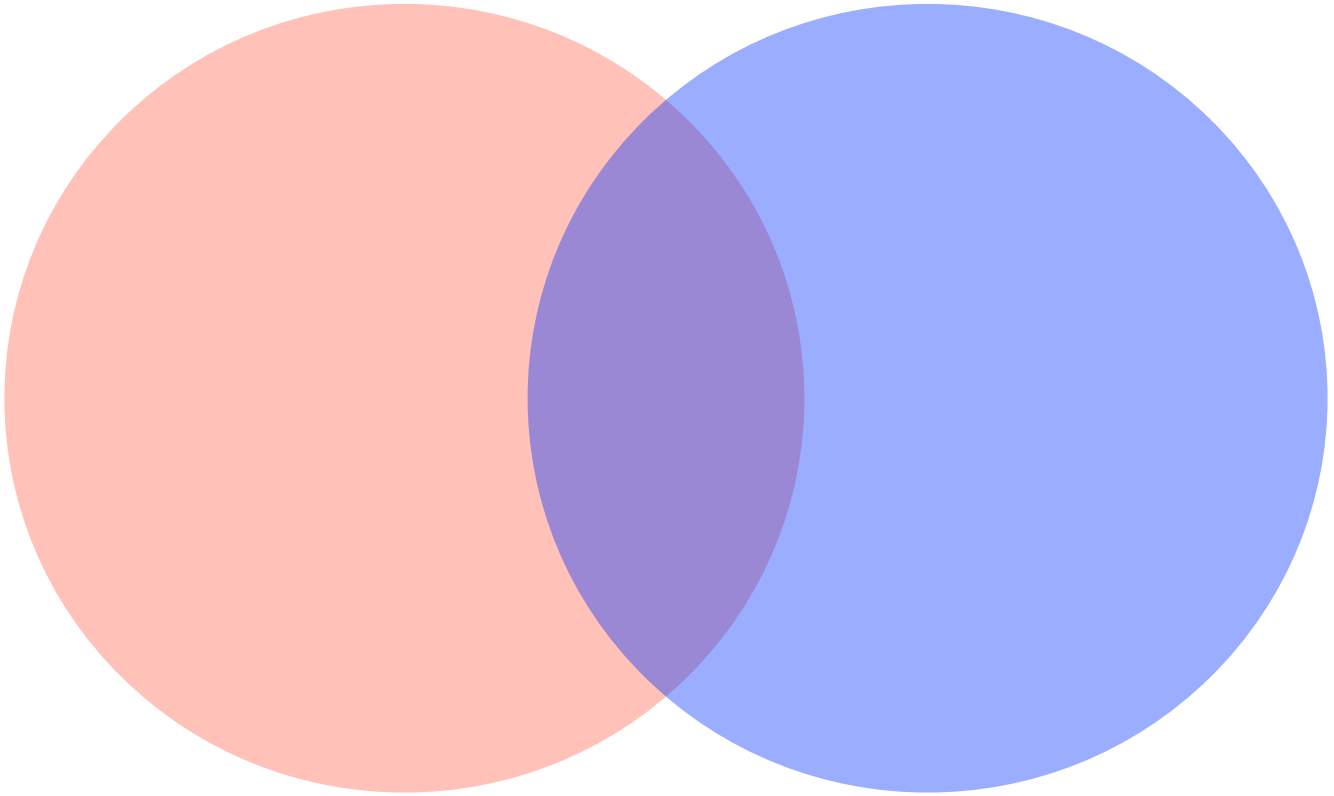
$|A \cup B|$

2	8
3	9
6	11
7	15

$$|A \cap B| \approx |S(A \cup B) \cap S(A) \cap S(B)|$$

Inclusion-Exclusion Principle

$$|A \cap B| =$$



Similarity Sketches

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3	11
6	17
7	23

$|A \cup B|$

2	8
3	9
6	11
7	15

kth minimum value (KMV) with $k = 8$, assuming hash range is integers in [0, 100):

$$= \frac{800/23 - 1 + 800/23 - 1 - 800/15 - 1}{800/15 - 1}$$

$$= \frac{34.782 + 34.782 - 53.333 - 1}{53.333 - 1}$$

$$\approx 0.29$$

$$\frac{|A| + |B| - |A \cup B|}{|A \cup B|}$$

Similarity Sketches

Claim: Can approximate the intersection of our sketches as our datasets!

