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PUFFINN

Parameterless and Universally Fast FInding of Nearest Neighbors

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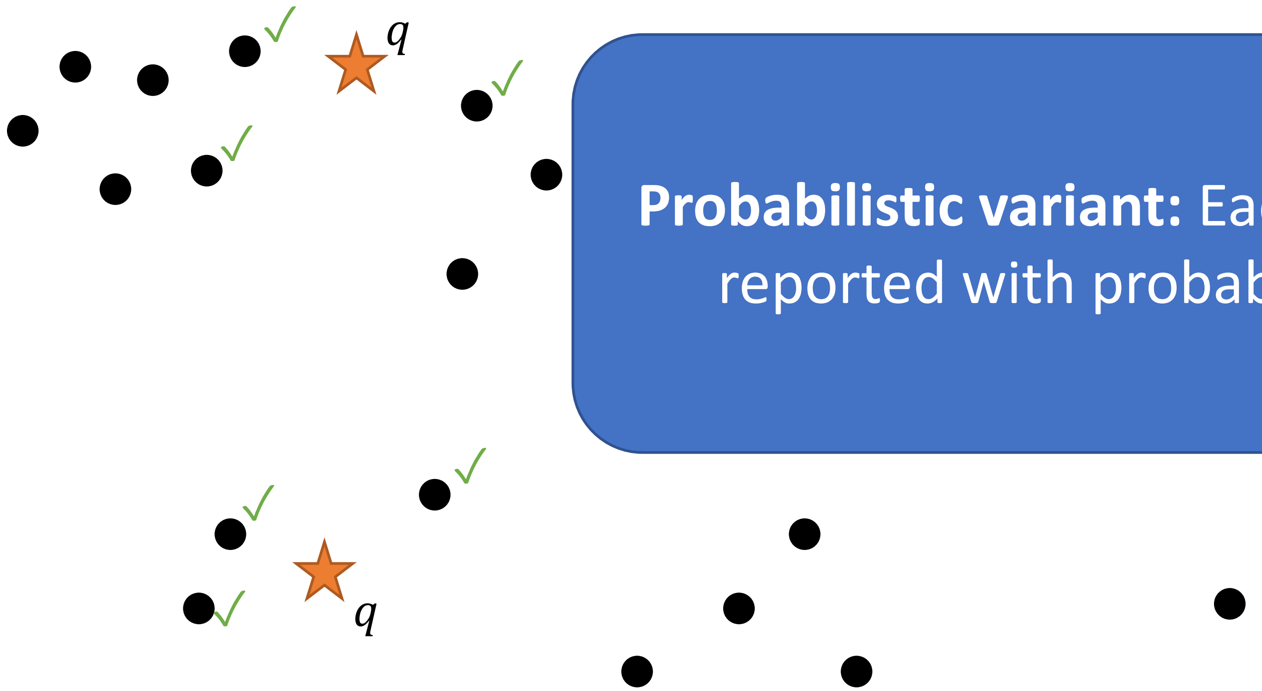
BASIC ALGORITHMS RESEARCH COPENHAGEN
BARC!

k-Nearest Neighbor Problem

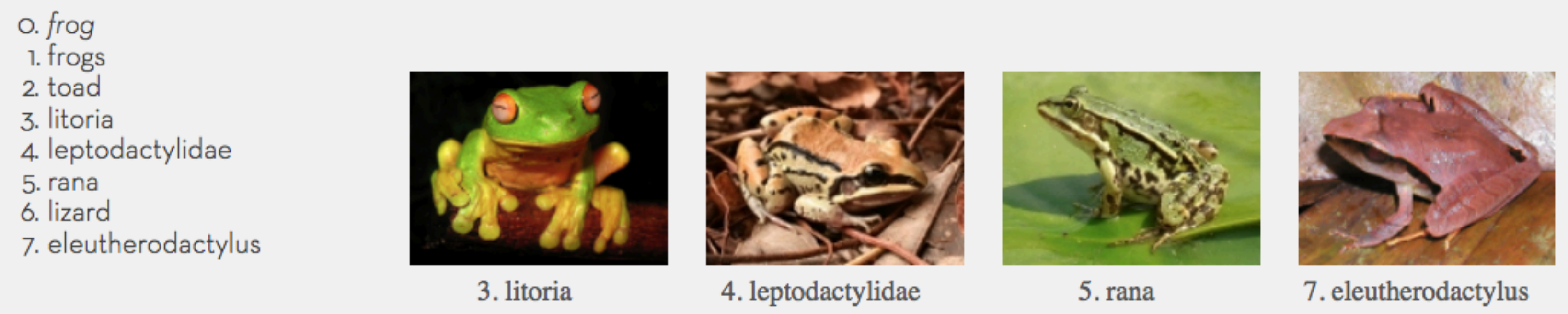
- **Preprocessing**: Build DS for set $S \subseteq \mathbb{R}^d$ of n data points
- **Task**: Given query point $q \in \mathbb{R}$, return k closest points to q in S



Probabilistic variant: Each nearest neighbor is reported with probability at least $1 - \delta$.

