

Falconnn++: A locality-sensitive filtering approach for approximate nearest neighbor search

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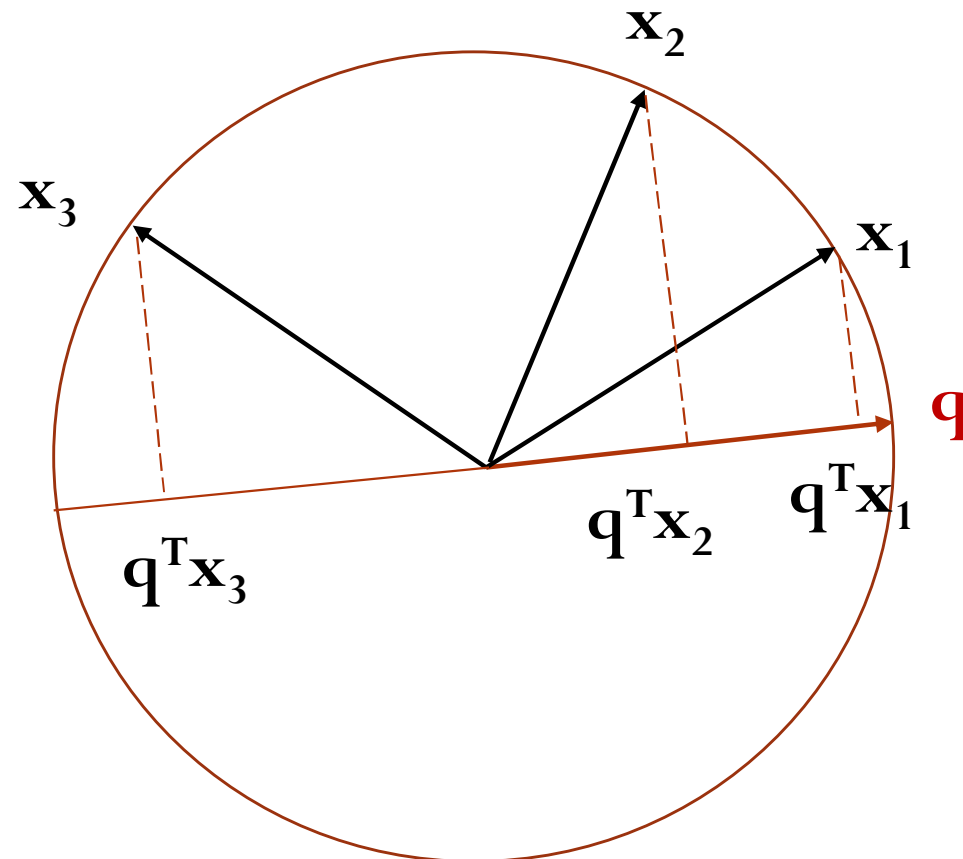
University of Auckland



MIT, Oct 15, 2022

Nearest neighbor search in sphere

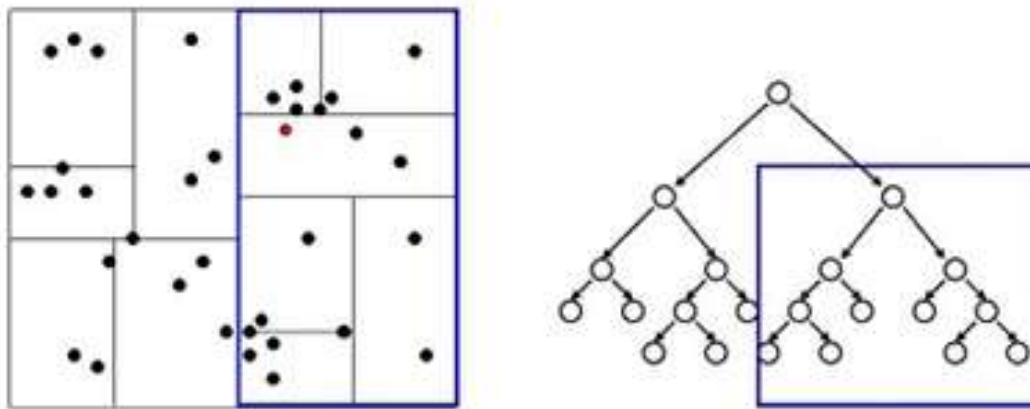
- Nearest neighbor search (NNS) in a unit sphere:
 - Given a data set \mathbf{X} of size \mathbf{n} and a query \mathbf{q} in \mathbf{d} dimensional unit sphere, return the point $\mathbf{x} \in \mathbf{X}$ such that the $\text{dist}(\mathbf{q}, \mathbf{x}) = \|\mathbf{x} - \mathbf{q}\|$ is minimum.



\mathbf{x}_1 is the top-1.

Challenges of NNS

- Curse of dimensionality:
 - Given a polynomial indexing space $n^{O(1)}d^{O(1)}$, existing a sublinear time algorithm to solve **exact** NNS refutes SETH [Wil18].
 - Indexing space or query time must be exponential in d .
- Classic solutions: KD Tree

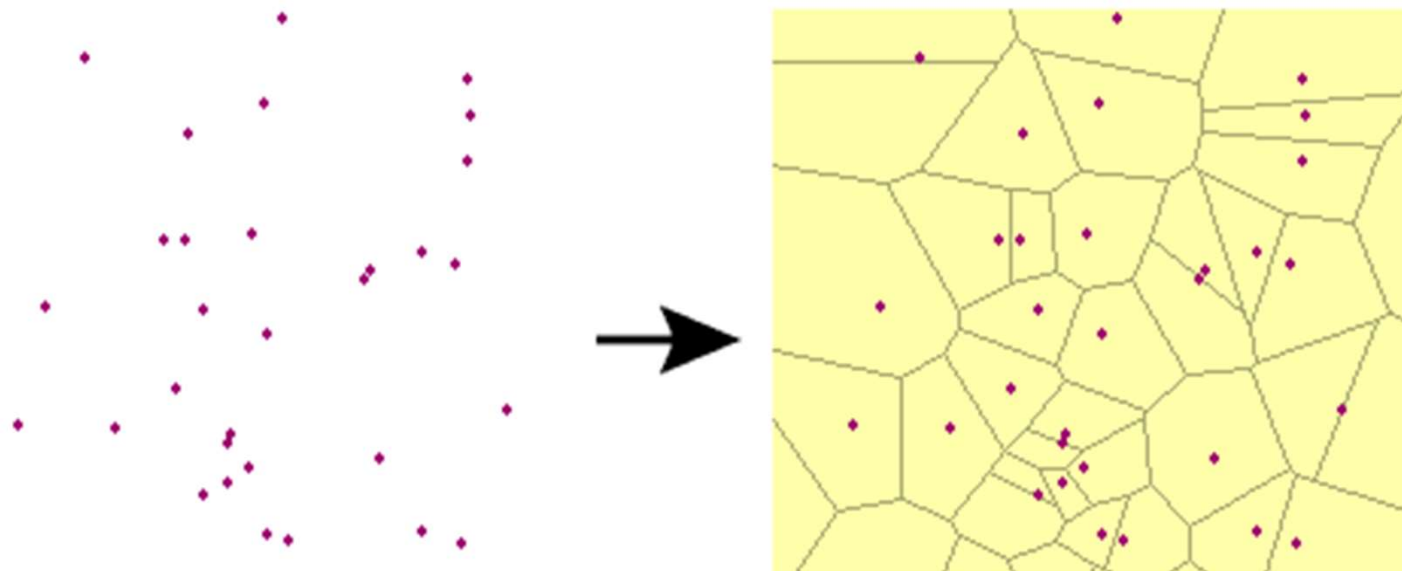


Space: $O(n)$
Range query: $O(dn^{1-1/d})$

Examine nearby points first: Explore the branch of the tree that is closest to the query point first.