Sketch A

3	15
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11	23

Sketch B

2	9
3	11
6	17
7	23

$|A \cup B|$

2	8
3	9
6	11
7	15

All computation here is simple

- Hash functions
- Bottom k (heap / sorted list)
- k^{th} minimum value (lookup)
- Get union sketch (merge heaps / lists)
- Calculate Jaccard (during merge)

1) Sequence decomposed into **kmers**

S_1 : CATGGACCGACCAG GCAGTACCGATCGT : S_2

CAT GAC GAC GTA CGA CGT

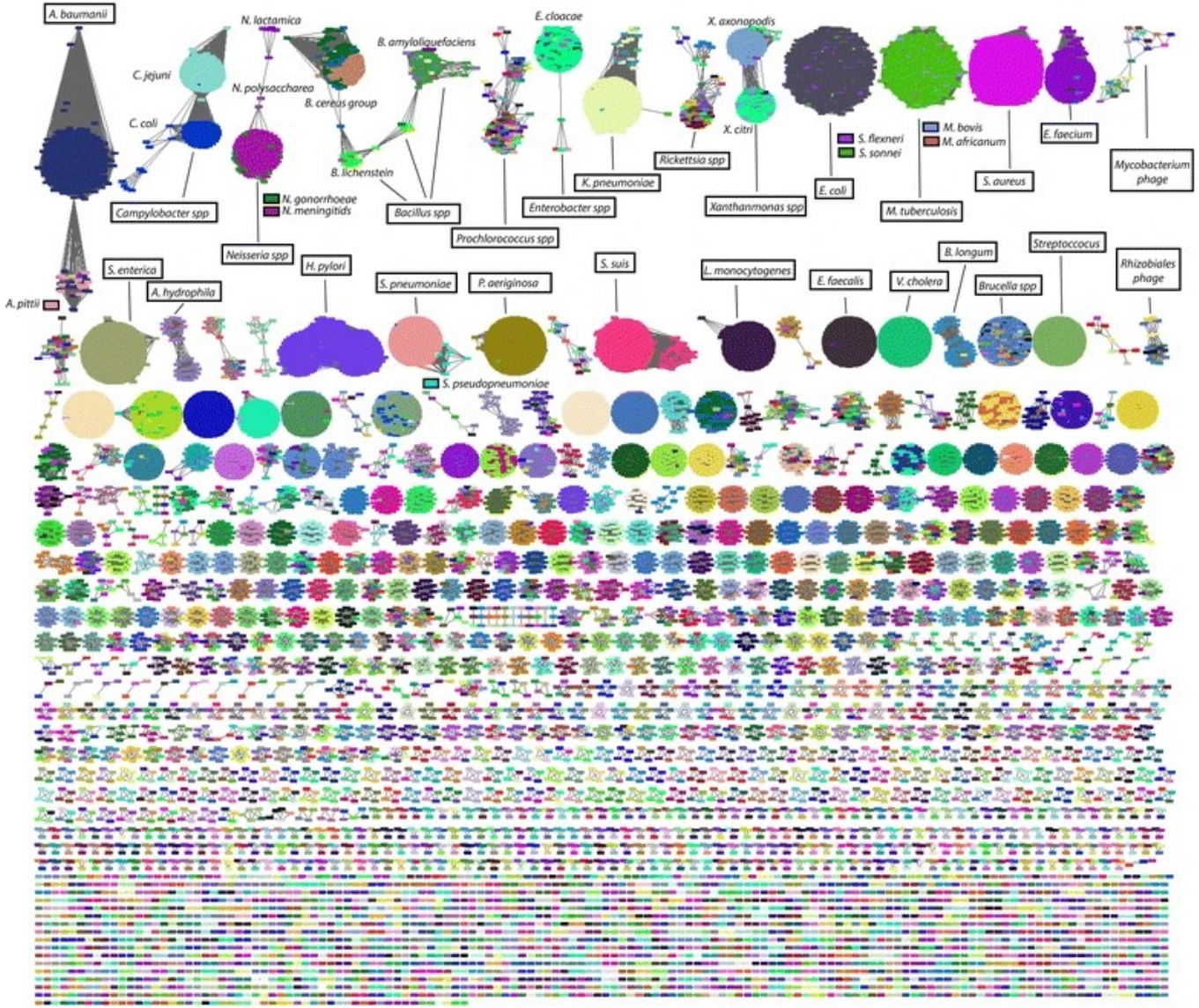
ATG ACC ACC AGT CCG TCG

TGG CCG CCA CAG ACC ATC

GGA CGA CAG GCA TAC GAT

Assembling large genomes with single-molecule sequencing and locality-sensitive hashing
Berlin et al (2015) *Nature Biotechnology*

Minhash in practice



Mash: fast genome and metagenome distance estimation using MinHash
Ondov et al (2016) *Genome Biology*

Sketching Summary

If my dataset is too large to handle, I can still answer many questions:

Does my object exist in a set?