Nearest neighbor search on words

- GloVe: learning algorithm to find vector representations for words
- *GloVe.twitter* dataset: **1.2M words**, vectors trained from **2B tweets**, **100 dimensions**
- Semantically similar words: nearest neighbor search on vectors



https://nlp.stanford.edu/projects/glove/

Jeffrey Pennington, Richard Socher, and Christopher D. Manning. 2014. GloVe: Global Vectors for Word Representation.

GloVe Examples (100d, 1.2M vectors)

“munich”	“germany”	“algorithm”
• “bayern”	• “austria”	• “algorithms”
• “cologne”	• “switzerland”	• “optimization”
• “stuttgart”	• “german”	• “approximation”
• “berlin”	• “europe”	• “iterative”
• “hamburg”	• “poland”	• “computation”

Our Results

Theory

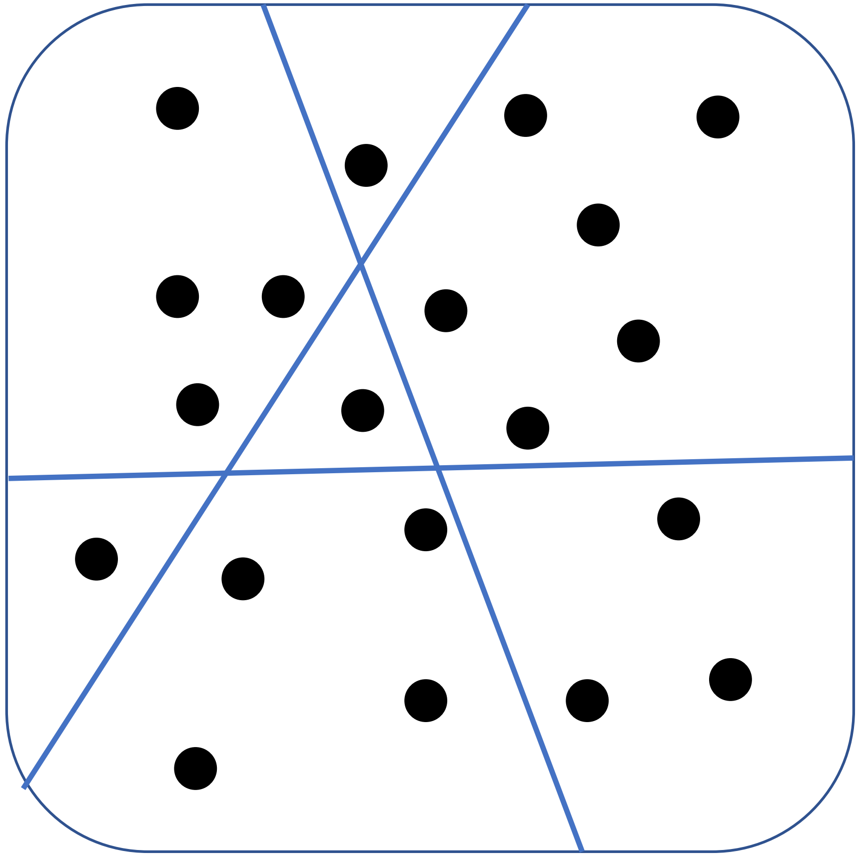
- A novel Locality-Sensitive Hashing (LSH)-based algorithm for probabilistic k-NN
- Avoids standard reduction approach by [Har-Peled et al., 2012]

Practice

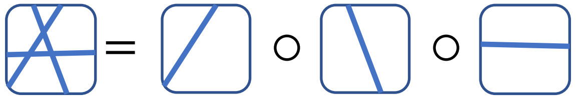
- Theory + algorithm engineering gives a fast implementation with provable guarantees
- in our experiments:
  - competitive with other state-of-the-art approaches (w/o guarantees)
  - faster than state-of-the-art LSH (w/o guarantees) [FALCONN]

How does it work?

Locality-Sensitive Hashing (LSH) [Indyk-Motwani, 1998]