Challenges of NNS

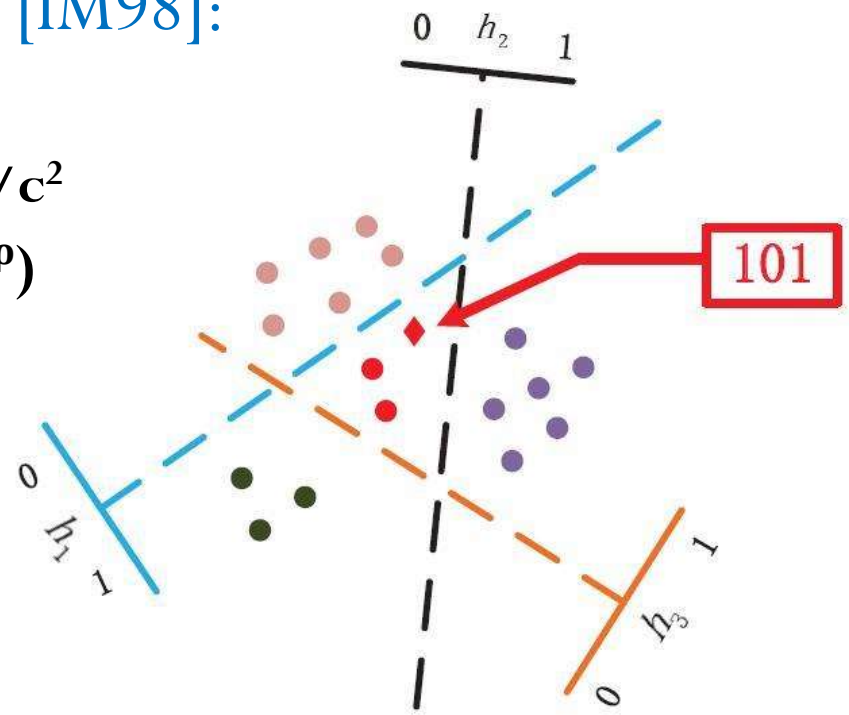
- Curse of dimensionality:
 - Given a polynomial indexing space $n^{O(1)}d^{O(1)}$, existing a sublinear time algorithm to solve **exact** NNS refutes SETH [Wil18].
 - Indexing space or query time must be exponential in d .
- Classic solutions: Voronoi decomposition



Space: $O(n^{O(d)})$
Time: $O(d^{O(1)} \log n)$

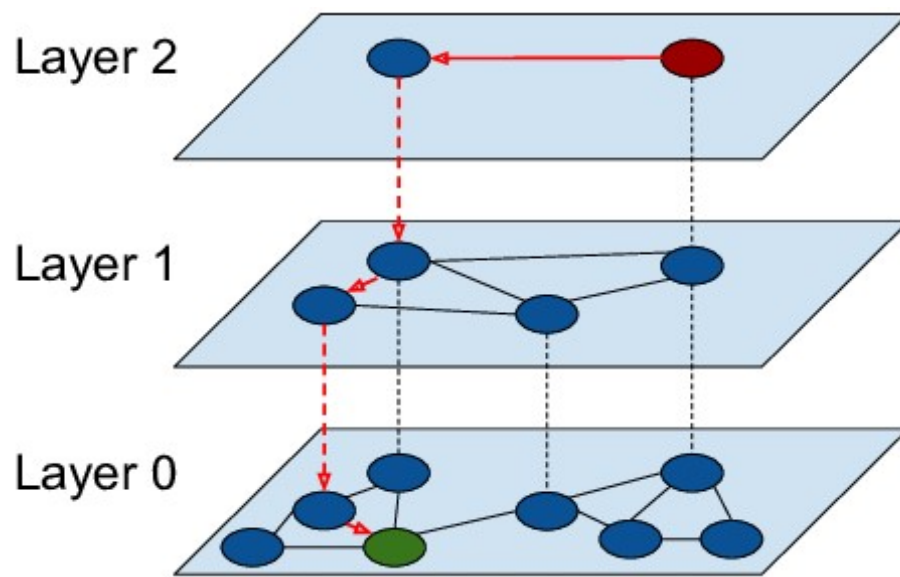
Approximate NNS

- Approximate NNS (ANNS):
 - Returns \mathbf{x}' such that $\text{dist}(\mathbf{q}, \mathbf{x}') \leq c \text{dist}(\mathbf{q}, \mathbf{x})$
- Locality-sensitive hashing (LSH) [IM98]:
 - Theoretical **guarantee** to find \mathbf{x}'
 - Sublinear query time $O(n^\rho)$, $\rho \approx 1/c^2$
 - Subquadratic indexing space $O(n^{1+\rho})$
 - **But...**

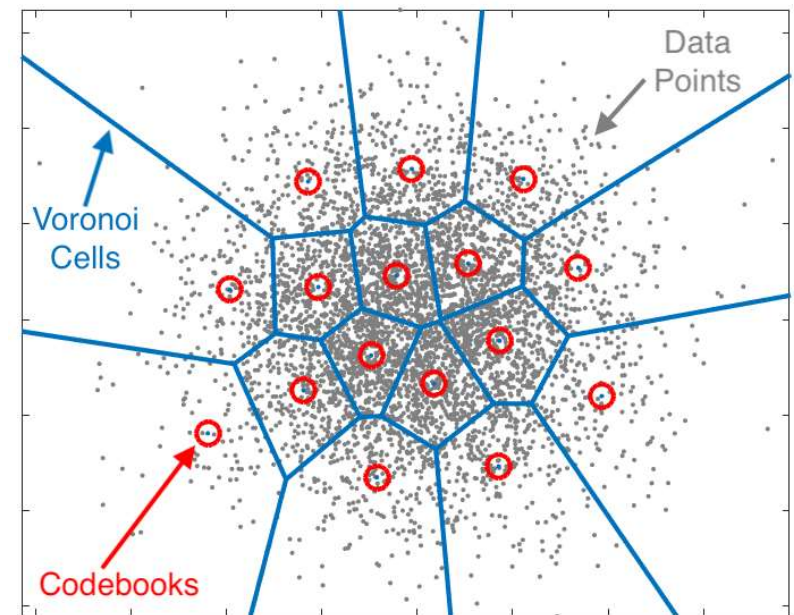


Approximate NNS

- Approximate NNS (ANNS):
 - Seek high **empirical** search recalls for top-**k** NNS (e.g. tiny c)
- Data-dependent approaches surpass LSH.