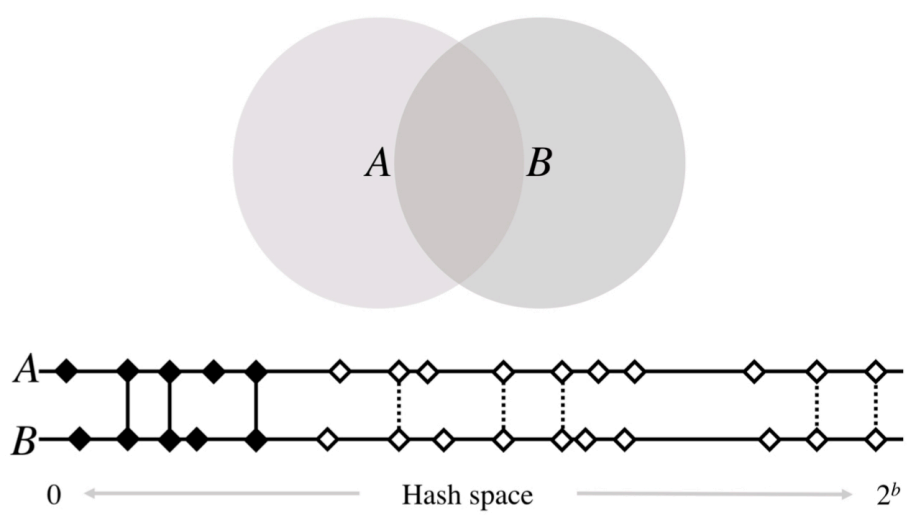
How often is a particular value repeated?

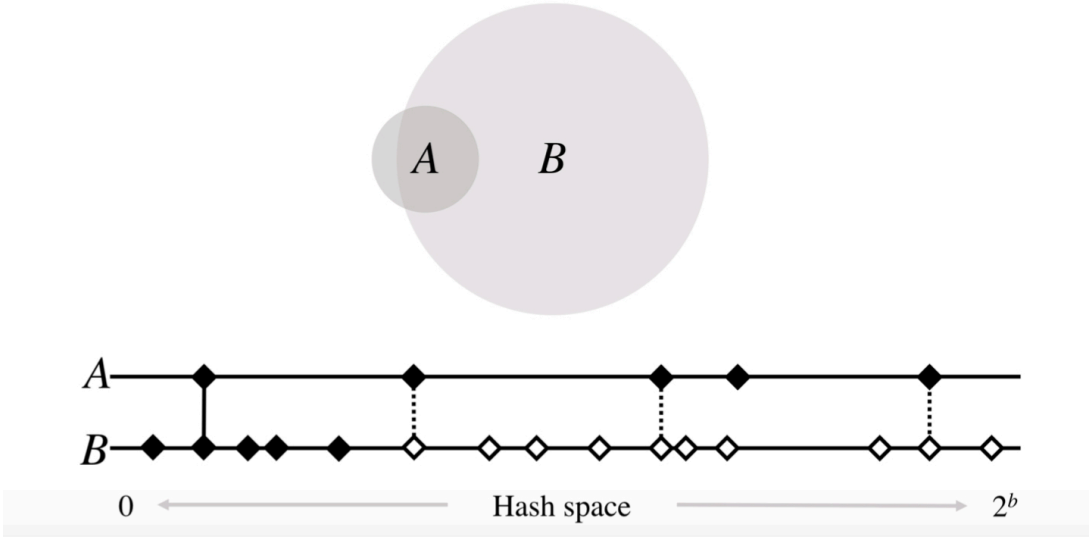
How many unique objects do I have?

How similar are two datasets?