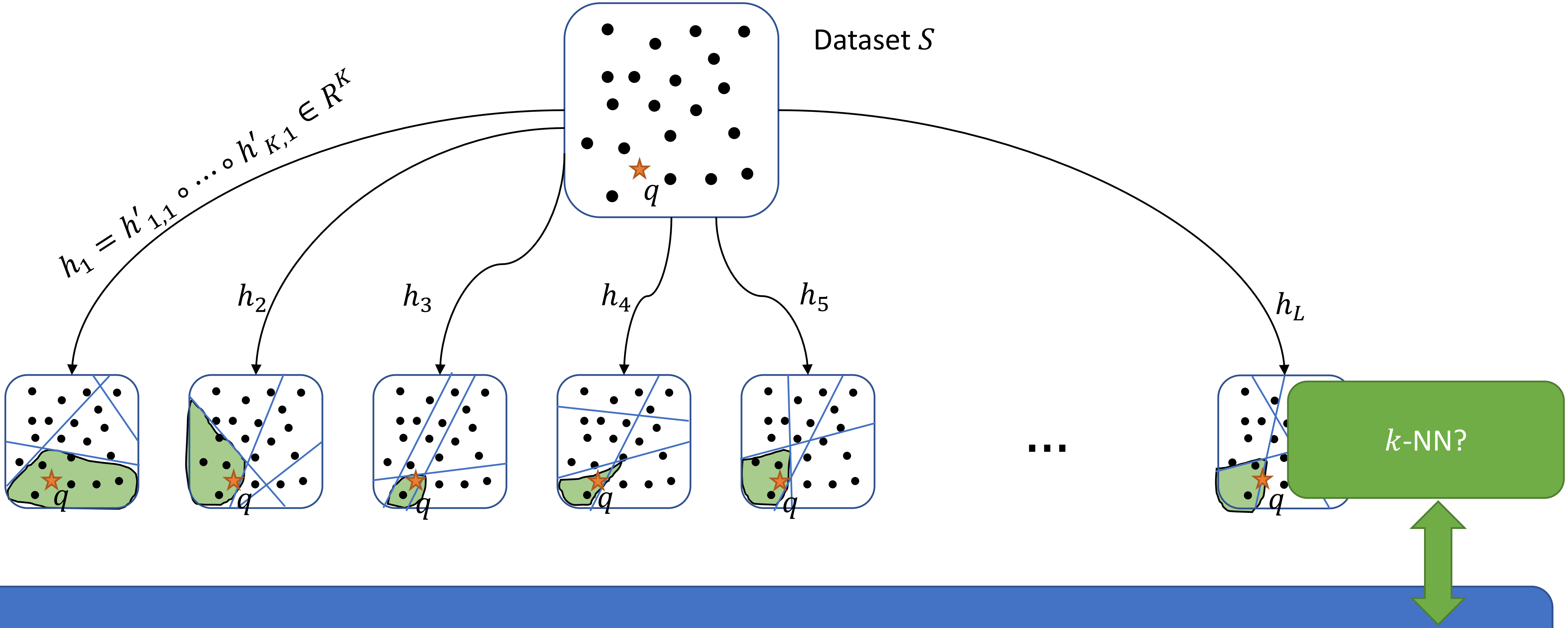


$$h(p) = h_1(p) \circ h_2(p) \circ h_3(p) \in \{0,1\}^3$$



A family $\mathcal{H}$ of hash functions is **locality-sensitive**, if the collision probability of two points is decreasing with their distance to each other.

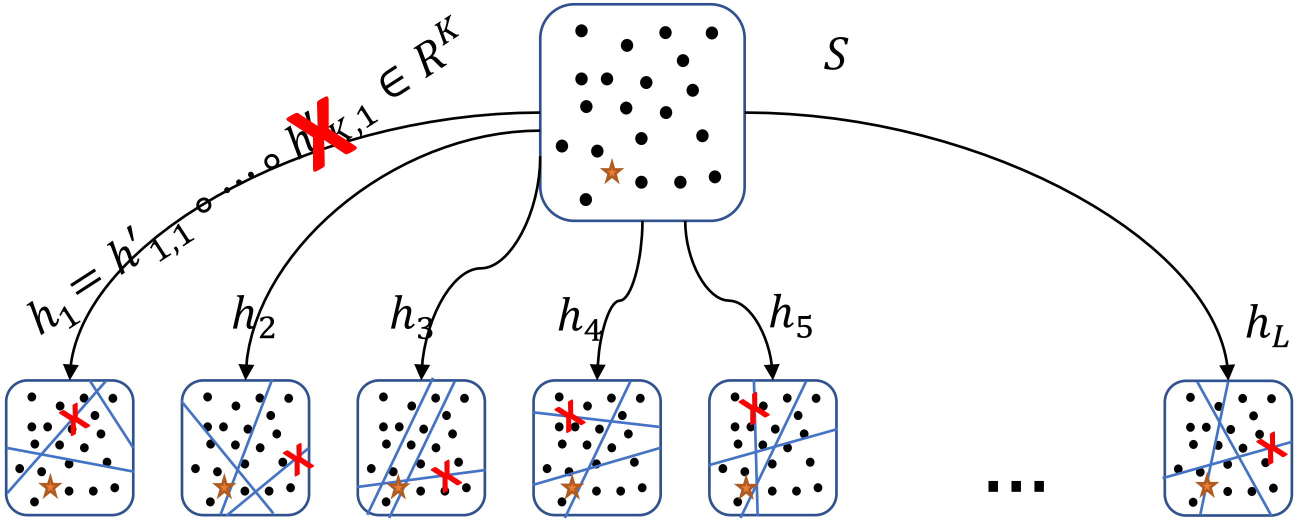
Standard LSH for Reporting Points at Distance $\leq r$



Query Algorithm: Collect all points that collide with q under $h_1, \dots, h_L$. Return all points at distance $\leq r$.

Our Approach: Solving k-NN using LSH

- Check buckets $j \in \{1, \dots, L\}$, one-by-one
- keep track of **current** k closest points
- **Goal**:
  Report with prob. $\geq 1 - \delta$



Termination: If $(1-p)^j \leq \delta$, report **current** top-k.

probability of the **current** k-th nearest neighbor to collide.