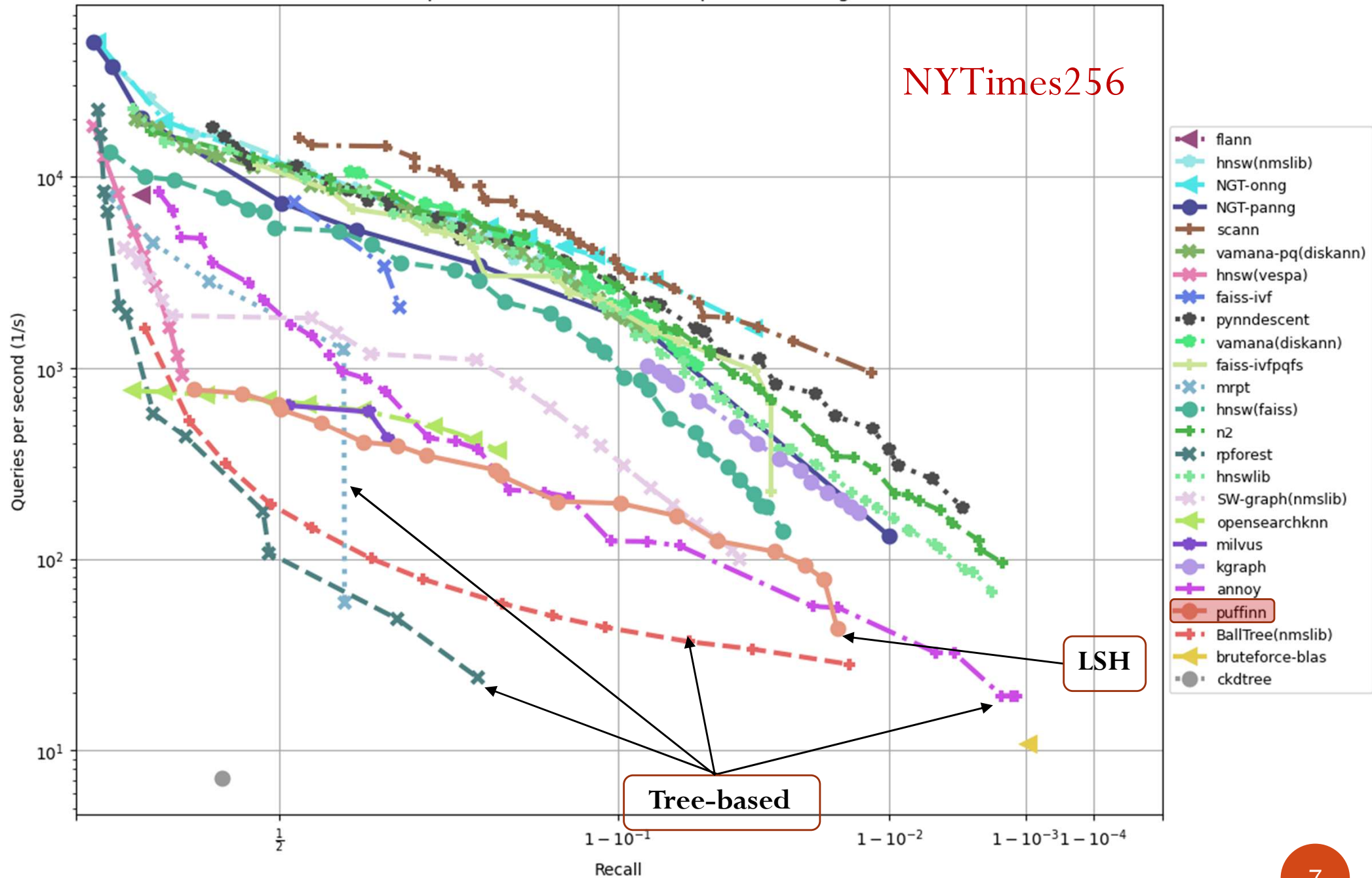
Graph-based index



Vector quantization

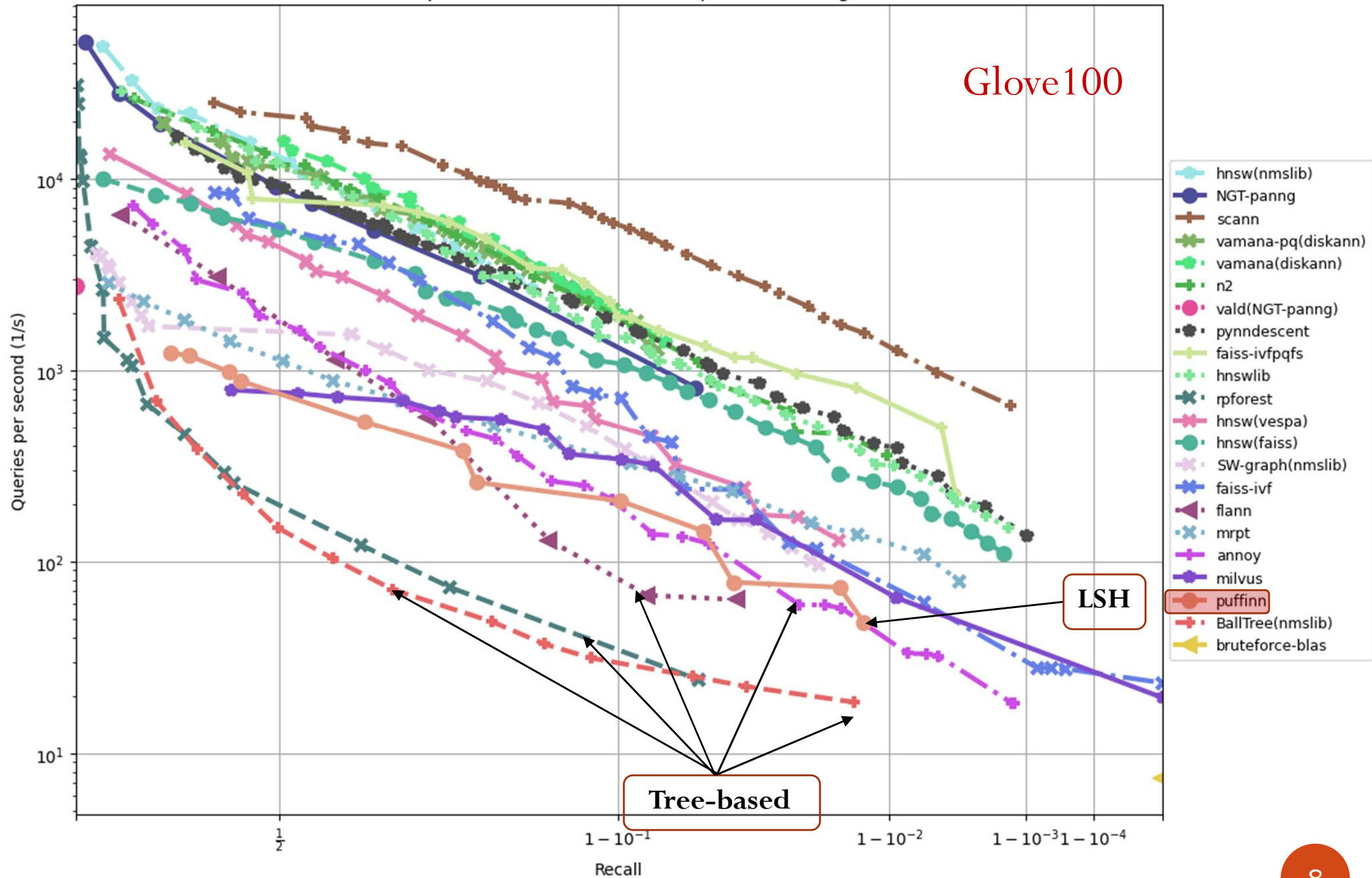
Recall-Queries per second (1/s) tradeoff - up and to the right is better