Bonus Slides (Taking it one step further…)

Bottom-k minhash has low accuracy if the cardinality of sets are skewed

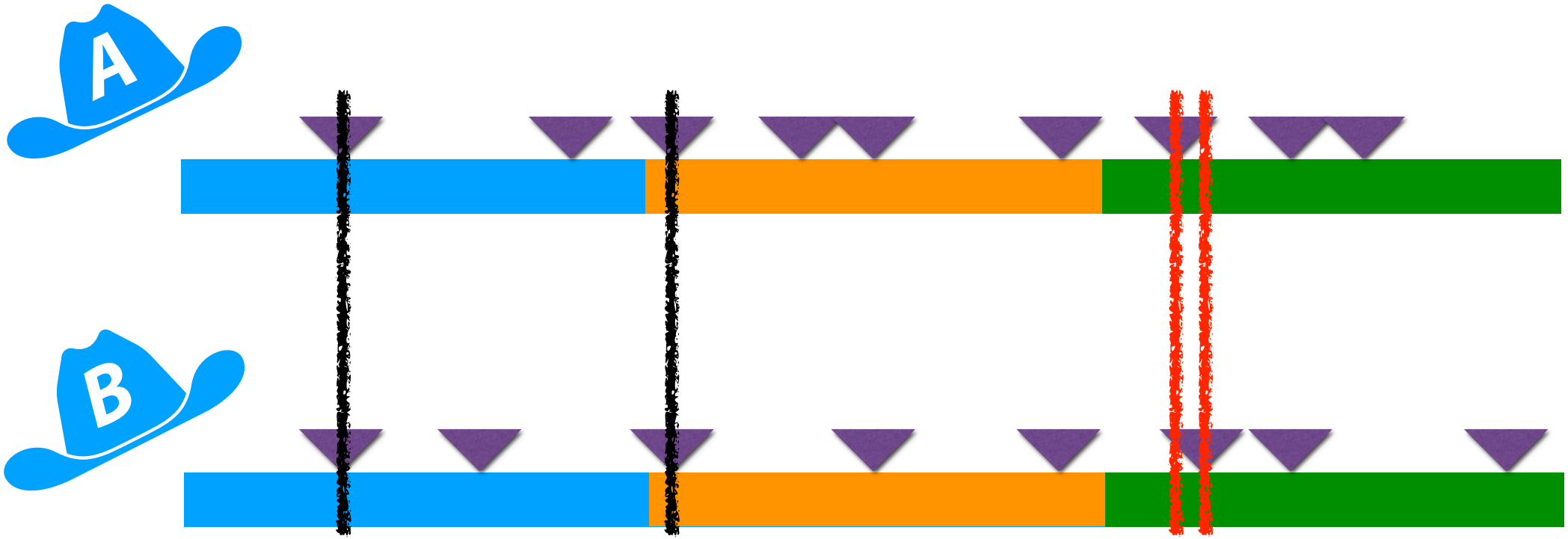




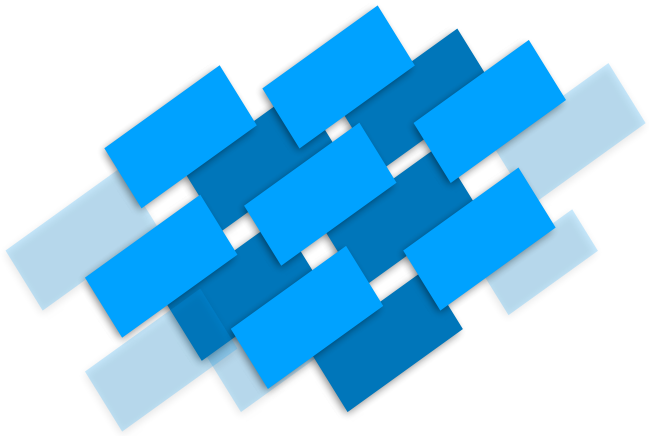
Ondov, Brian D., Gabriel J. Starrett, Anna Sappington, Aleksandra Kostic, Sergey Koren, Christopher B. Buck, and Adam M. Phillippy. **Mash Screen: High-throughput sequence containment estimation for genome discovery**. *Genome biology* 20.1 (2019): 1-13.

K-Partition Minhash

What if we instead took the minimum of k-partitions?



