Data Structures and Algorithms

MinHash Sketch

CS 225

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December 4, 2024

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

Department of Computer Science

Thursday OH Time Change

Will be 10 - 10:50 AM instead of 11-12 PM

A hard time limit on OH

Learning Objectives

Review the concept of cardinality and cardinality estimation

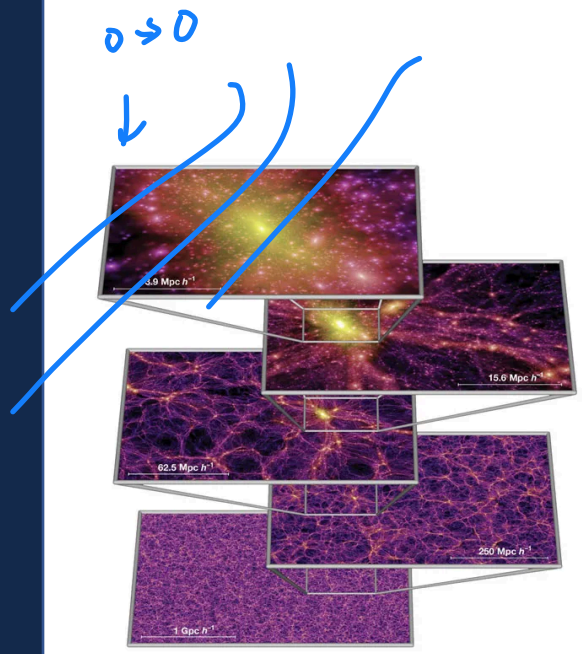
Improve our cardinality estimation approach

Demonstrate the relationship between cardinality and similarity

Introduce the MinHash Sketch for set similarity detection

Big Picture of Sketching

If you cant store or analyze a data collection using exact approaches…



Cannot store this!

Bloom Filter Sketch

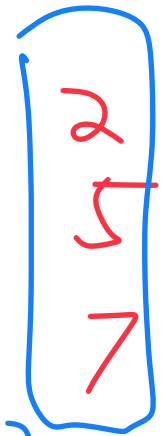
1) Hash every item one at a time
2) Store in a bloom filter

Query presence absense

Space efficient

Cardinality Sketch

1) Hash every item one at a time
2) Store the k-th minimum hash value

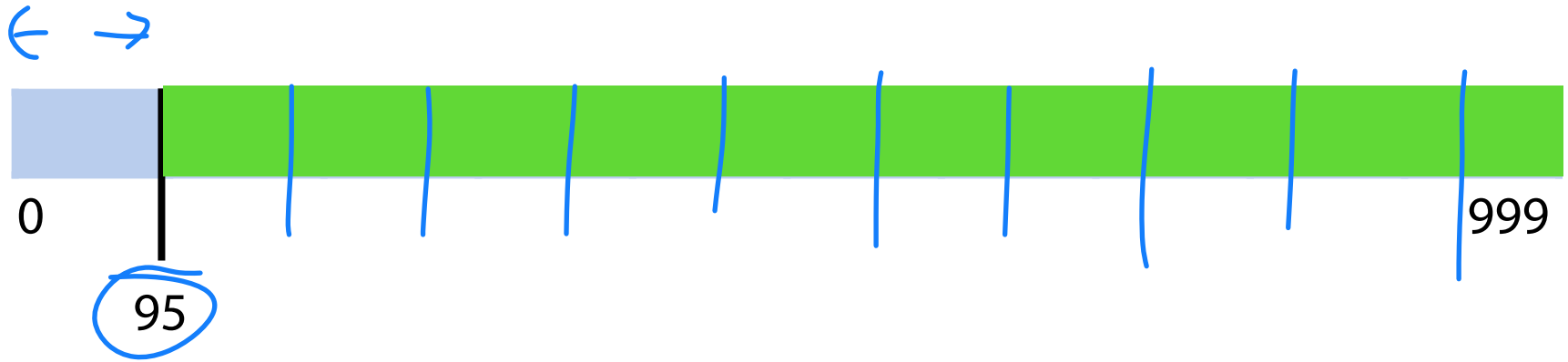


3rd minhash Val

Space efficient

Cardinality Estimation

Let min = 95. Can we estimate N, the cardinality of the set?



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

Assuming our first 'partition' is about average:

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

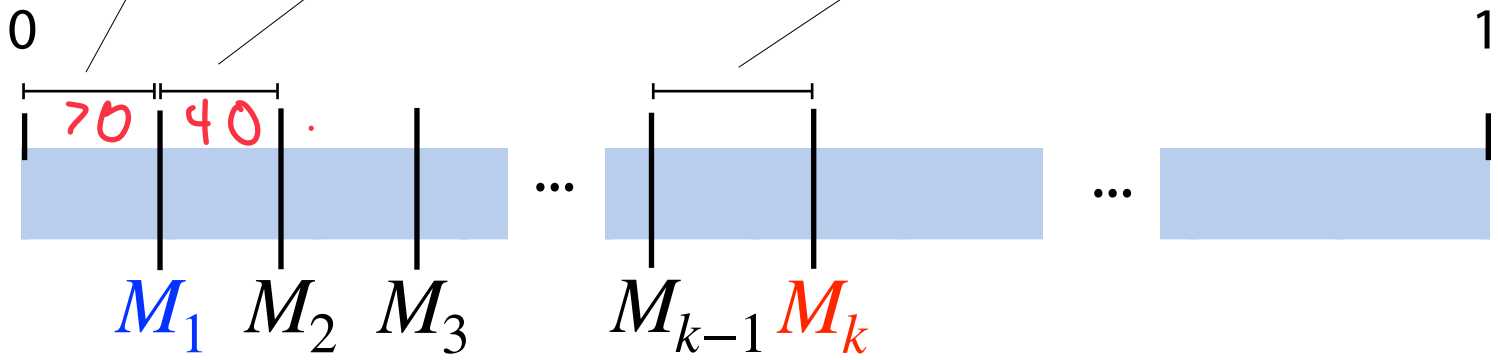
$$N+1 \approx 10.5$$

$$N \approx 9.5$$

Cardinality Sketch

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

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



k^{th} minimum value (KMV)

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

Cardinality Sketch

Given any dataset and a SUHA hash function, we can **estimate the number of unique items** by tracking the **k-th minimum hash value**.