NYTimes256



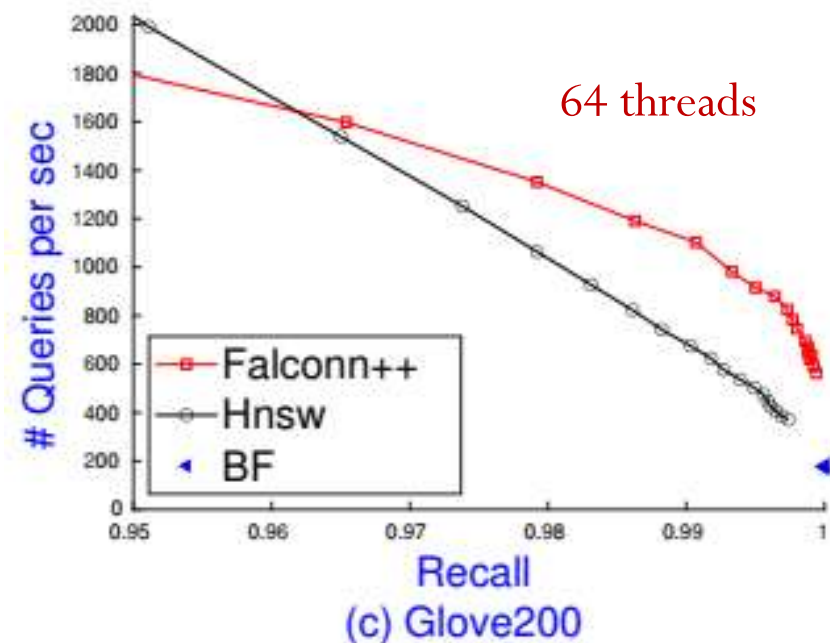
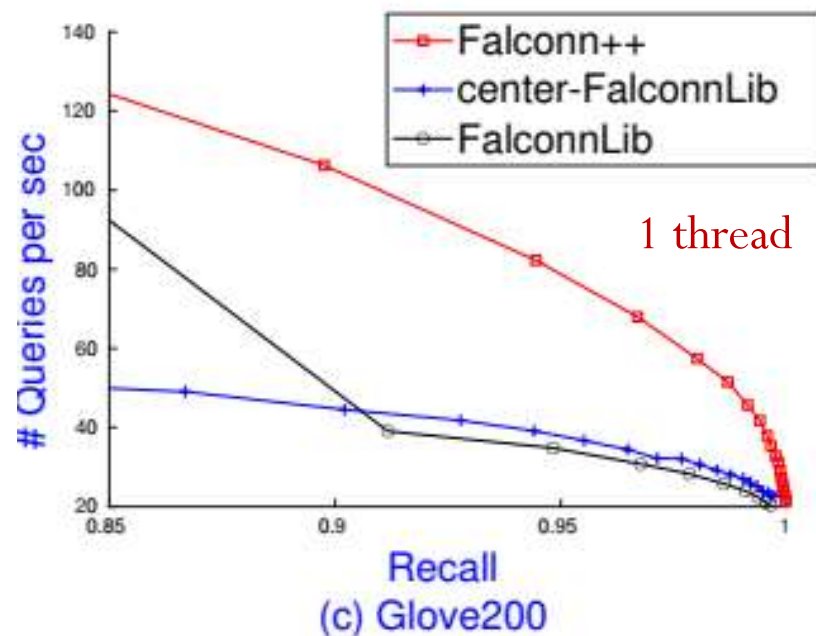
Recall-Queries per second (1/s) tradeoff - up and to the right is better

Glove100



Falconn++

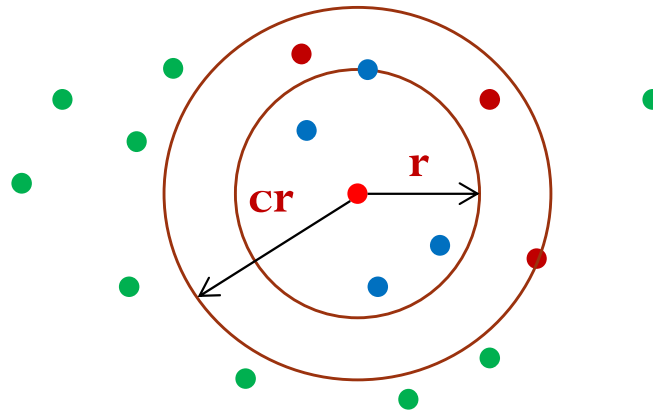
- A practical locality-sensitive filtering approach
 - Lower query time complexity than Falconn, an optimal LSH scheme on angular distance.
 - Empirical higher recall-speed tradeoffs than Falconn
 - Competitive with HNSW on high recall regimes



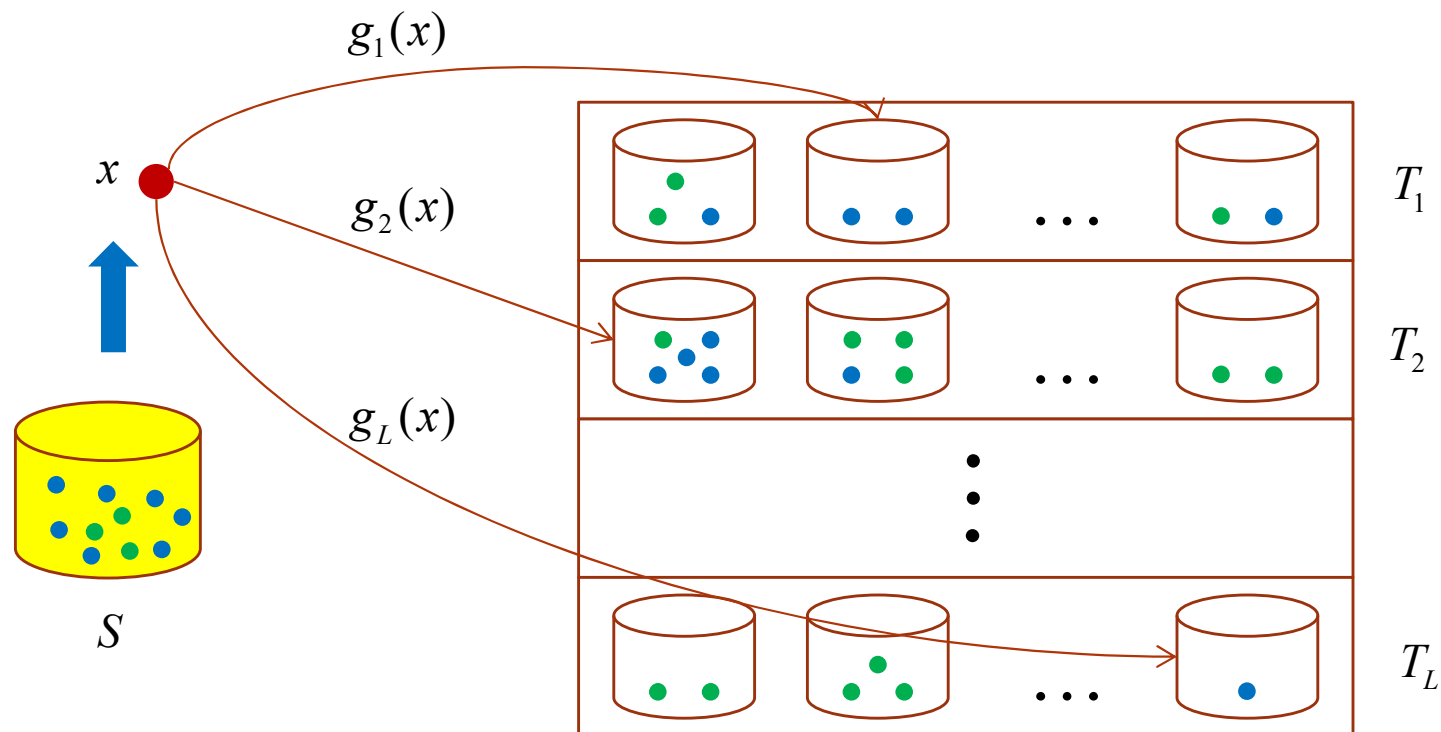
Locality-sensitive hashing (LSH)