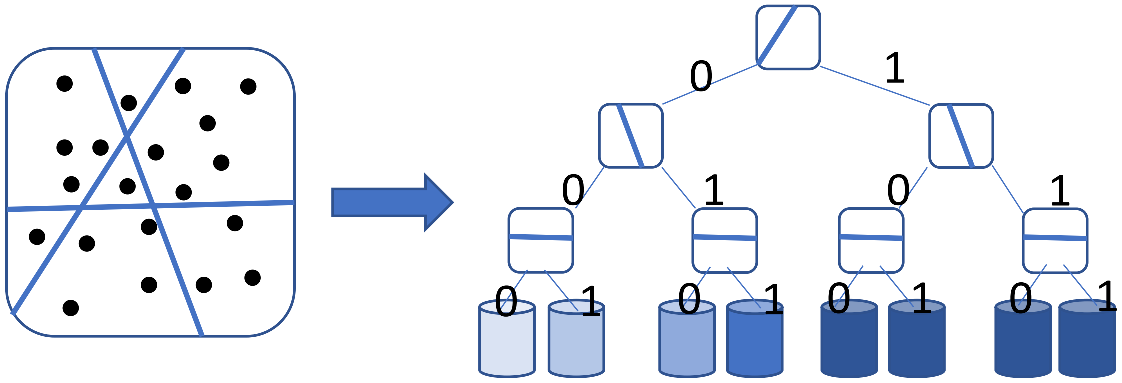
- What if there is no such j?
  - Try again with smaller K

Why does that work? **Monotonicity** of the LSH collision prob.

The Data Structure

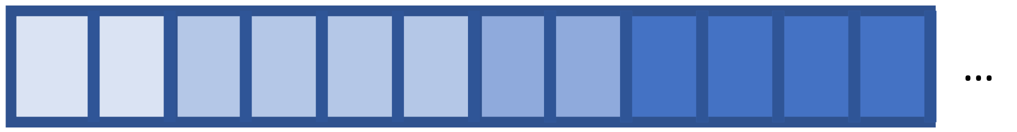
Theoretical

- **LSH Forest:** Each repetition is a Trie build from LSH hash values [Bawa et al., 2005]



Practical

- Store indices of data set points sorted by hash code
- ”Traversing the Trie” by binary search
- use lookup table for first levels



Works with any kind of LSH

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“space parameter” + “quality parameter”

no **internal** parameters

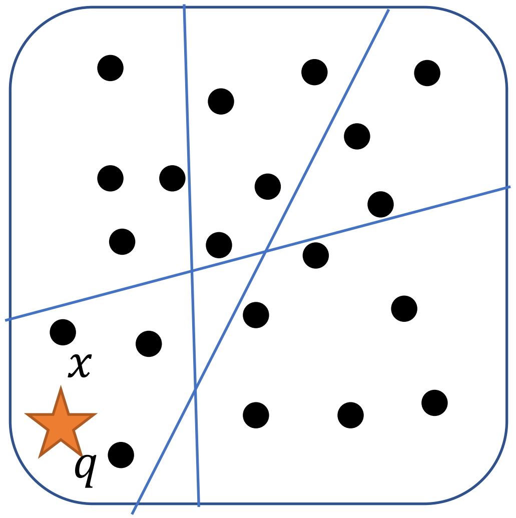
Implicit Tries + Recycling LSH values + ???

[Christiani, 2019]

Sketching to avoid distance computations

SimHash [Charikar, 2002]
1-BitMinHash [König-Li, 2010]

- Have to carry out (expensive) distance computations on candidates
- Can be reduced by storing compact sketch representations