Hash

0.253	0.839	0.327	0.655	0.491

.1 .1 .2

$\frac{1}{.253} - 1 \approx 3$ $\frac{2}{.327} - 1 \approx 5.1$

$\frac{3}{.491} - 1 \approx 5$

Applied Cardinalities

Cardinalities

$$|A|$$

$$|B|$$

$$|A \cup B|$$

$$|A \cap B|$$

Set similarities

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

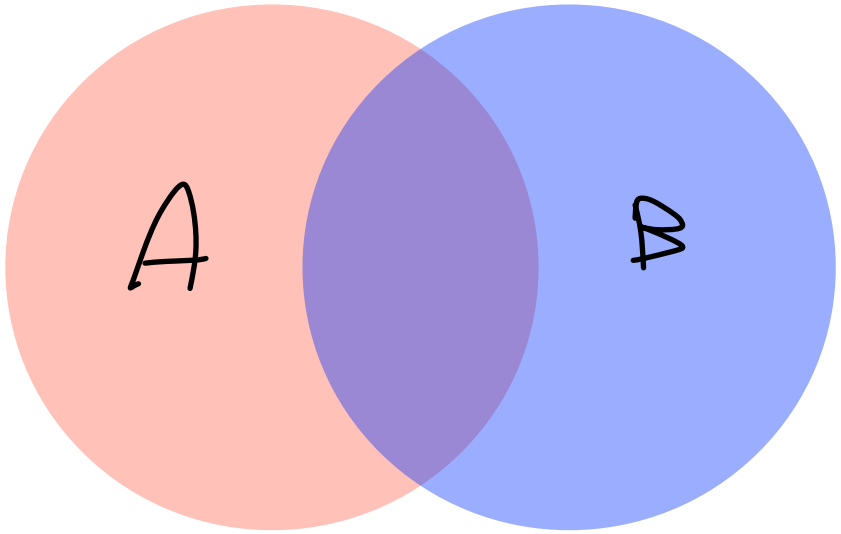
$$J = \frac{|A \cap B|}{|A \cup B|}$$

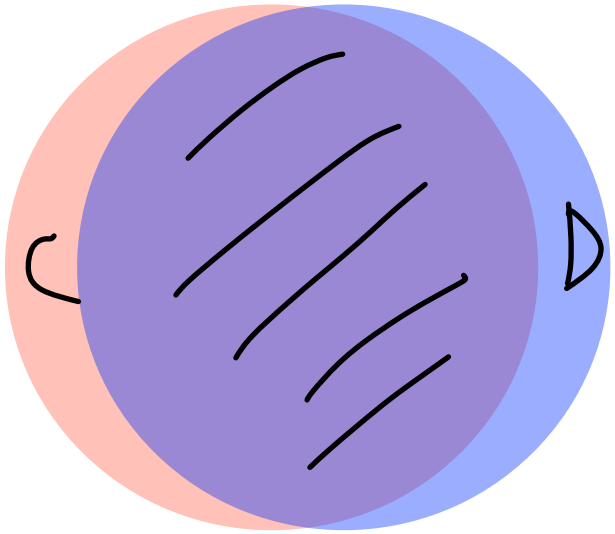
Real-world Meaning

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

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

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

Set Similarity Review

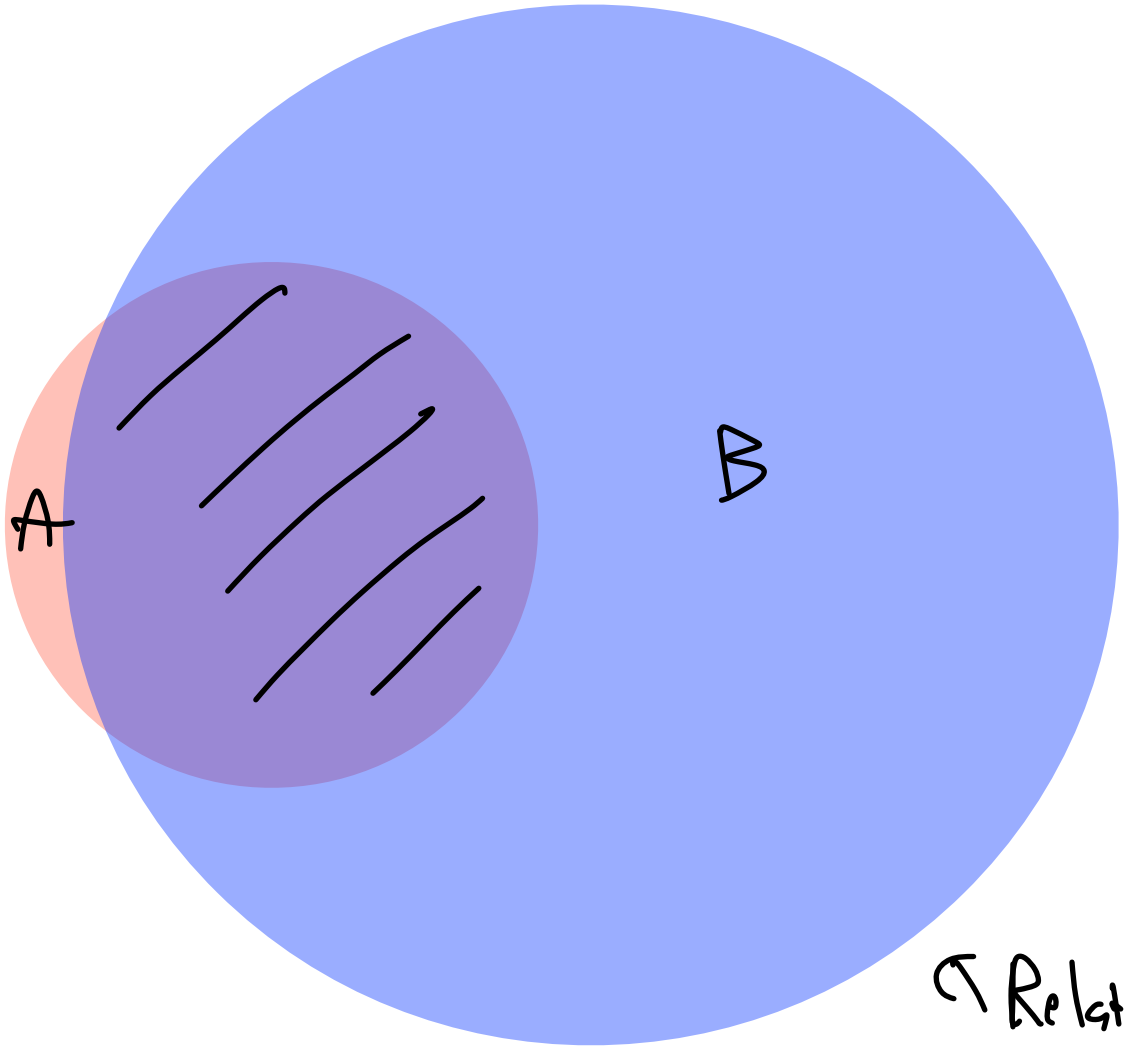
How can we describe how ***similar*** two sets are?

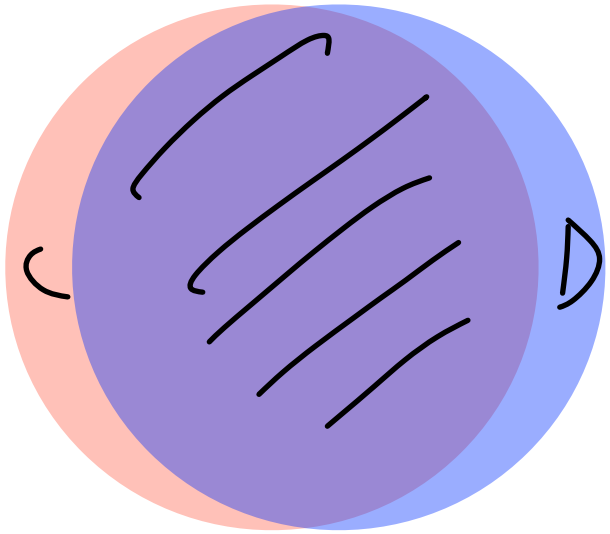




Set Similarity Review

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



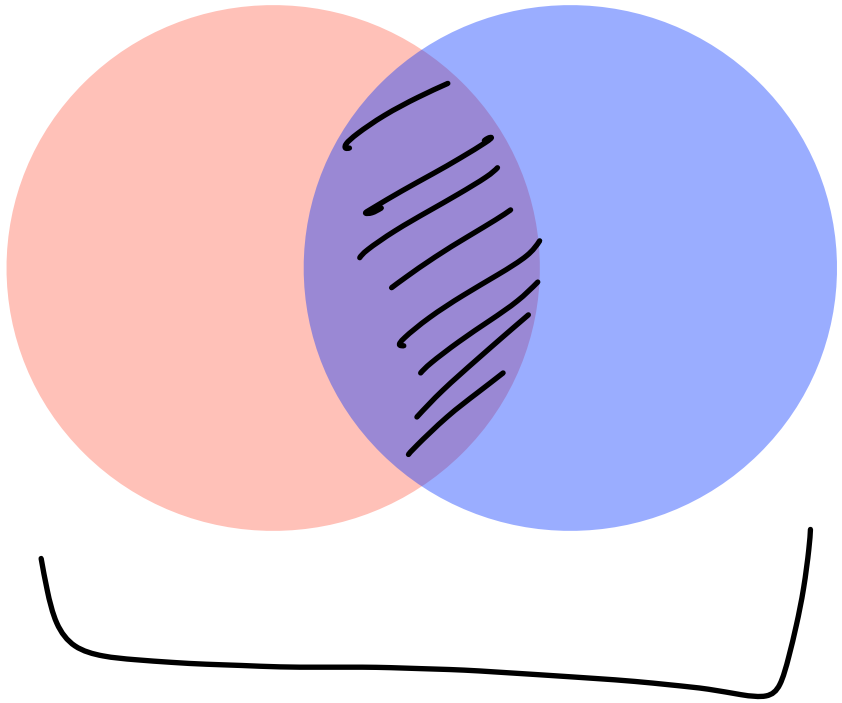


↑
More similar

↑ Relative # of values in total is larger

Set Similarity Review

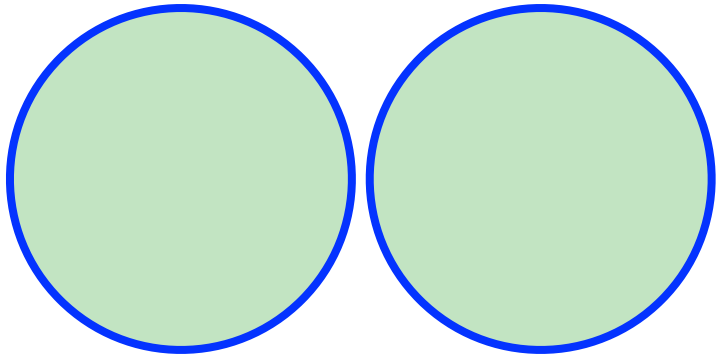
To measure **similarity** of A & B, we need both a measure of how similar the sets are but also the total size of both sets.