- Definition [IM98]:

- Given a distance function $\text{dist}(\cdot, \cdot)$ and positive values r, c, p_1, p_2 where $p_1 > p_2, c > 1$. A family of functions \mathbf{H} is called (r, cr, p_1, p_2) -sensitive if for uniformly chosen $h \in \mathbf{H}$ and all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$:
 - If $\text{dist}(\mathbf{x}, \mathbf{y}) \leq r$ then $\Pr [h(\mathbf{x}) = h(\mathbf{y})] \geq p_1$; (close points)
 - If $\text{dist}(\mathbf{x}, \mathbf{y}) \geq cr$ then $\Pr [h(\mathbf{x}) = h(\mathbf{y})] \leq p_2$. (far away points)



Hash tables construction



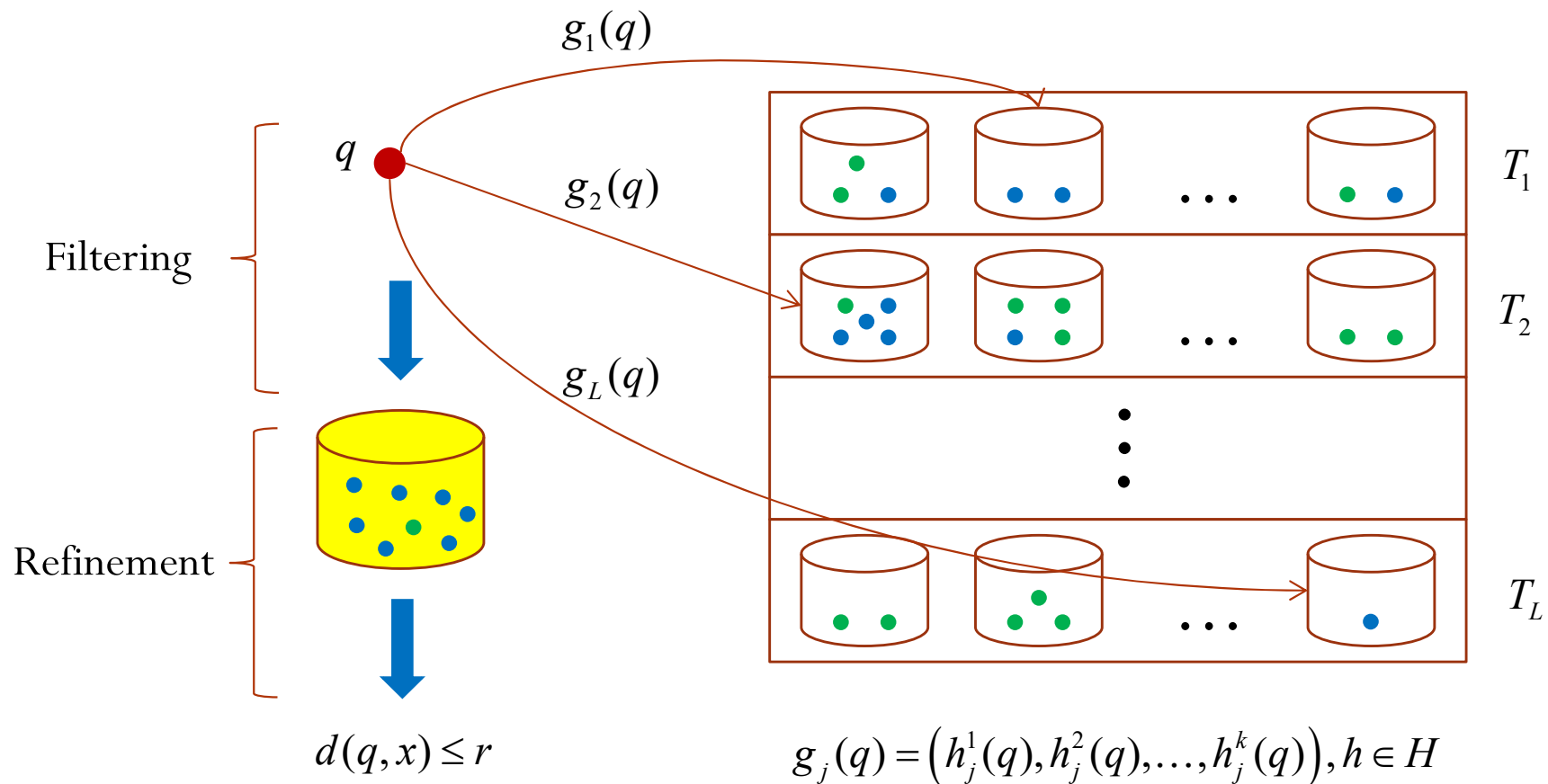
Parameter settings:

$$\begin{aligned} \mathbf{k} &= \ln(n)/\ln(1/p_2) \\ \rho &= \ln(1/p_1)/\ln(1/p_2) \\ \mathbf{L} &= n^\rho \end{aligned}$$

$$g_j(q) = (h_j^1(q), h_j^2(q), \dots, h_j^k(q)), h \in H$$

$$\text{Space: } O(dn + n^{1+\rho})$$

Hash tables lookup



Time: Hashing time + $O(dn^\rho)$

Falconn [AIL+15]