Sketch representation

q 1011100101

x 0101110101

Easy to analyze:
Sum of Bernoulli trials of
$\Pr(X = 1) = f(\text{dist}(q, x))$

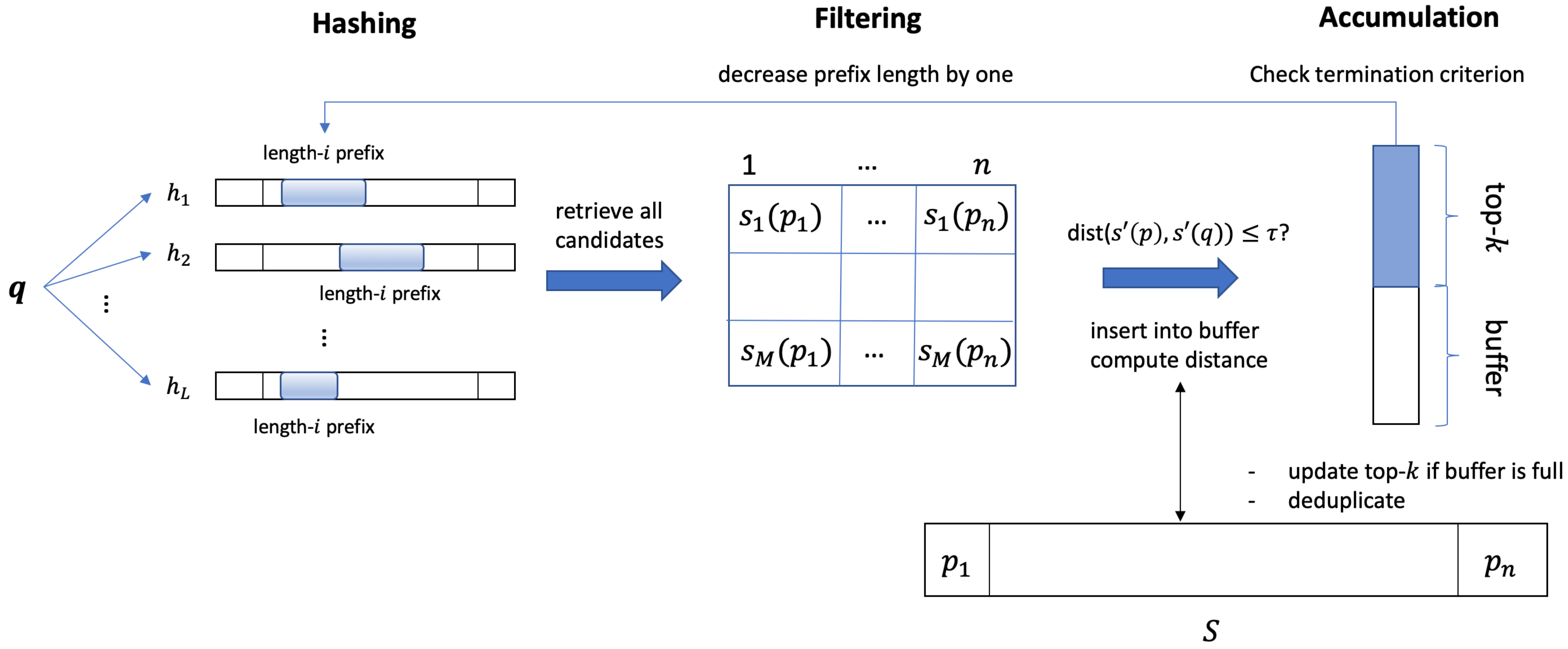
At least τ collisions?

Yes → compute $\text{dist}(q, x)$

No → skip

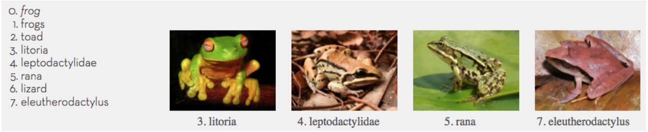
Set τ such that with probability at least $1 - \varepsilon$ we don't disregard point that could be among NN.