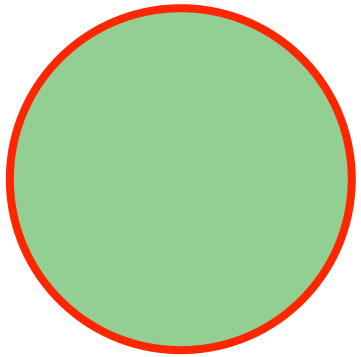
$$J = \frac{|A \cap B|}{|A \cup B|}$$

J is the ***Jaccard coefficient***

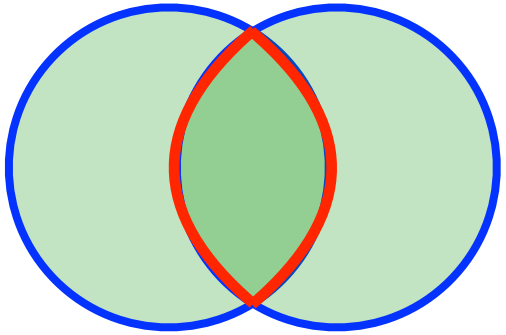
Set Similarity Review



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



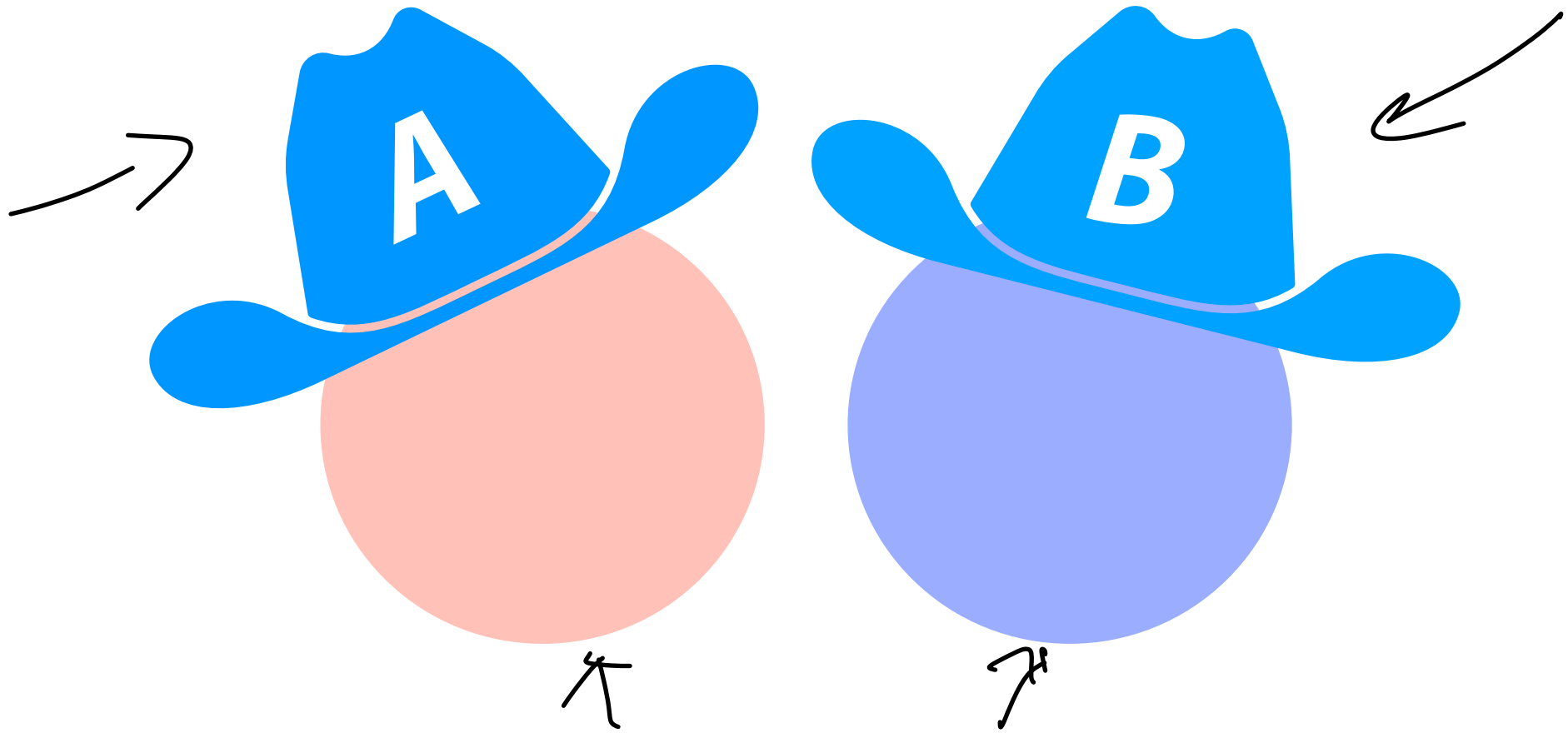
$$\frac{|A \cap B|}{|A \cup B|} = 1$$



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

Similarity Sketches

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



Similarity Sketches

Imagine we have two datasets represented by their kth minimum values

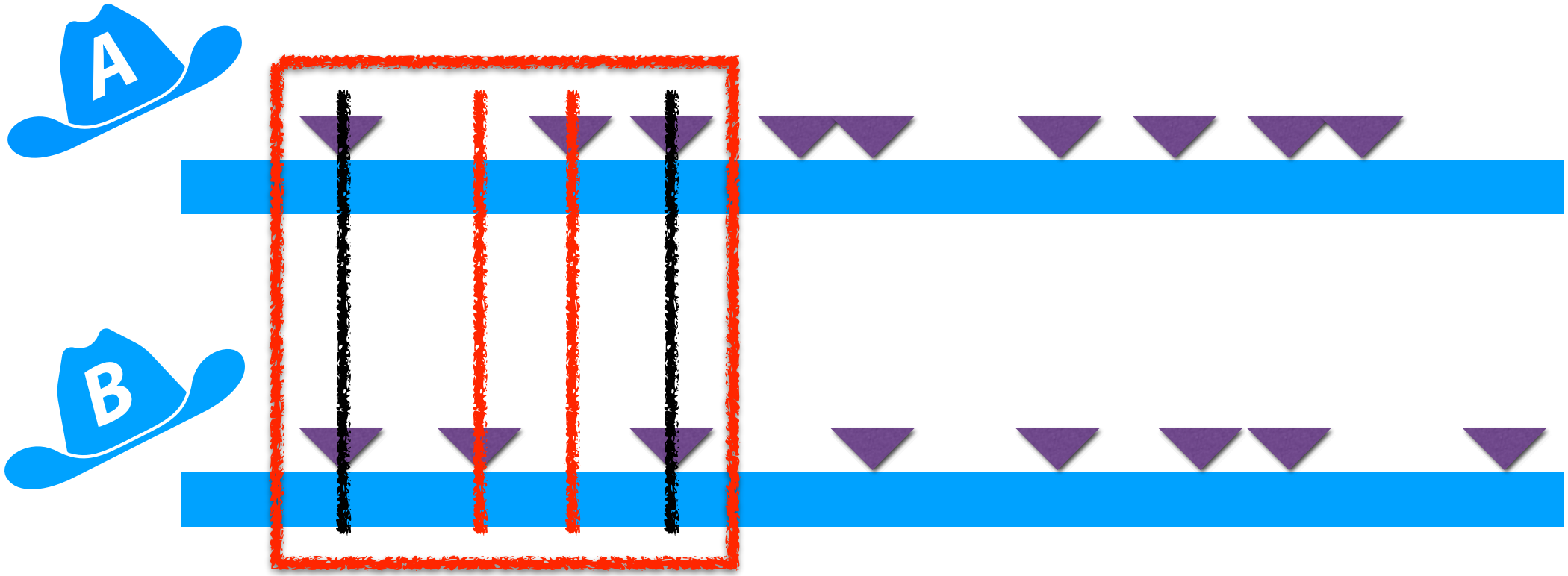


Image inspired by: Ondov B, Starrett G, Sappington A, Kostic A, Koren S, Buck CB, Phillippy AM. **Mash Screen: high-throughput sequence containment estimation for genome discovery**. *Genome Biol* 20, 232 (2019)

Similarity Sketches

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

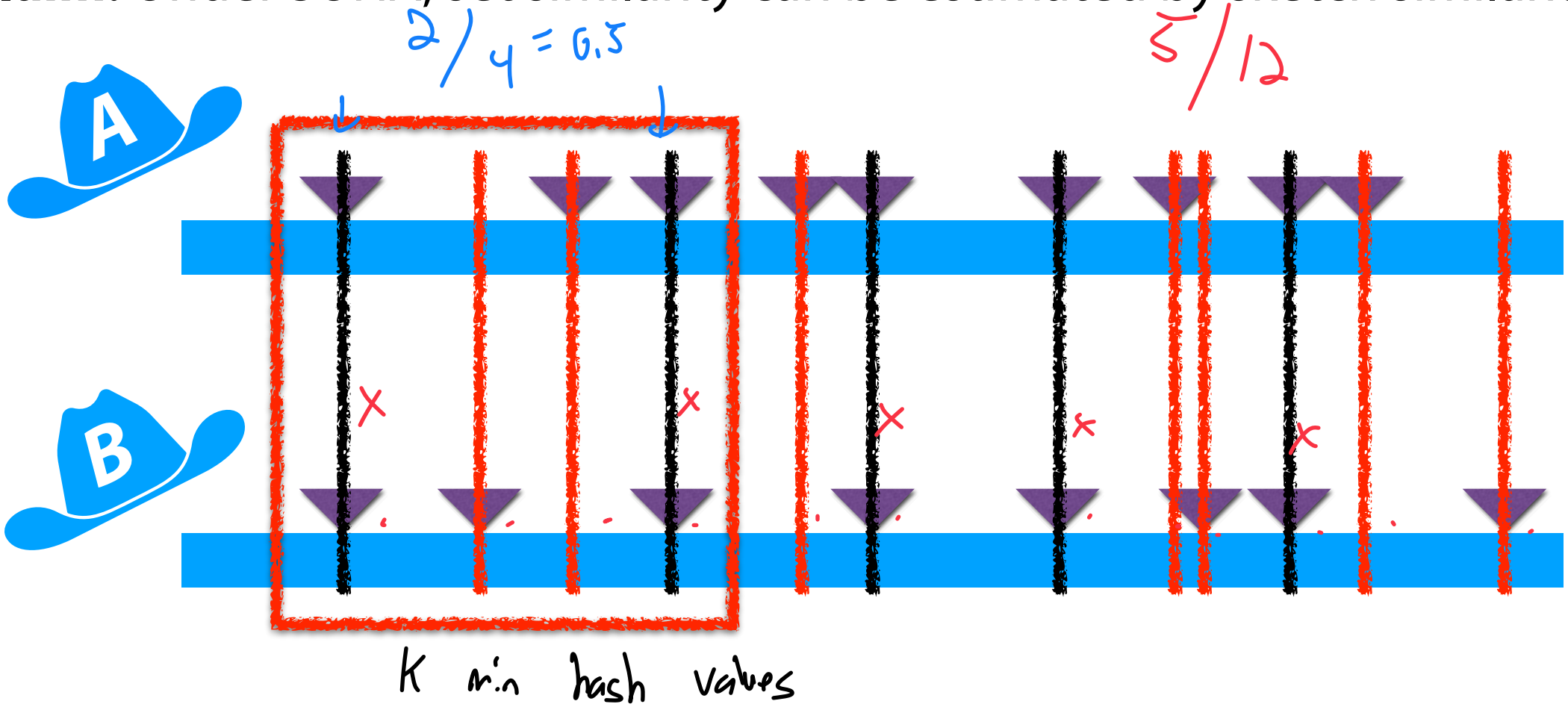
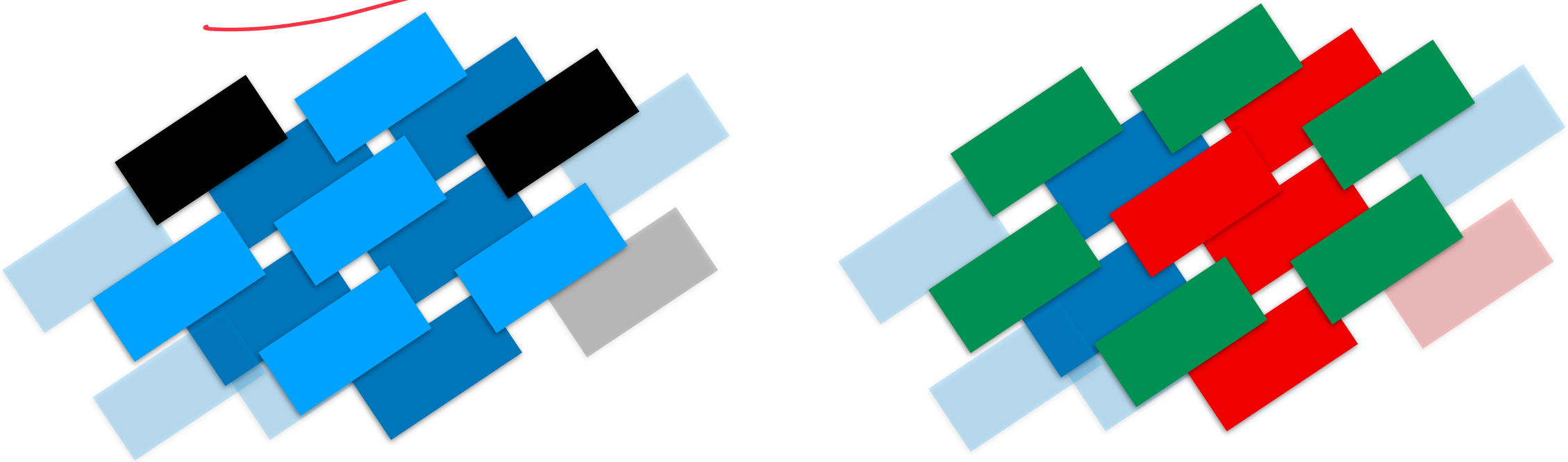