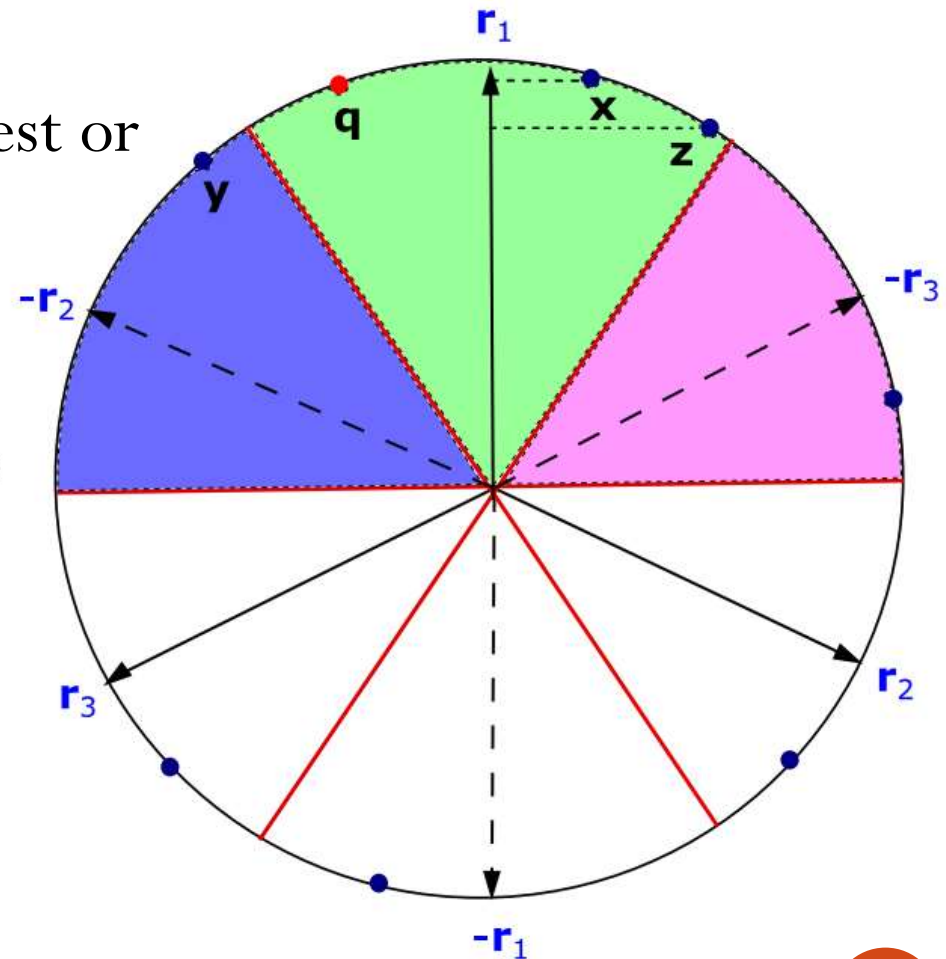
- Construct a spherical Voronoi using \mathbf{D} random vectors $\mathbf{r}_i \sim \mathbf{N}^d(\mathbf{0}, 1)$
- \mathbf{x} and \mathbf{q} collide if sharing the closest or furthest random vector.

- Assume $\mathbf{r}_1 = \arg \max_{\mathbf{r}_i} |\mathbf{q}^\top \mathbf{r}_i|$,

$$h(\mathbf{q}) = \begin{cases} \mathbf{r}_1 & \text{if } \text{sgn}(\mathbf{q}^\top \mathbf{r}_1) \geq 0, \\ -\mathbf{r}_1 & \text{otherwise.} \end{cases}$$

- Example:

- $h(\mathbf{x}) = h(\mathbf{z}) = h(\mathbf{q}) = \mathbf{r}_1$
- $h(\mathbf{y}) = -\mathbf{r}_2$



Falconn's takeaways

- Given \mathbf{D} random vectors, if $\text{dist}(\mathbf{x}, \mathbf{q}) = r$, then

$$\Pr [h(\mathbf{x}) = h(\mathbf{q})] \approx D^{-\frac{1}{4/r^2 - 1}}$$

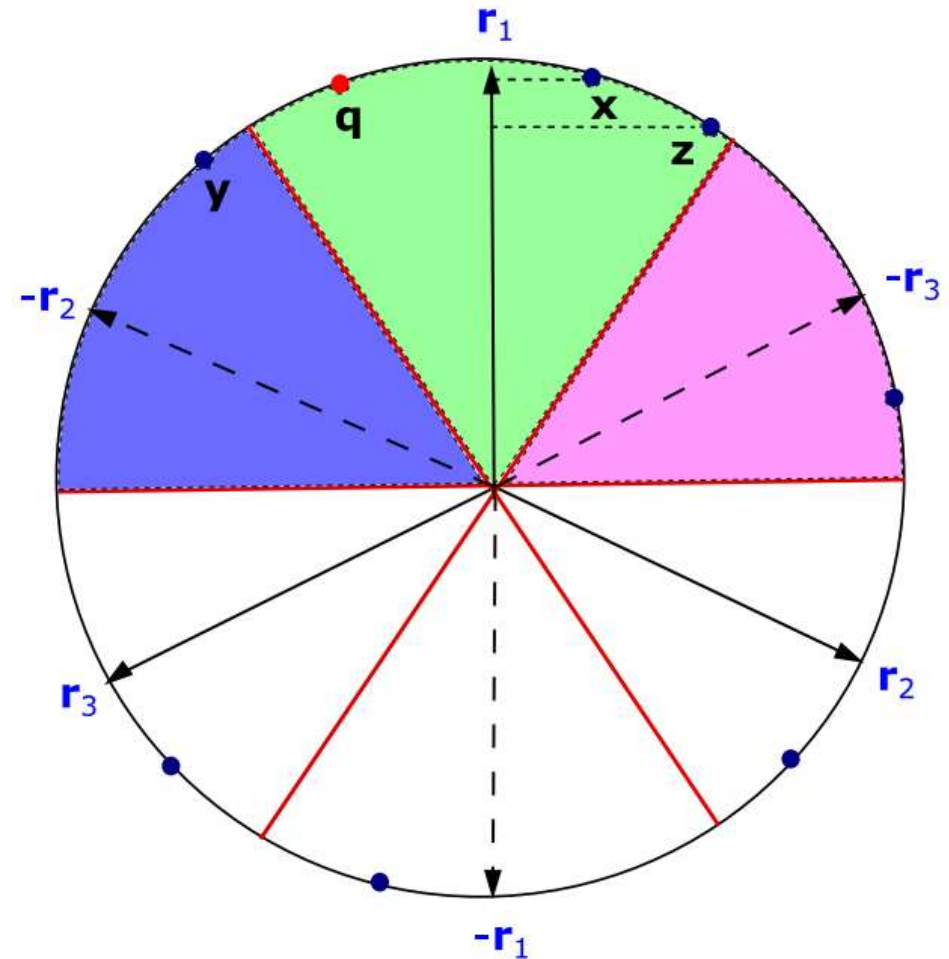
- Given a small \mathbf{c} , (r, cr, p_1, p_2) -sensitive Falconn has