Overall System Design

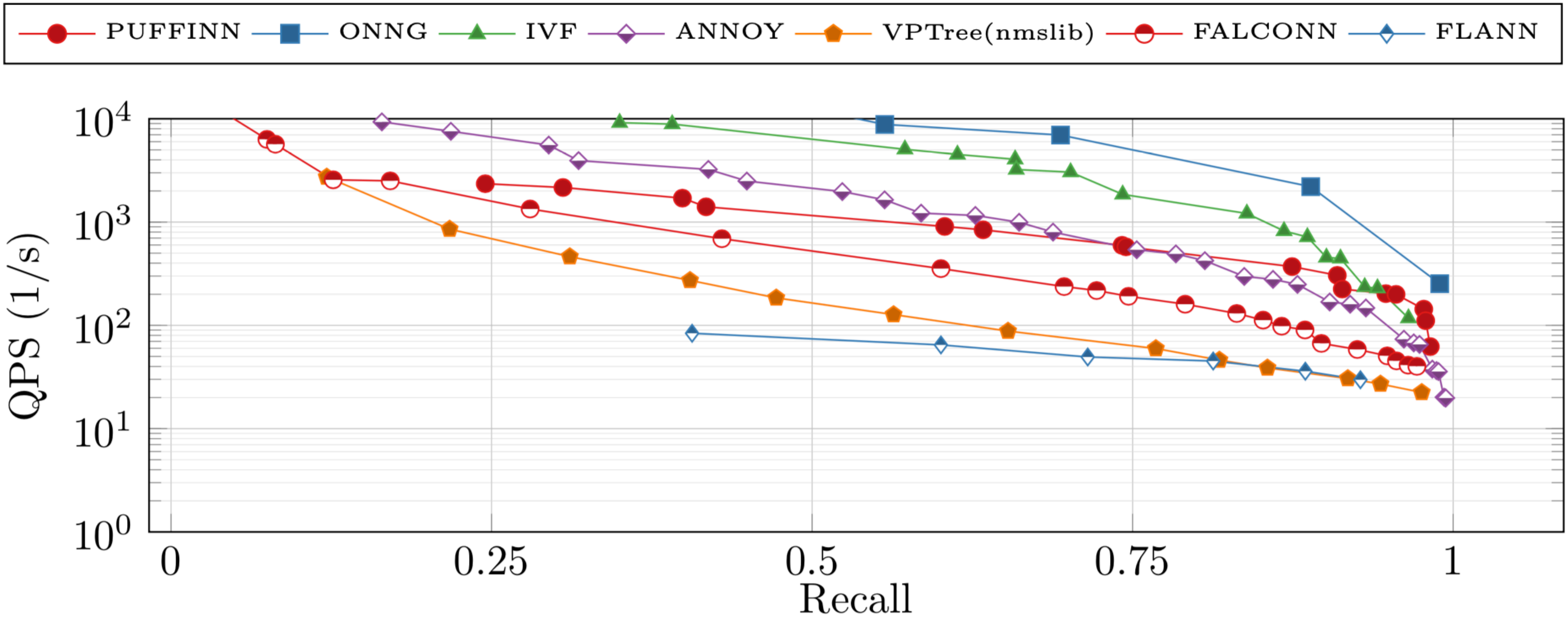


Experimental Evaluation

- Design choices in the implementation
  - Which LSH family to use? Cross-Polytope LSH [Andoni et al., 2015]
  - Which evaluation strategy to use? Pooling
  - Use sketches? Yes
  - Influence of parameters? More space helps, but saturates quickly
- Comparison to other existing k-NN implementations



Running time (Glove 100d, 1.2M, 10-NN)



A difficult (?) data set in $\mathbb{R}^{3d}$

n data points

$$x_1 = (0^d, y_1, z_1)$$

$$\vdots$$

$$x_{n-1} = (0^d, y_{n-1}, z_{n-1})$$
$$x_n = (v, w, 0^d)$$

m query points

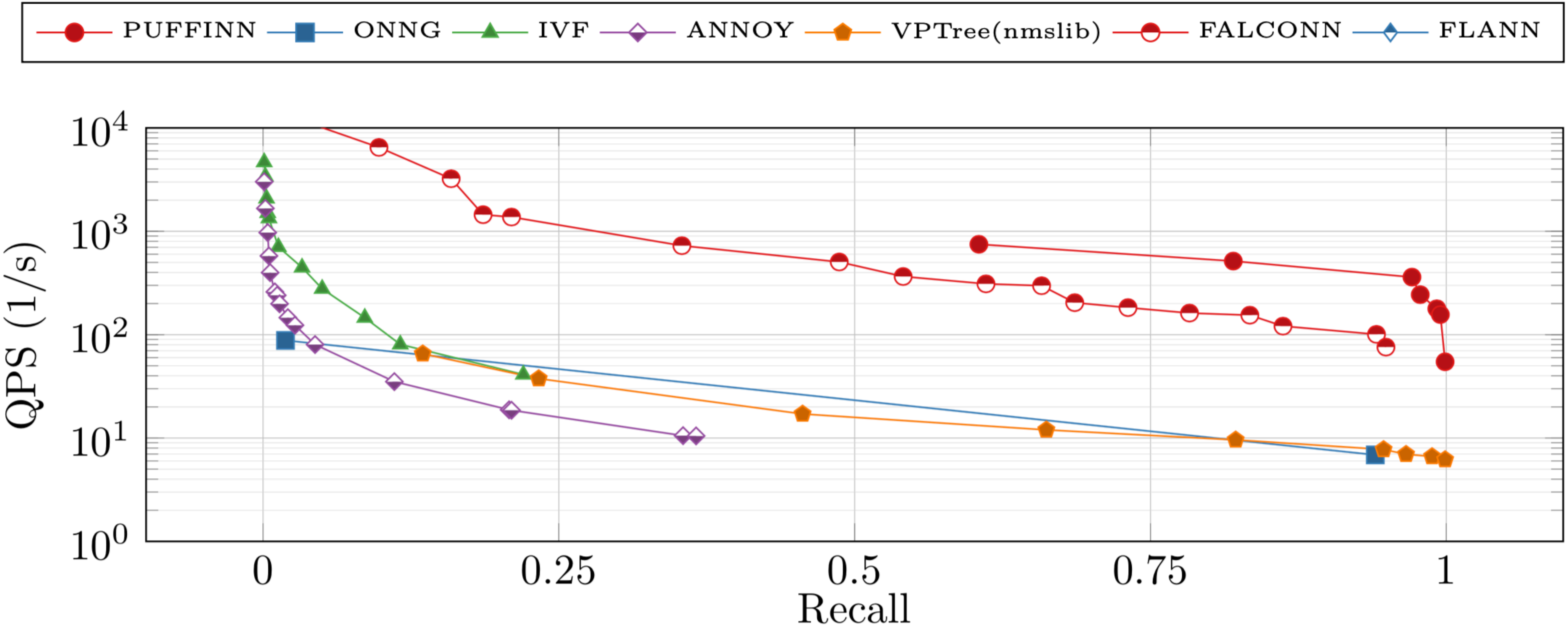
$$q_1 = (v, 0^d, r_1)$$

$$\vdots$$

$$q_m = (v, 0^d, r_m)$$

$$y_i, z_i, v, w, r_i \sim \mathcal{N}^d\left(0, \frac{1}{2d}\right)$$

Running time (“Difficult”, 1M, 10-NN)



Summary

- Using LSH to solve exact k-NN (with probabilistic guarantees)
- Adaptive query algorithm
- Engineering tricks to make it fast (more in the paper!)