Image inspired by: Ondov B, Starrett G, Sappington A, Kostic A, Koren S, Buck CB, Phillippy AM. **Mash Screen: high-throughput sequence containment estimation for genome discovery**. *Genome Biol* 20, 232 (2019)

MinHash Sketch

The **k-th minimum value sketch** is built by tracking k minima but only uses one value (the k-th minima) to get **cardinality!**

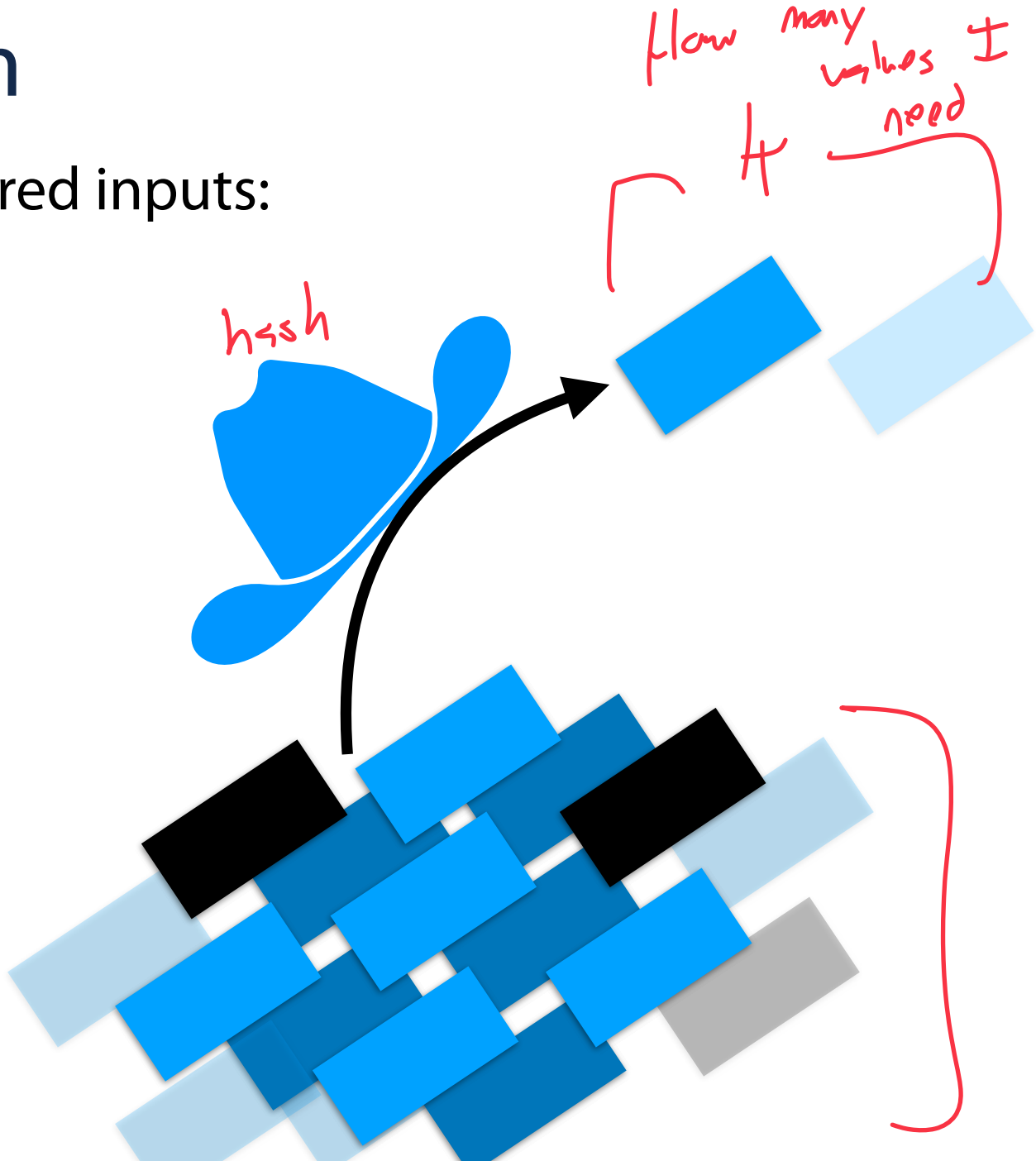
We can extend this approach into a full **MinHash sketch** that can also estimate **set similarities.**



MinHash Construction

A MinHash sketch has three required inputs:

1. A hashable dataset
2. A hash function
   ↳ This is hard!
3. The size of k



MinHash Construction

S = { 16, 8, 4, 13, 15}

h(x) = x % 7

k = 3

Algorithm is trivial:

1. Hash each item
2. Keep the k-minimum values in memory
   (Ignore collisions / duplicates)

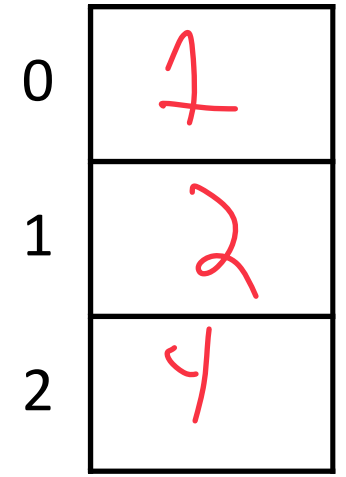
16 → 2

8 → 1

4 → 4

13 → 6

15 → 1



MinHash Jaccard Estimation

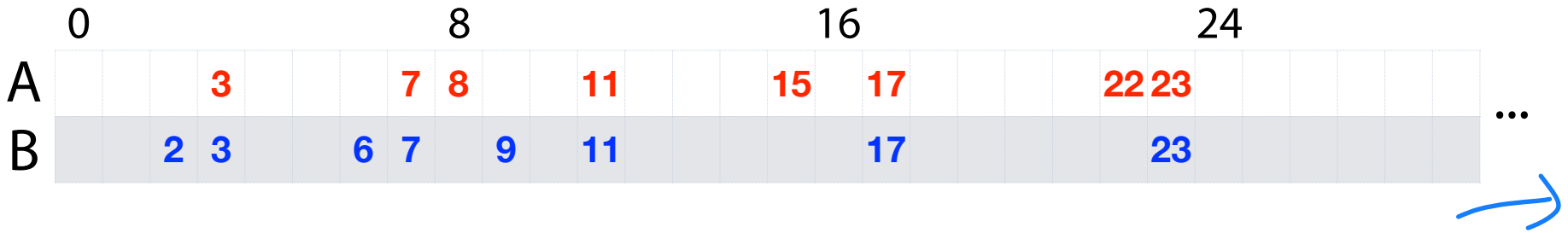
Given sets A and B sampled uniformly from [0, 100], store the bottom-8 **MinHash:**

Sketch A

3	15
7	17
8	22
11	23

Sketch B

2	9
3	11
6	17
7	23



MinHash Jaccard Estimation

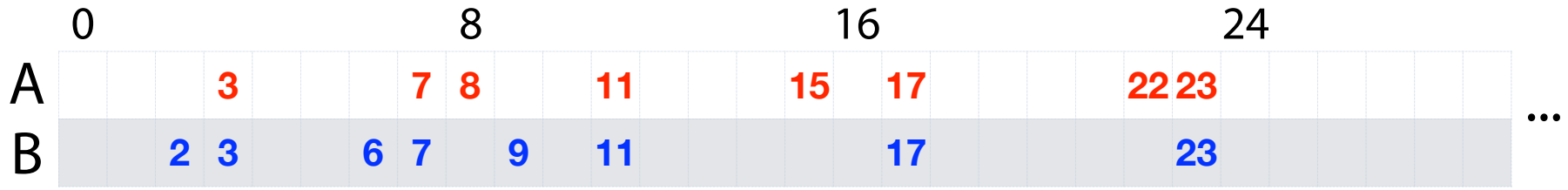
We want to estimate the Jaccard Coefficient: $\frac{|A \cup B|}{|A \cap B|}$

Sketch A

3	15
7	17
8	22
11	23

Sketch B

2	9
3	11
6	17
7	23



MinHash Jaccard Estimation

What do we know about $A \cup B$?

Sketch A

3	15
7	17
8	22
11	23

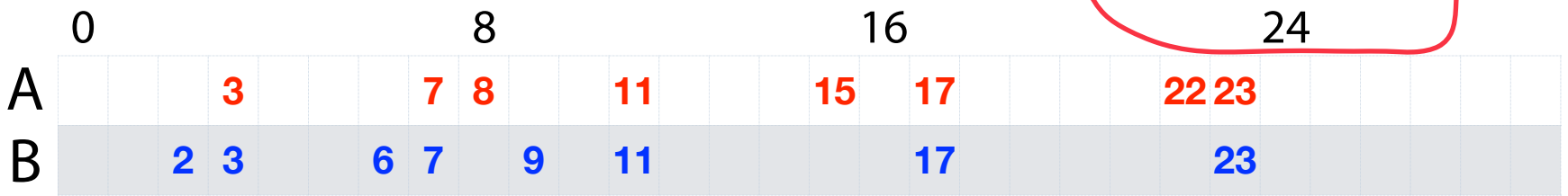
Sketch B

2	9
3	11
6	17
7	23

$A \cup B$

2	8	17
3	9	22
6	11	23
7	15	

...