$$\rho \approx \frac{4/c^2 r^2 - 1}{4/r^2 - 1} \approx 1/c^2$$

- Lower bound [OZW14]: $\rho \geq 1/c^2 - o(1)$ if $p_2 \geq 1/n$

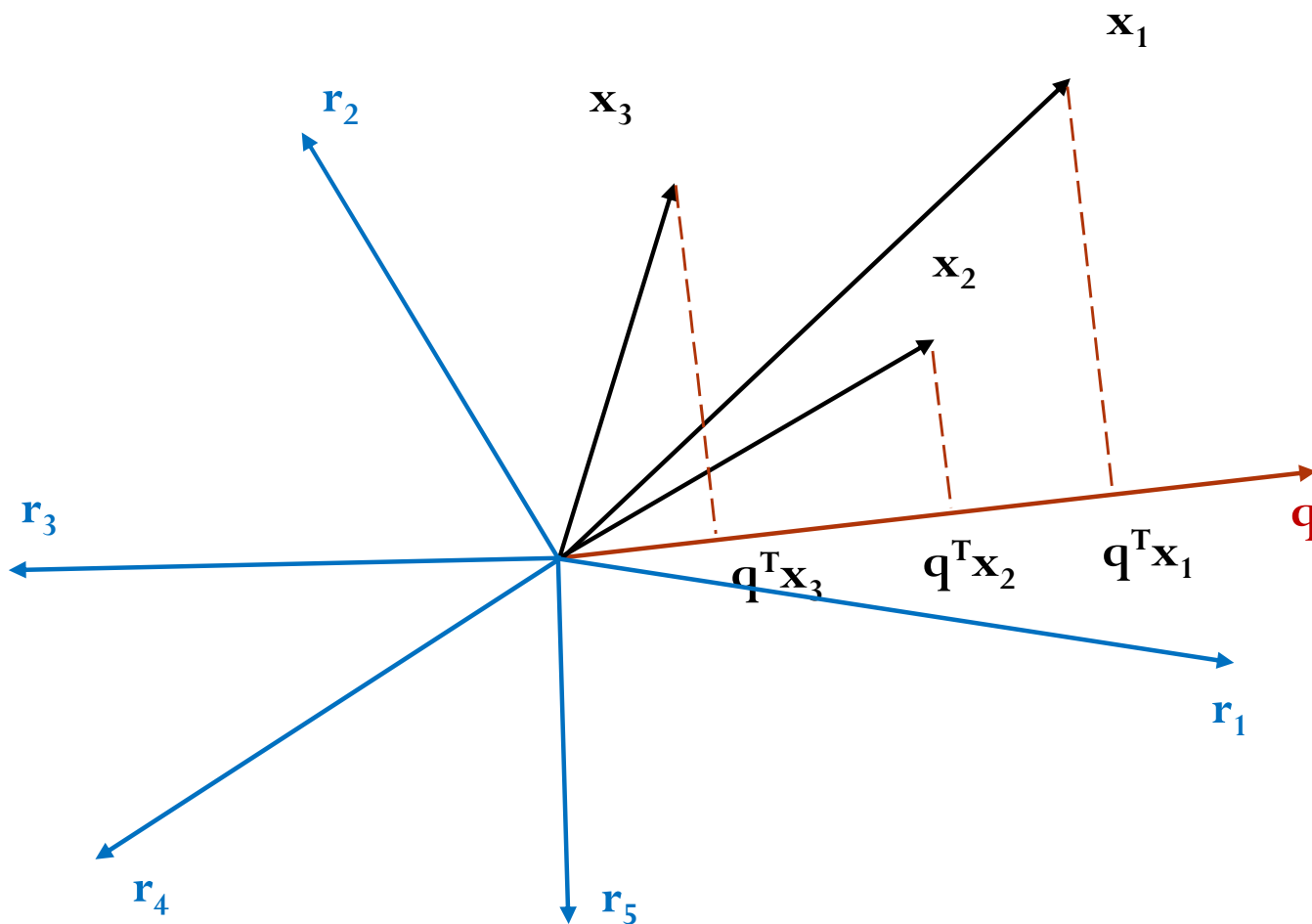
Practical multi-probe Falconn

- To reduce \mathbf{L} , probe the bucket of the next closest or furthest random vectors
 - Require a large $\mathbf{qProbes}$
 - Compute up to $0.1n$ distances to achieve recall of 90% in Glove300
- Example:
 - \mathbf{q} is next closest to $-\mathbf{r}_2$
 - The blue wedge is the next probe



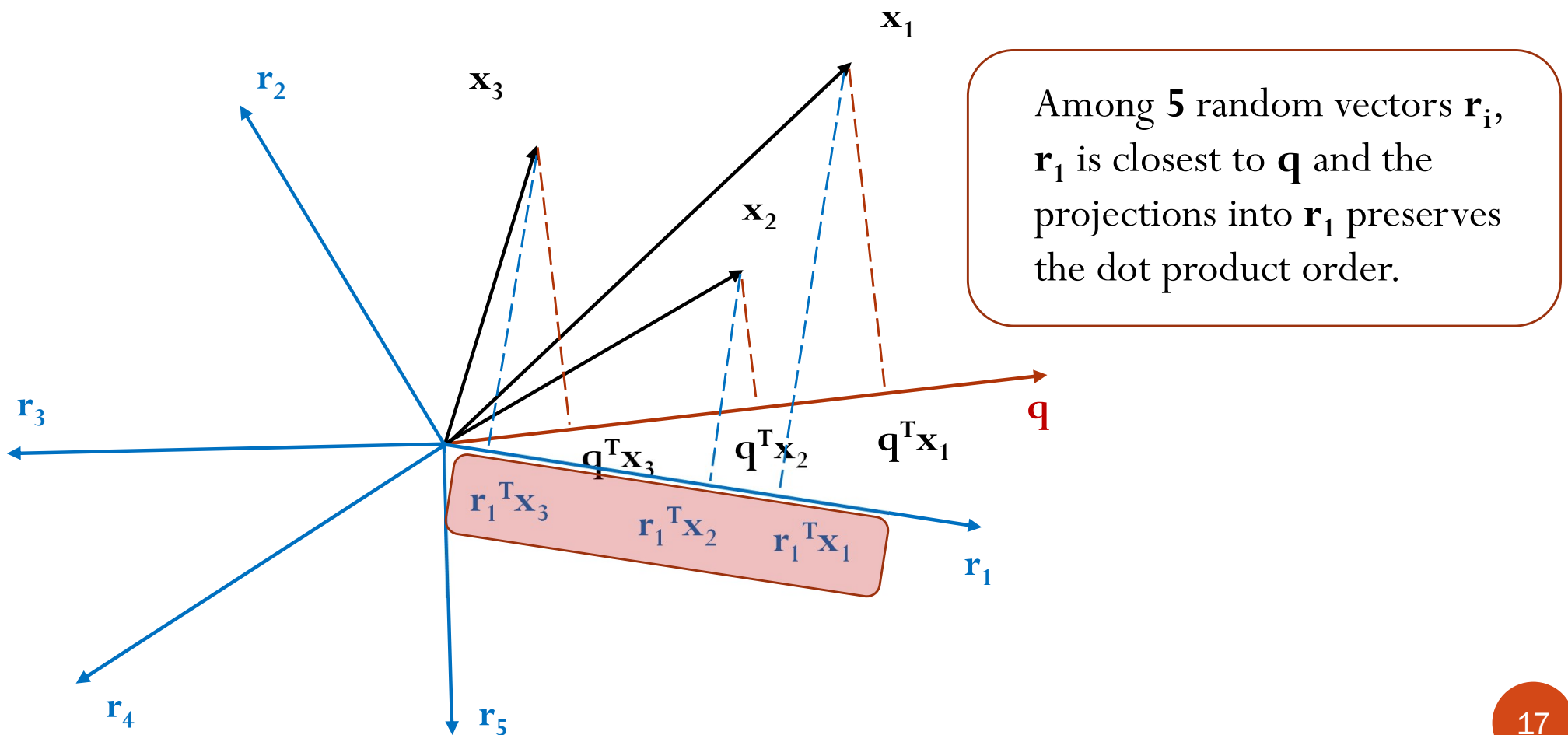
Geometric intuition

- Use random projections to find \mathbf{x} s.t. $\mathbf{x}^T \mathbf{q}$ is maximum.