K-Partition Minhash



Hash

1010110101

0001111010

1101101011

1011010110

0101100000

0010001101

Partition

00

01111010

10001101

01

01100000

10

10110101

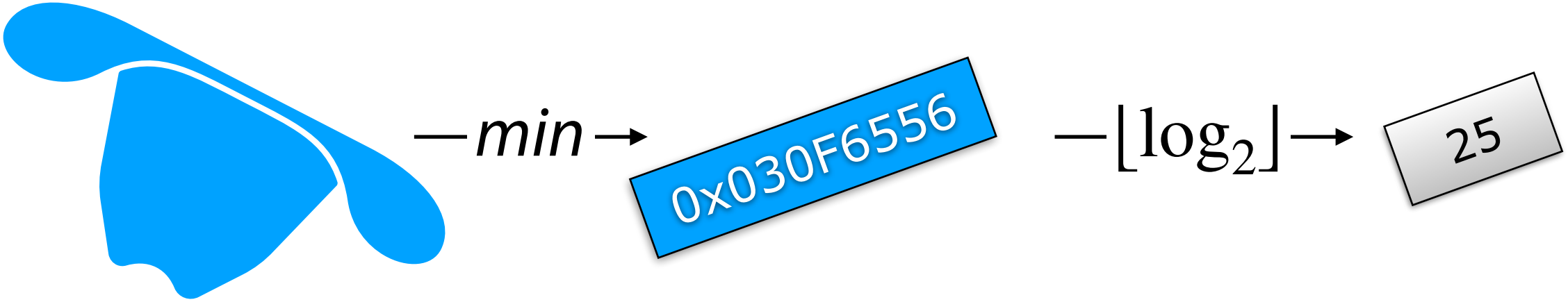
11010110

11

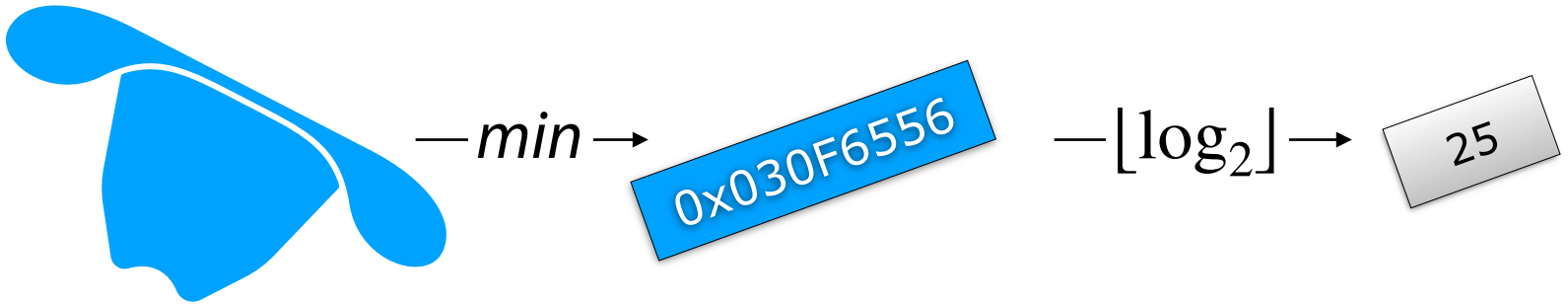
01101011

HyperLogLog

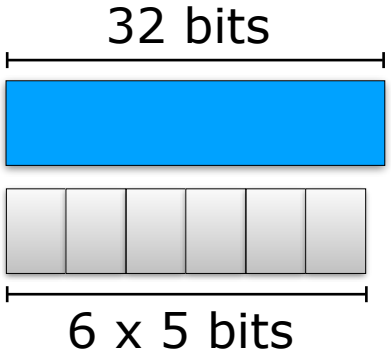
Instead of *minimum*, say we use *log-minimum*