MinHash Jaccard Estimation

We dont *know* $A \cup B$, but we can make a sketch!

min 8 A

Sketch A

3	15
7	17
8	22
11	23

$\cup$

min 8 B

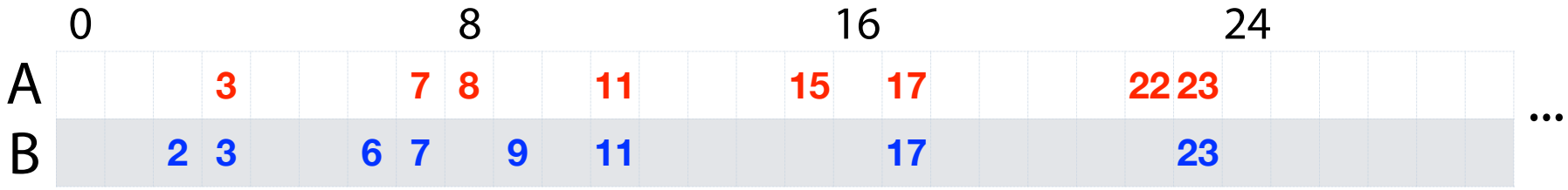
Sketch B

2	9
3	11
6	17
7	23

$=$

Sketch $A \cup B$

2	8
3	9
6	11
7	15



MinHash Jaccard Estimation

Estimate $|A \cup B|$ (the cardinality of the union) from sketch:

Sketch $A \cup B$

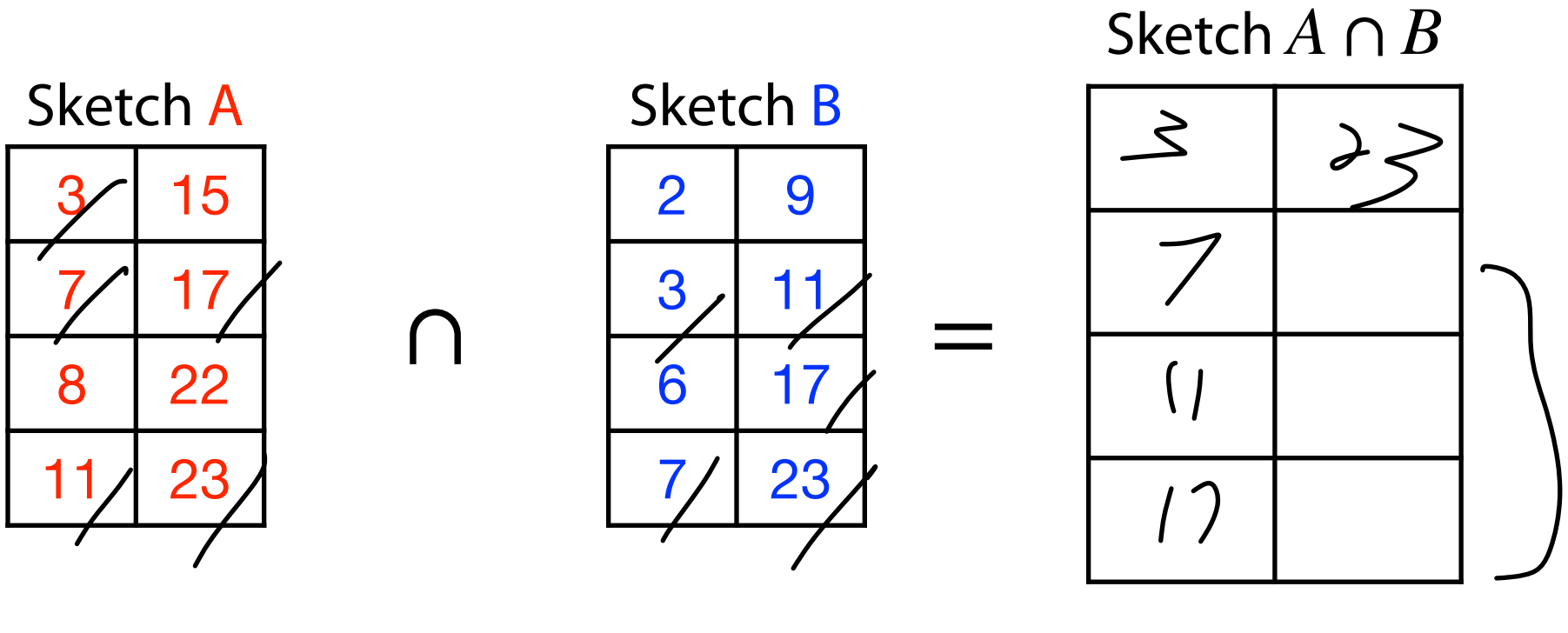
2	8
3	9
6	11
7	15

Our sets sampled from [0, 100].

$$\frac{15}{100} = \frac{8}{N+1} \rightarrow N = \frac{800}{15} - 1 = 52.3$$

MinHash Jaccard Estimation

Can we build a 8-Minhash of $A \cap B$?



MinHash Jaccard Estimation

Not guaranteed to be able to get a full sketch of the intersection!

Sketch A

3	15
7	17
8	22
11	23

$\cap$

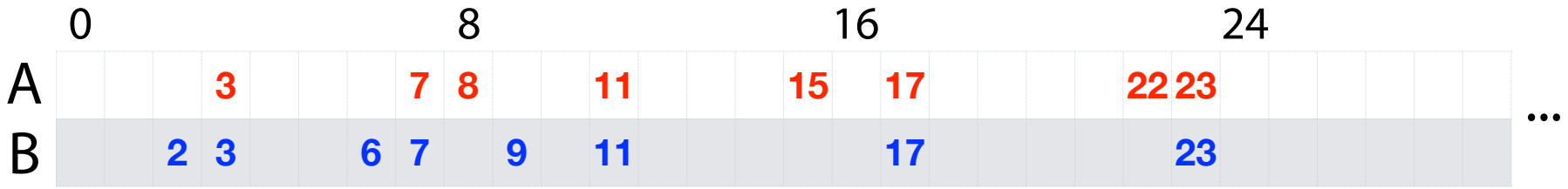
Sketch B

2	9
3	11
6	17
7	23

$=$

Sketch $A \cap B$

3	23
7	
11	
17	



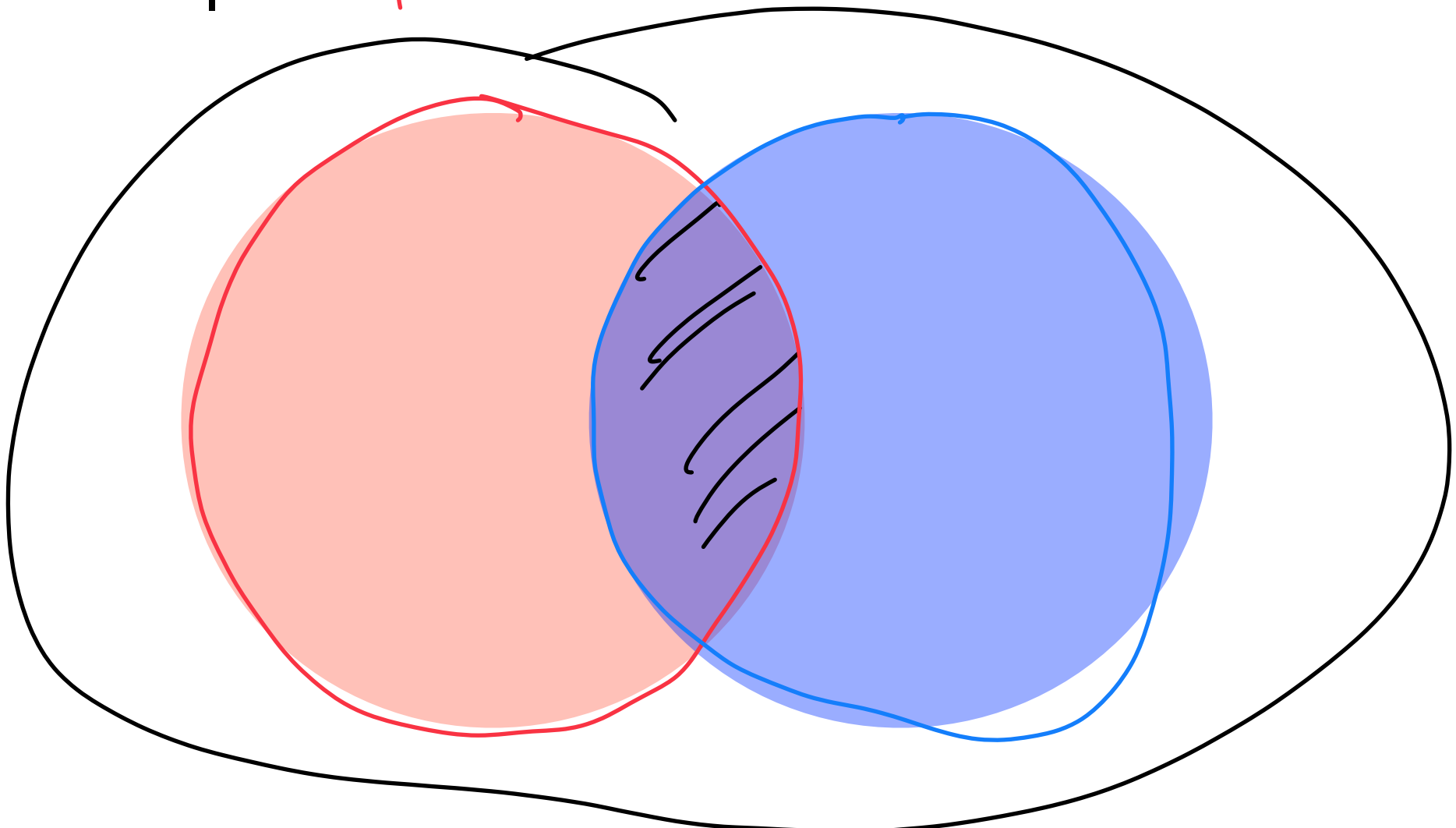
MinHash Jaccard Estimation

Using MinHash sketches, we can estimate $|A|$, $|B|$, and $|A \cup B|$

Is this enough to estimate the Jaccard?