- Can ideas be applied to other settings?
  - Similarity Joins

https://github.com/puffinn/puffinn
https://github.com/puffinn/esa-paper

A Bound on the Expected Running Time

- **knows for each query $\boldsymbol{q}$**
  best stopping point in data structure

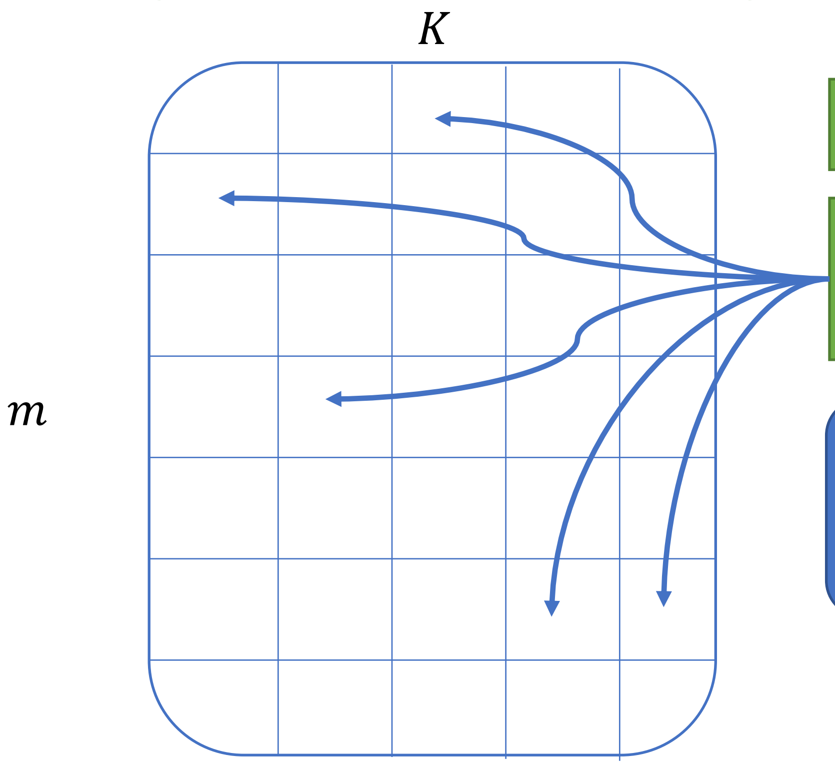
$$OPT(L,K,k,\delta) = \min\left\{ \frac{\ln(1/\delta)}{p(q,x_k)^i}\left(i + \sum_{x\in P} p(q,x)^i\right) \mid 0 \le i \le K, \frac{\ln(1/\delta)}{p(q,x_k)^i} \ge L \right\}$$

- **Lemma**: In expectation, proposed algorithm takes time

$$O(OPT(L,K,k,\delta/k) + L(K+k))$$

Fast Hash Function Evaluation

- **Main Bottleneck**: Computation of Hash Values
- Adapt the "pooling" technique of [Dahlgaard et al., 2017] and [Christiani, 2019]



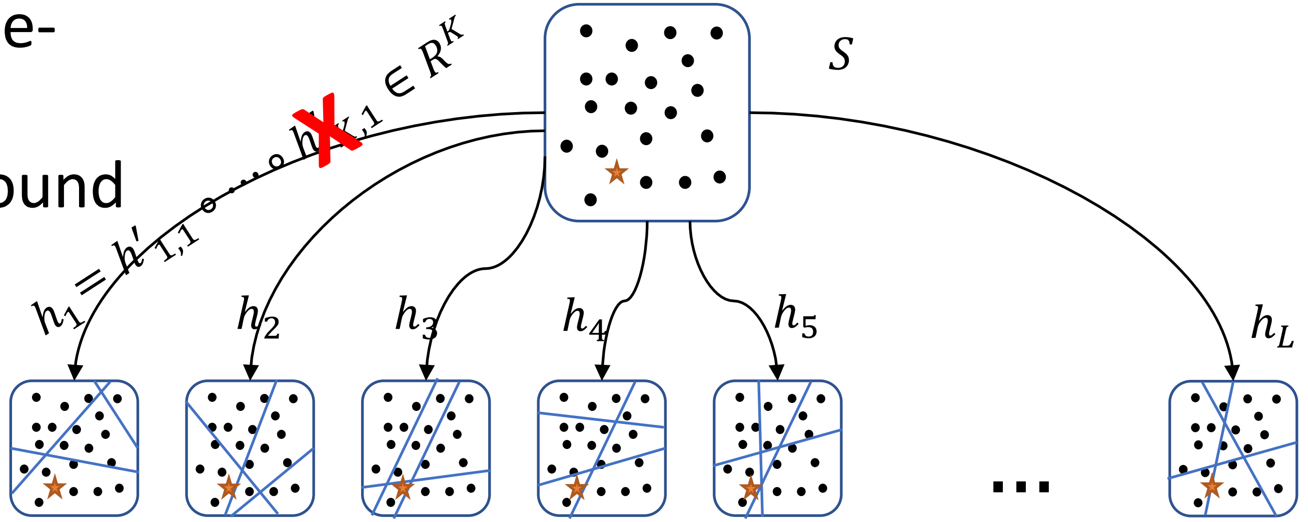
$K \cdot m$ independent hash functions from LSH family, $m \ll L$.