HyperLogLog

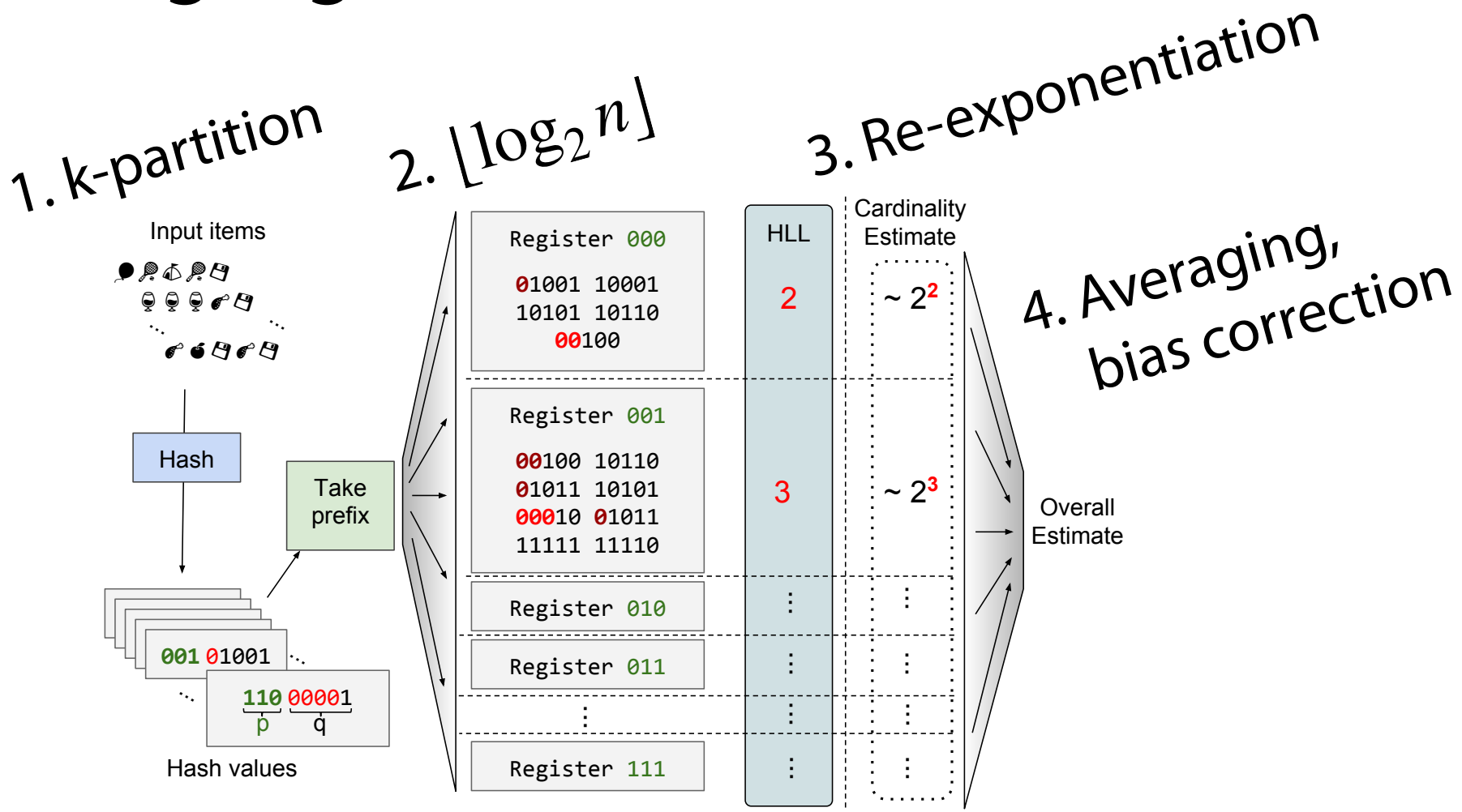


Pro: Representatives take $\log \log U$ rather than $\log U$ bits



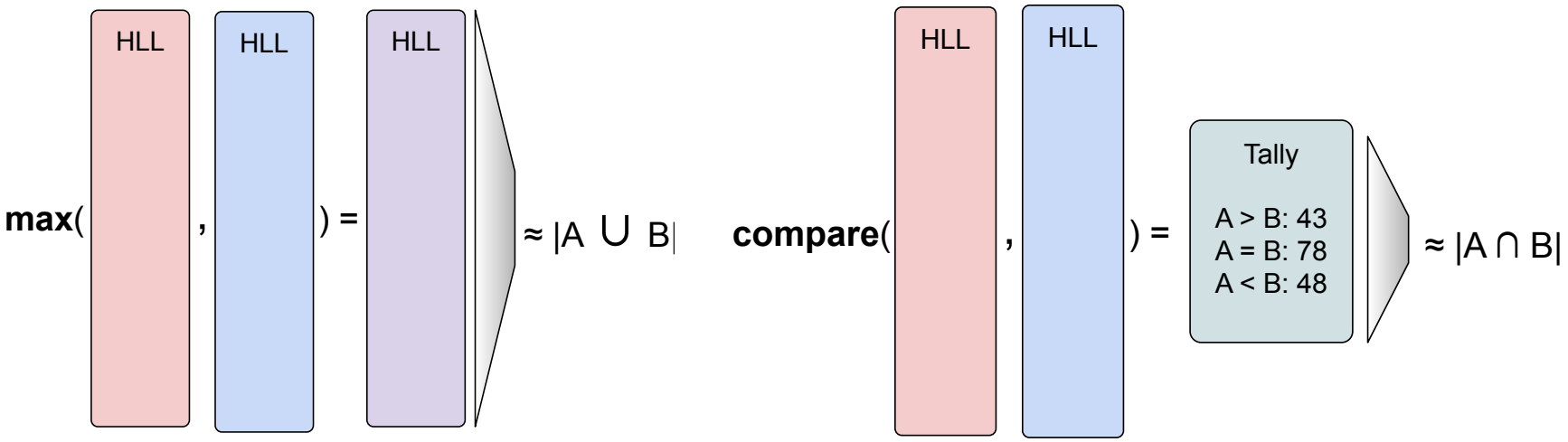
Con: Estimate is of $\lfloor \log_2 n \rfloor$; can re-exponentiate later, but with added variance & bias