Inclusion-Exclusion Principle

$$|A \cap B| = |A| + |B| - |A \cup B|$$



MinHash Indirect Jaccard Estimation

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

$k = 8$ MinHash sketches

Our sets sampled from [0, 100]

Sketch A

3	15
7	17
8	22
11	23

Sketch B

2	9
3	11
6	17
7	23

Sketch of $|A \cup B|$

2	8
3	9
6	11
7	15

~35 + ~53

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

$$= \frac{34.782 + 34.782 - 53.333 - 1}{53.333 - 1} \approx 0.29$$

MinHash Direct Jaccard Estimate

We can also estimate cardinality directly using our sketches!

Sketch A

3	15
7	17
8	22
11	23

Sketch B

2	9
3	11
6	17
7	23

Intersection

3	23
7	
11	
17	

5

Union

2	8	17
3	9	23
6	11	23
7	15	

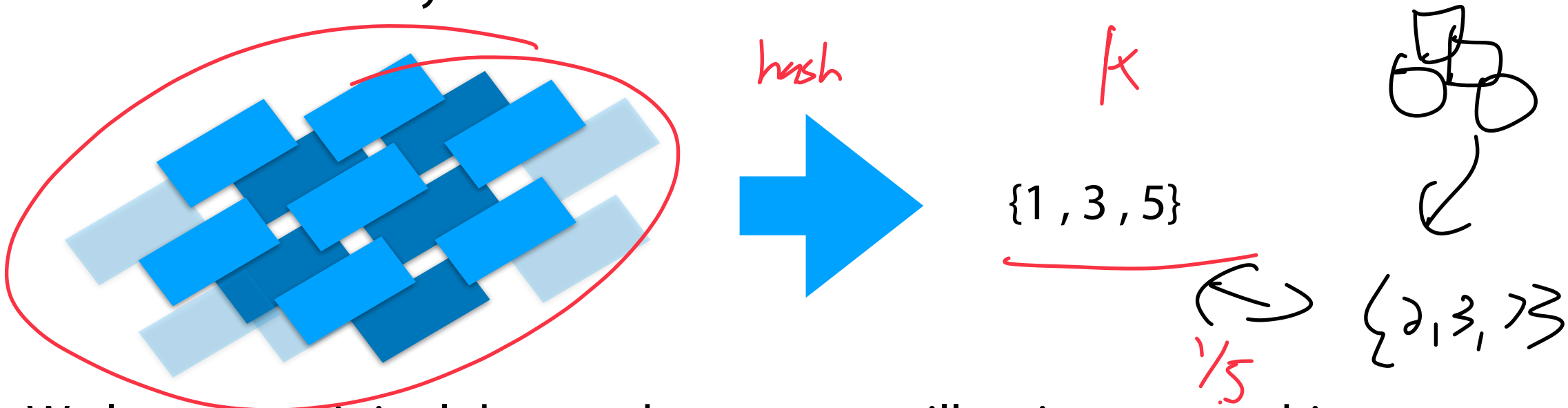
11

Good random sub-samples

5/11

MinHash Sketch

We can convert any hashable dataset into a **MinHash sketch**



We lose our original dataset, but we can still estimate two things:

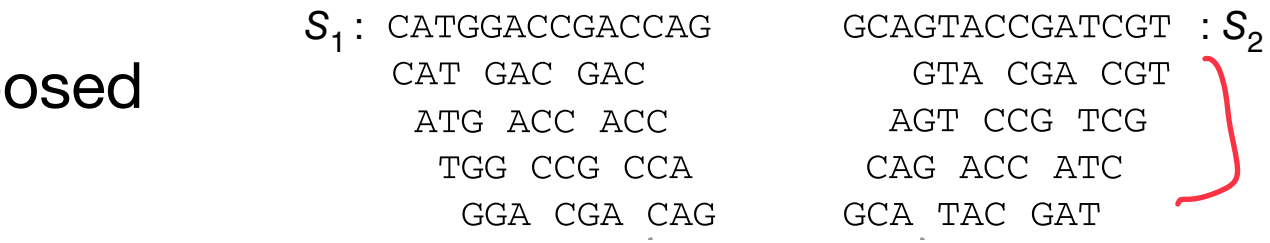
1. (cardinality (# of items)

2. Set Similarit

Alternative MinHash Sketch Approaches

Rather than use one single hashes and take bottom-k, we can also use k hashes — **if you have access to that many independent hashes**!

1) Sequence decomposed into **kmers**



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

1) Sequence decomposed into **kmers**

2) Multiple hash functions (**Γ**) map kmers to values.

S_1 : CATGGACCGACCAG

CAT GAC GAC

ATG ACC ACC

TGG CCG CCA

GGA CGA CAG

Γ_1	Γ_2	Γ_3	Γ_4	
19	14	57	36	CAT
14	57	36	19	ATG
58	37	16	15	TGG
40	23	2	61	GGA
33	28	11	54	GAC
5	48	47	26	ACC
22	1	60	43	CCG
24	7	50	45	CGA
33	28	11	54	GAC
5	48	47	26	ACC
20	3	62	41	CCA
18	13	56	39	CAG

GCAGTACCGATCGT : S_2

GTA CGA CGT

AGT CCG TCG

CAG ACC ATC

GCA TAC GAT

	Γ_1	Γ_2	Γ_3	Γ_4
GCA	36	19	14	57
CAG	18	13	56	39
AGT	11	54	33	28
GTA	44	27	6	49
TAC	49	44	27	6
ACC	5	48	47	26
CCG	22	1	60	43
CGA	24	7	50	45
GAT	35	30	9	52
ATC	13	56	39	18
TCG	54	33	28	11
CGT	27	6	49	44

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

1) Sequence decomposed into **kmers**

2) Multiple hash functions (**Γ**) map kmers to values.

3) The smallest values for each hash function is chosen

S_1 : CATGGACCGACCAG

CAT GAC GAC

ATG ACC ACC

TGG CCG CCA

GGA CGA CAG

Γ_1	Γ_2	Γ_3	Γ_4	
19	14	57	36	CAT
14	57	36	19	ATG
58	37	16	15	TGG
40	23	2	61	GGA
33	28	11	54	GAC
5	48	47	26	ACC
22	1	60	43	CCG
24	7	50	45	CGA
33	28	11	54	GAC
5	48	47	26	ACC
20	3	62	41	CCA
18	13	56	39	CAG

[5, 1, 2, 15]

Sketch (S_1)

GCAGTACCGATCGT : S_2

GTA CGA CGT

AGT CCG TCG

CAG ACC ATC

GCA TAC GAT

	Γ_1	Γ_2	Γ_3	Γ_4
GCA	36	19	14	57
CAG	18	13	56	39
AGT	11	54	33	28
GTA	44	27	6	49
TAC	49	44	27	6
ACC	5	48	47	26
CCG	22	1	60	43
CGA	24	7	50	45
GAT	35	30	9	52
ATC	13	56	39	18
TCG	54	33	28	11
CGT	27	6	49	44

[5, 1, 6, 6]

Sketch (S_2)

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

1) Sequence decomposed into **kmers**

2) Multiple hash functions (**Γ**) map kmers to values.

3) The smallest values for each hash function is chosen

4) The Jaccard similarity can be estimated by the overlap in the **Min**imum **Hash**es (**MinHash)**

S_1 : CATGGACCGACCAG

CAT GAC GAC
ATG ACC ACC
TGG CCG CCA
GGA CGA CAG

Γ_1	Γ_2	Γ_3	Γ_4	
19	14	57	36	CAT
14	57	36	19	ATG
58	37	16	15	TGG
40	23	2	61	GGA
33	28	11	54	GAC
5	48	47	26	ACC
22	1	60	43	CCG
24	7	50	45	CGA
33	28	11	54	GAC
5	48	47	26	ACC
20	3	62	41	CCA
18	13	56	39	CAG

[5, 1, 2, 15]
Sketch (S_1)

GCAGTACCGATCGT : S_2

GTA CGA CGT
AGT CCG TCG
CAG ACC ATC
GCA TAC GAT

	Γ_1	Γ_2	Γ_3	Γ_4
GCA	36	19	14	57
CAG	18	13	56	39
AGT	11	54	33	28
GTA	44	27	6	49
TAC	49	44	27	6
ACC	5	48	47	26
CCG	22	1	60	43
CGA	24	7	50	45
GAT	35	30	9	52
ATC	13	56	39	18
TCG	54	33	28	11
CGT	27	6	49	44