Pick K hash functions in repetition j using universal hash functions in each column.

Analysis using Cantelli's inequality →
Requires different stopping criteria (factor 2 slowdown)

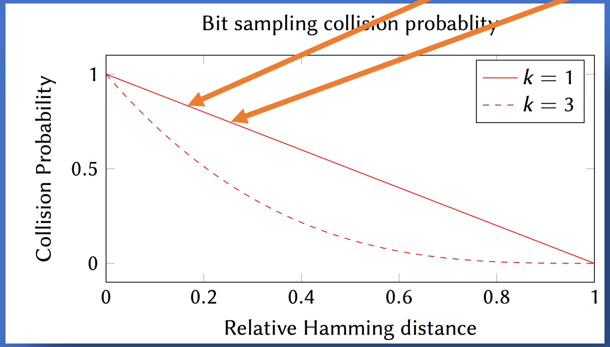
Our Approach: Solving k-NN using LSH

- Check buckets $j \in \{1, \dots, L\}$, one-by-one
- keep track of closest k points found so far



Want: $(1-p^*)^j \leq \delta$,
(p^* collision prob. of true k-NN)

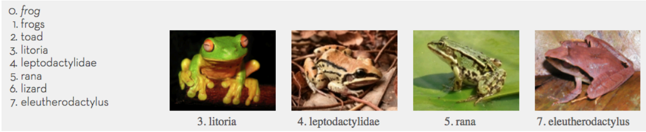
Montonocity of LSH: $p^* \geq p$.



Termination: If $(1-p)^j \leq \delta$, report top-k.

probability of the current k-th nearest neighbor to collide.

Why does that work? Monotonicity of the LSH collision prob.



Influence of Index Size (Glove 100d, 1.2M, 10-NN)

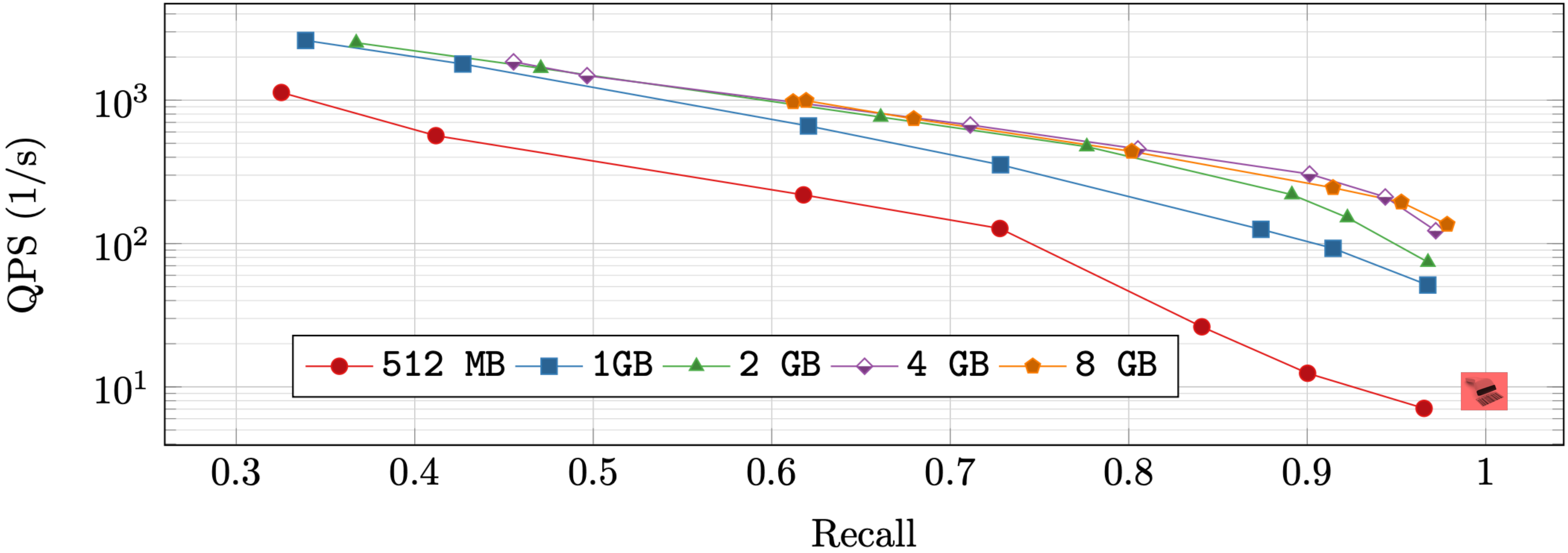


Figure 3 Influence of index size to quality-performance trade-off.