HyperLogLog



Baker DN, Langmead B. **Dashing: fast and accurate genomic distances with HyperLogLog**. In press, *Genome Biology*.

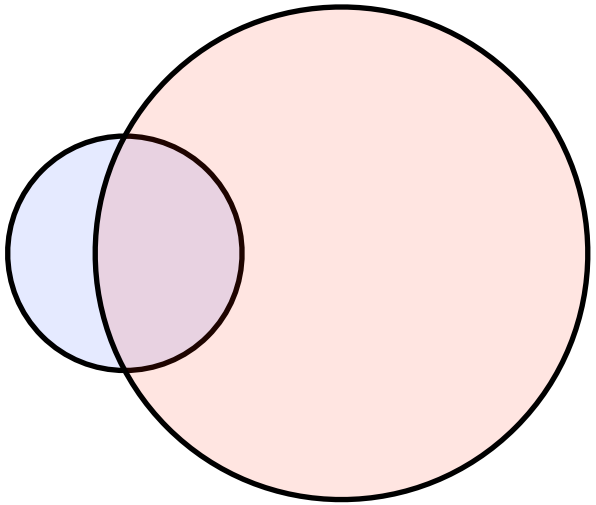
HyperLogLog

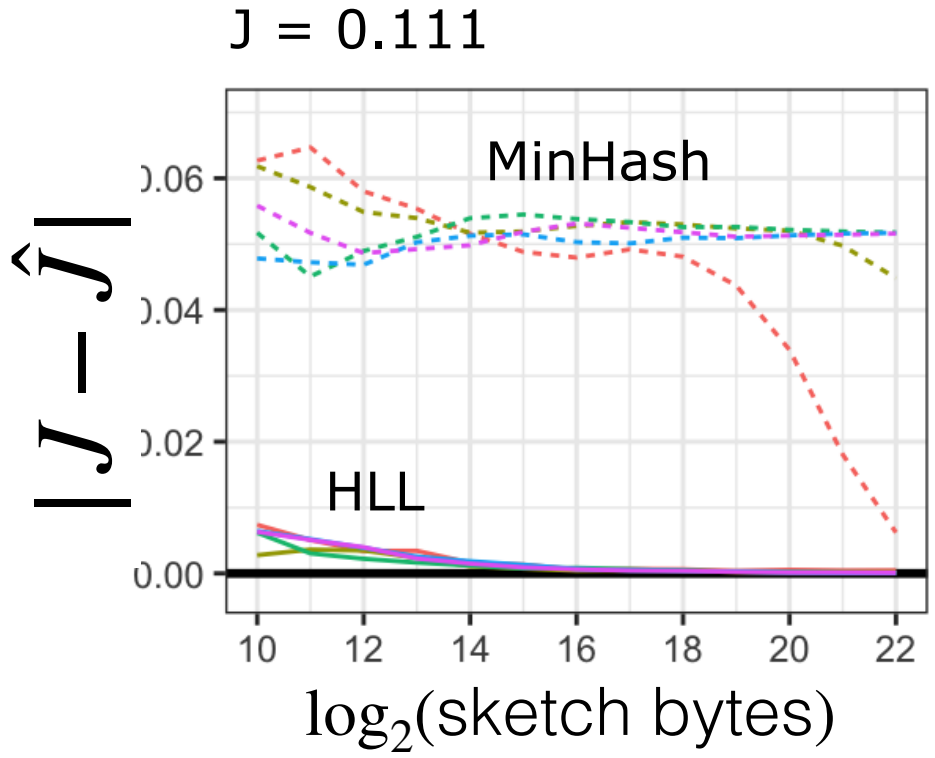


Union *and intersection* cardinalities can be estimated *directly*. No need for $|A \cap B| \approx |S(A \cup B) \cap S(A) \cap S(B)|$.