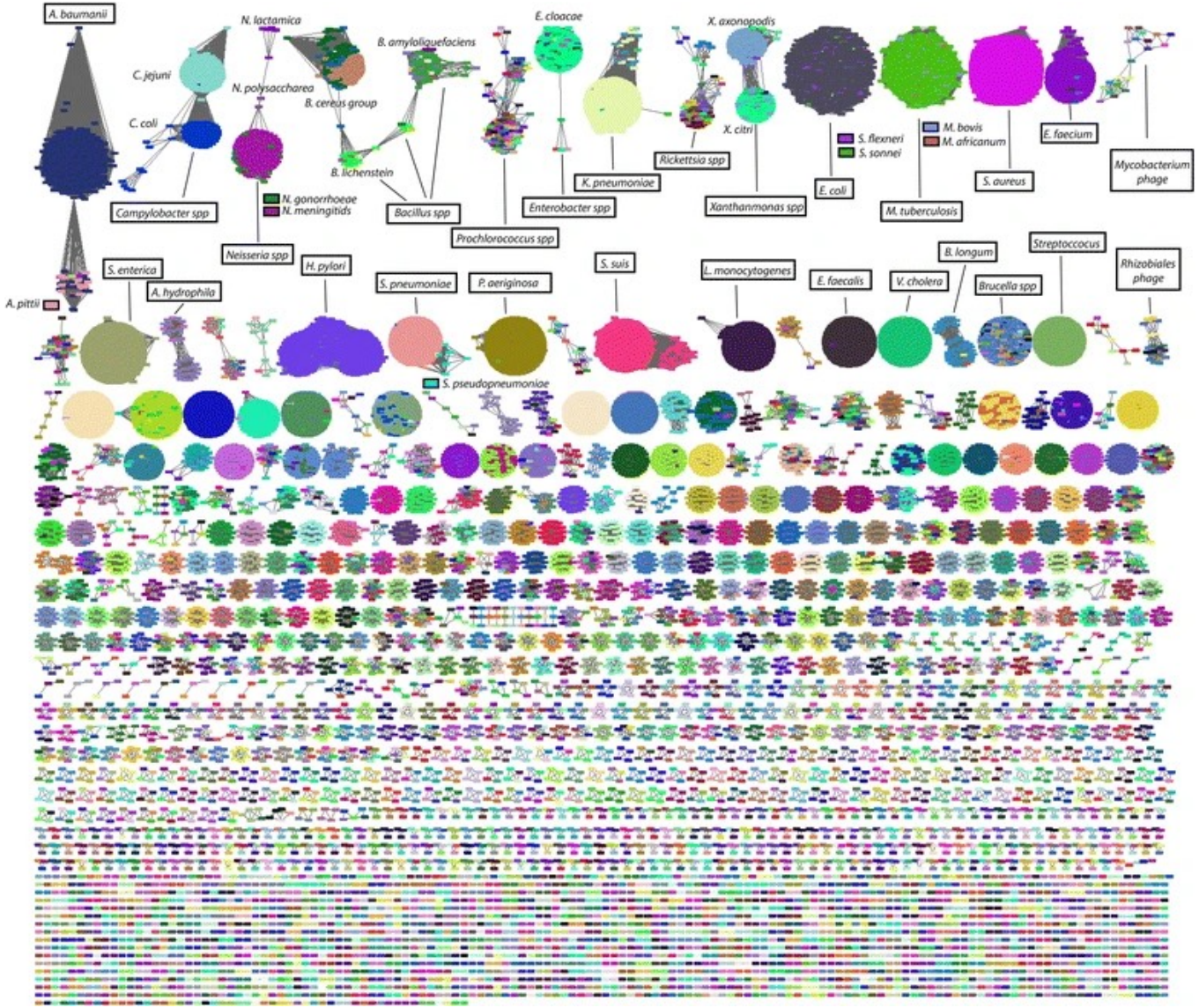
[5, 1, 6, 6]
Sketch (S_2)

$J(S_1, S_2) \approx 2/4 = 0.5$

S_1 : CATGGACCGACCAG
S_2 : GCAGTACCGATCGT

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

MinHash in practice



Microbial genes

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

Alternative MinHash Sketch Approaches

What if I have a dataset which is **much** larger than another?

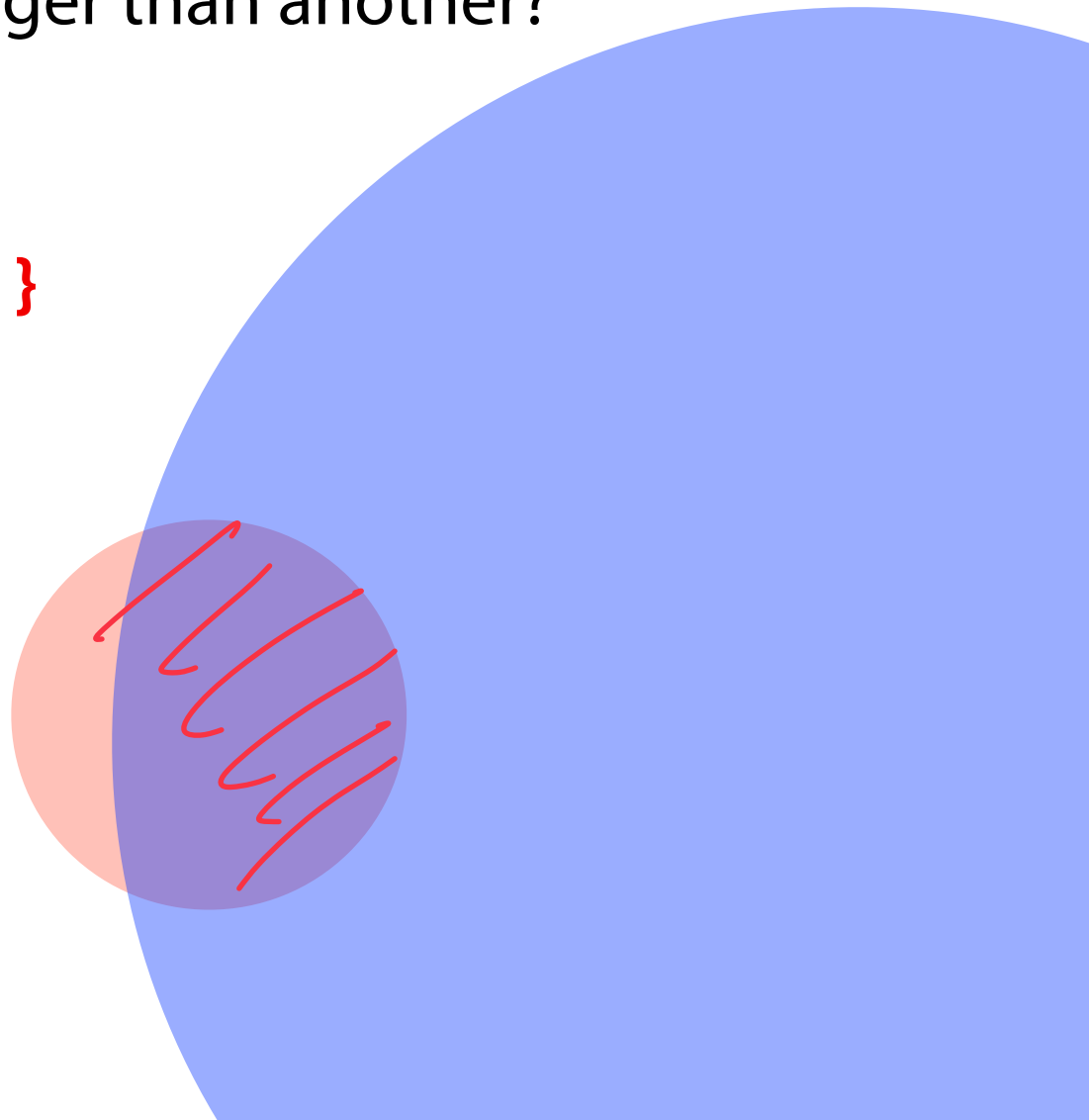
$S_1 = \{ 1, 3, 40, 59, 82, 101 \}$

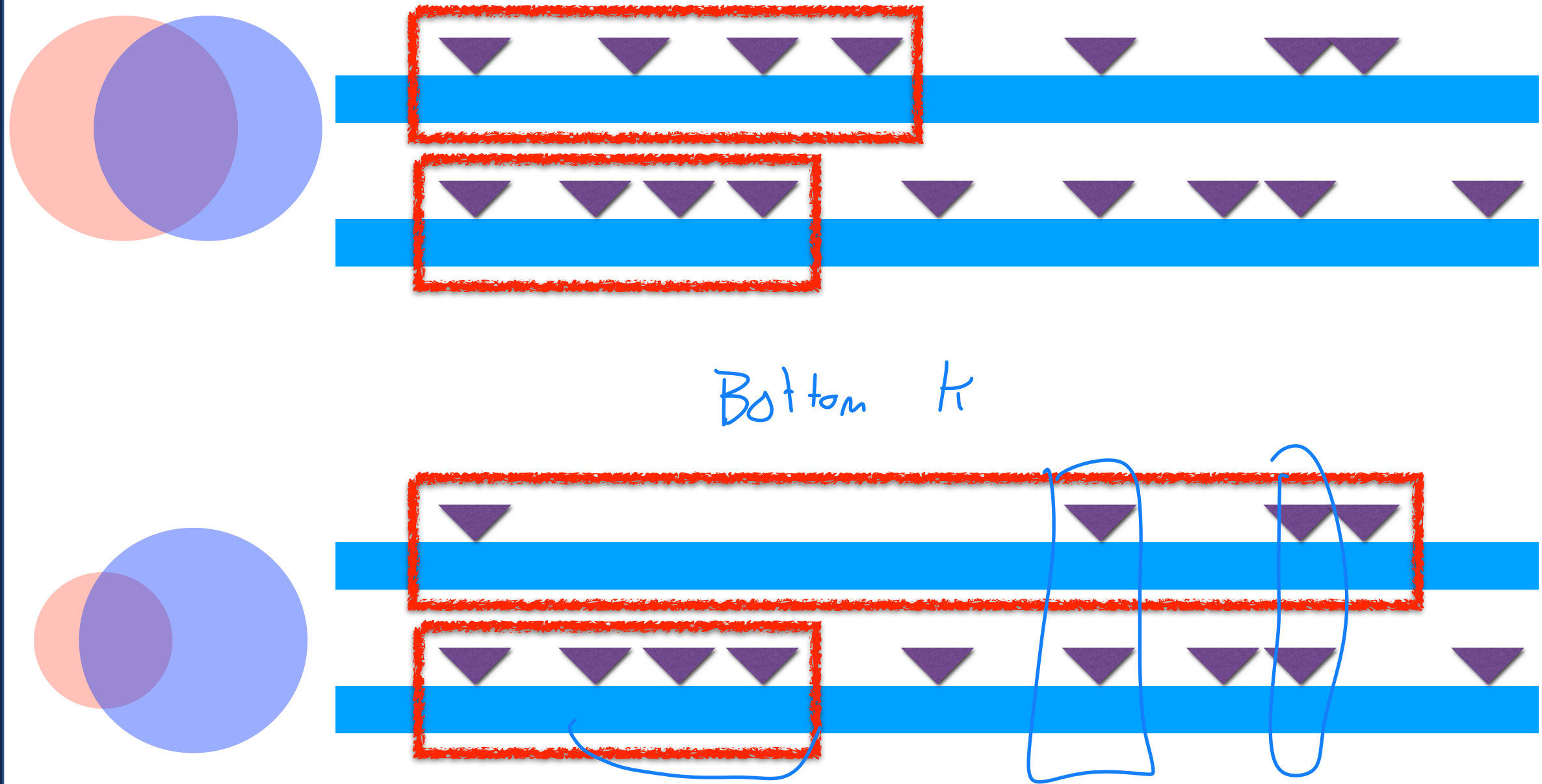
$S_2 = \{ 1, 2, 3, 4, 5, 6, 7, \ldots 59, 82, 101, \ldots \}$

$k = 5$

$S_1 = 1, 3, 40, 59, 82$

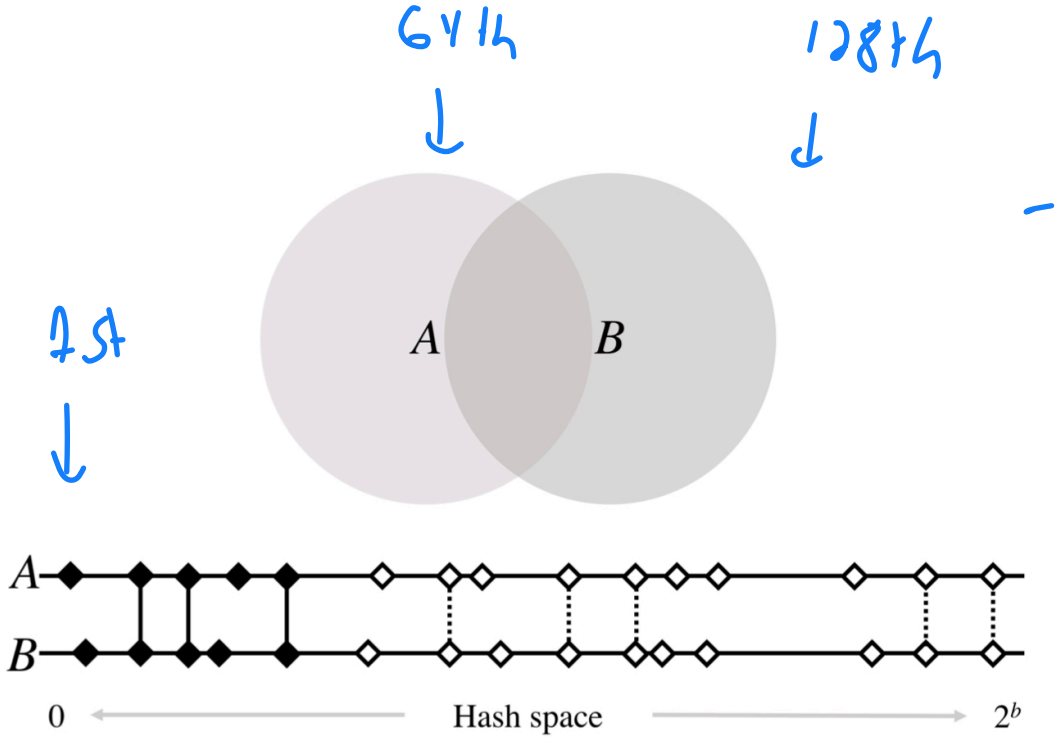
$S_2 = 1, 2, 3, 4, 5$

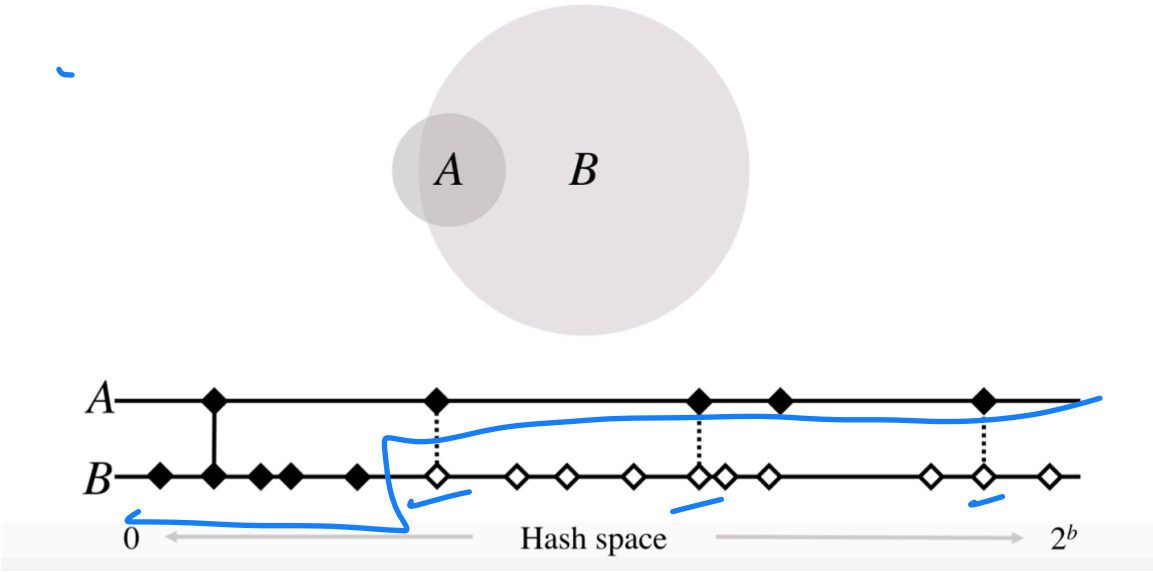



Bottom

Alternative MinHash sketches

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

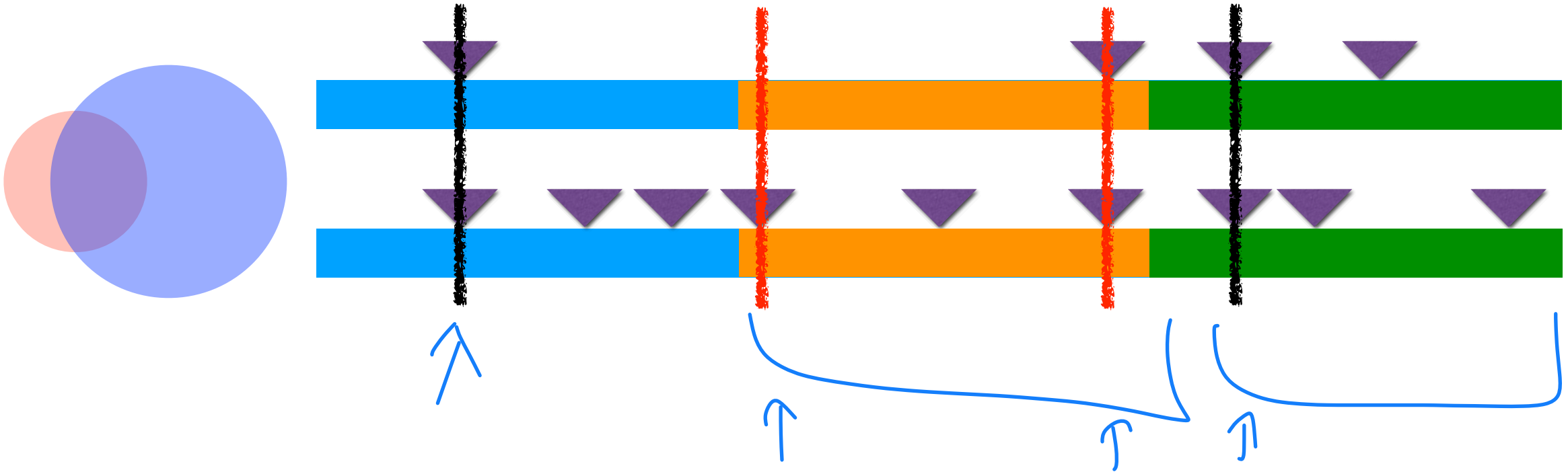




Ondov, Brian D., Gabriel J. Starrett, Anna Sappington, Aleksandra Kostic, Sergey Koren, Christopher B. Buck, and Adam M. Phillippy. **Mash Screen: High-throughput sequence containment estimation for genome discovery**. *Genome biology* 20.1 (2019): 1-13.

Alternative MinHash Sketch Approaches

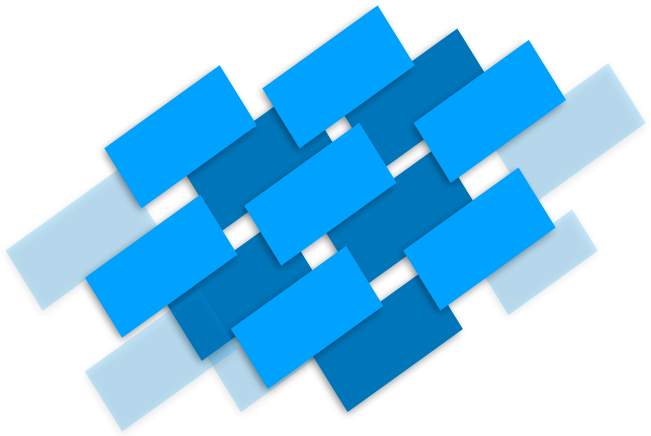
If there is a large cardinality difference, **use k-partitions!**



H(x) → int → 0x00000001

K-Partition Minhash

↳ This only works if actually uniform dist



Hash

10110110101
0001111010
1101101011
1011010110
0101100000
0010001101

Partition

k=4

2 bits

00
01111010
10001101

01
01100000

10
10110101
11010110

11
01101011

Probabilistic Data Structures

Probabilistic data structures trade accuracy for efficiency

Most can maintain surprisingly good accuracy

"Cheat" Big O limitations on conventional data analysis

↳ Expectation under SUHA