HyperLogLog

HLL handles lopsided sets better than bottom-k MinHash [1,2]

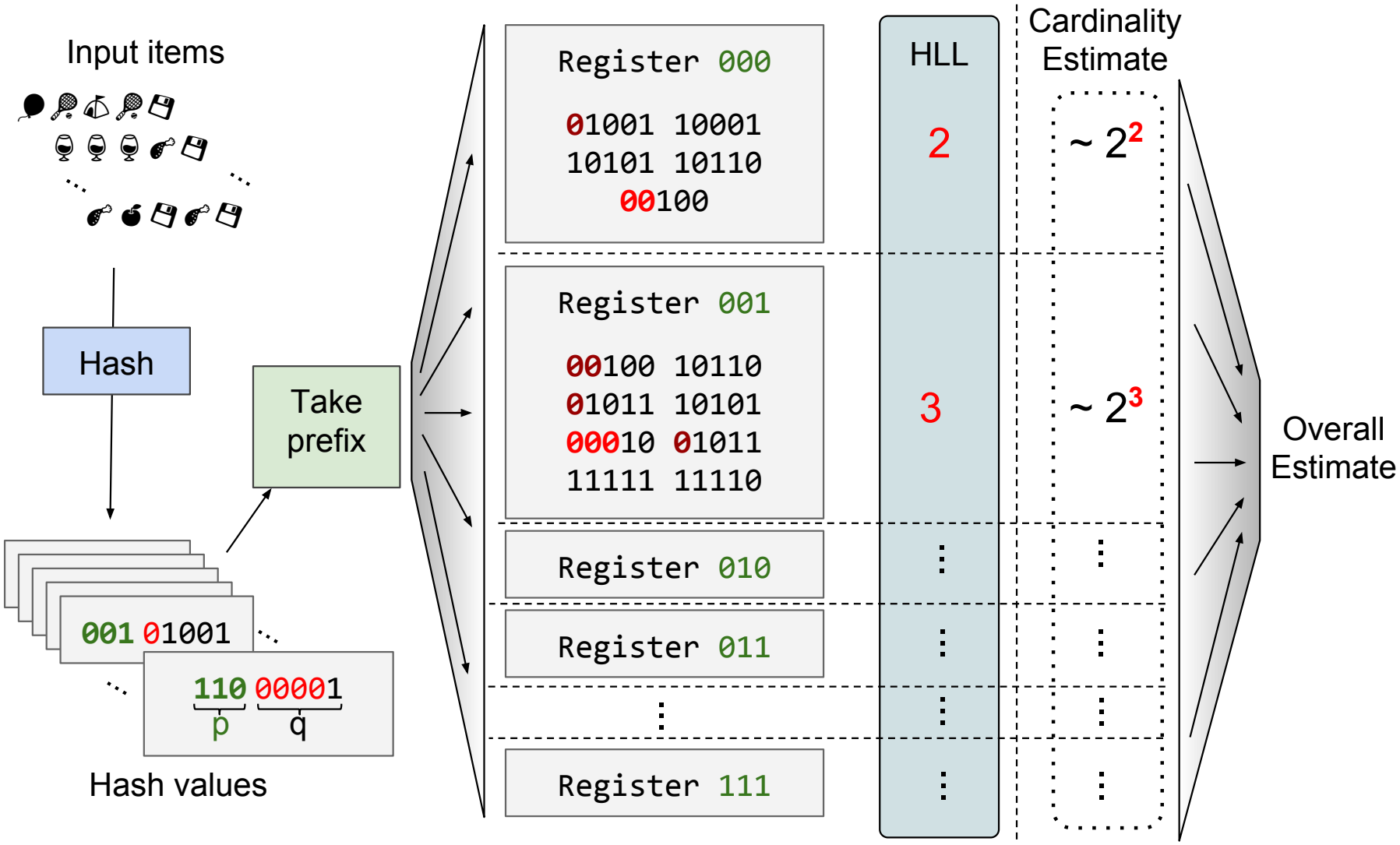




1. Koslicki, David, and Hooman Zabeti. **Improving MinHash via the containment index with applications to metagenomic analysis**. *Applied Mathematics and Computation* 354 (2019): 206-215.

2. Ondov B, Starrett G, Sappington A, Kostic A, Koren S, Buck CB, Phillippy AM. **Mash Screen: high-throughput sequence containment estimation for genome discovery**. *Genome Biol* 20, 232 (2019)

HyperLogLog



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