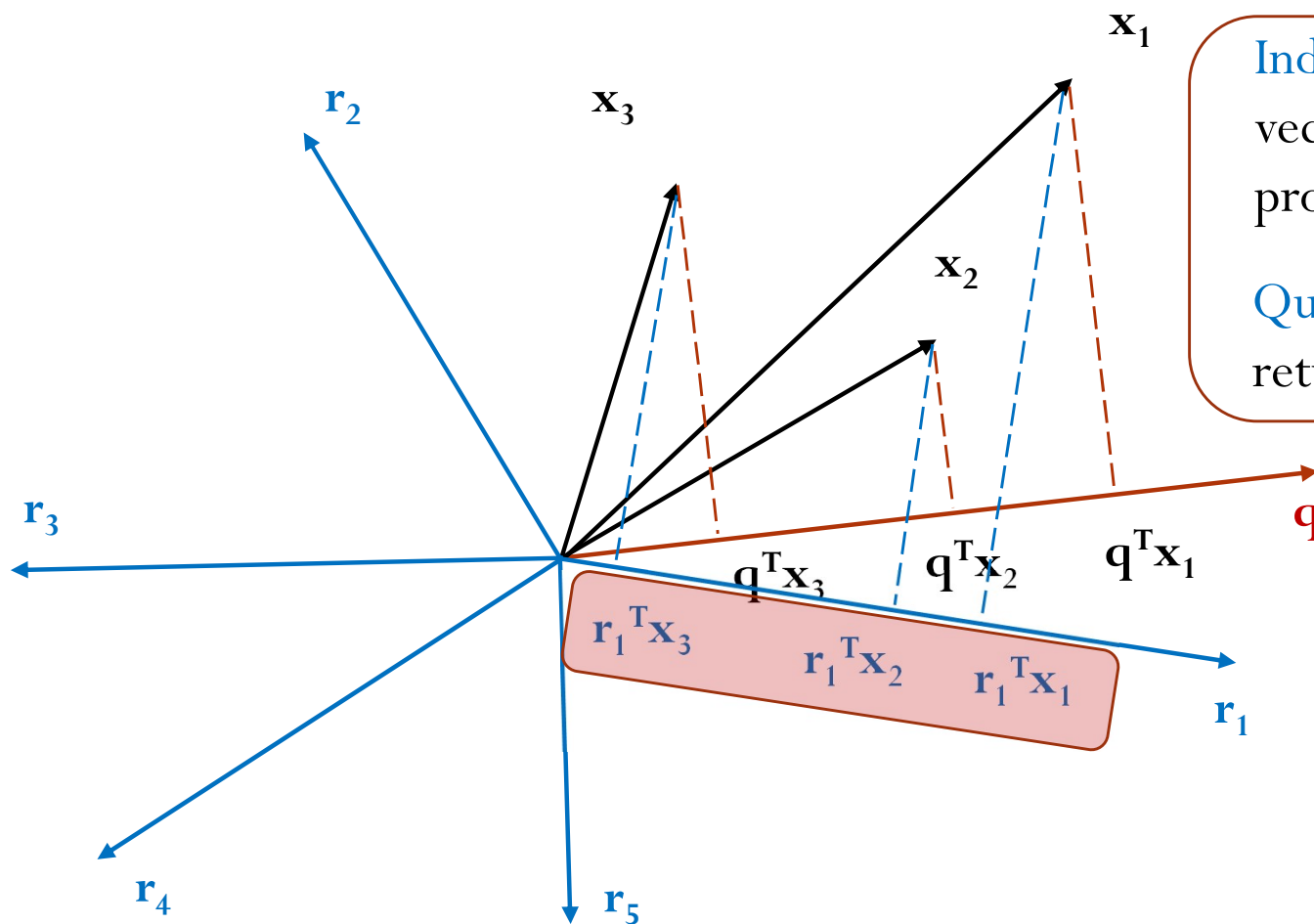
Geometric intuition

- Use a **large** number of random projections.



CEOs [Pha21]

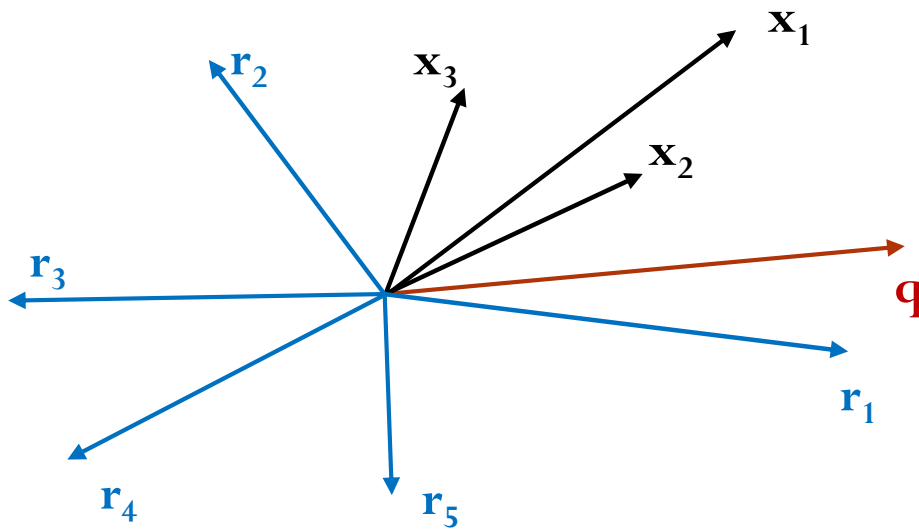
- Use a **large** number of random projections.





Indexing: Generate many random vectors r_i , **precompute** the dot product order L_i for r_i

Querying: Find r_i **closest** to q and return the top-1 NNS from L_i

CEOs: Dimensionality reduction



Among 5 random vectors \mathbf{r}_i , we only use \mathbf{r}_1 to estimate dot products.

\mathbf{x}_1		1.2	0.9
\mathbf{x}_2		0.5	0.5
\mathbf{x}_3		0.1	0.7

\mathbf{q}		1.5	0.1
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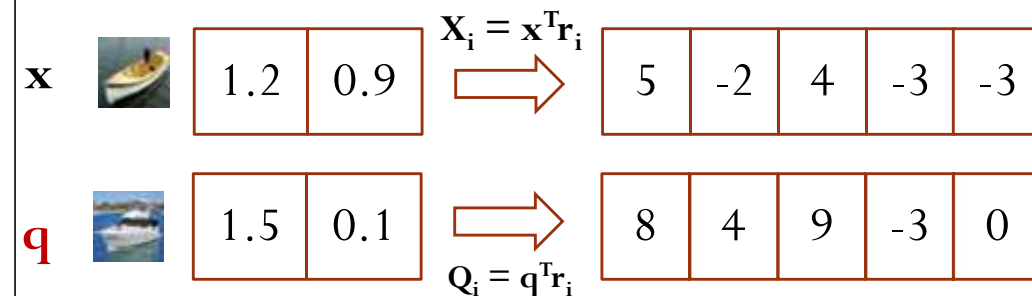
\mathbf{r}_1	\mathbf{r}_2	\mathbf{r}_3	\mathbf{r}_4	\mathbf{r}_5
4	-2	-4	-3	-3
3	-1	-3	-4	-4
1	-3	-2	-3	-3



9	4	-8	-3	0
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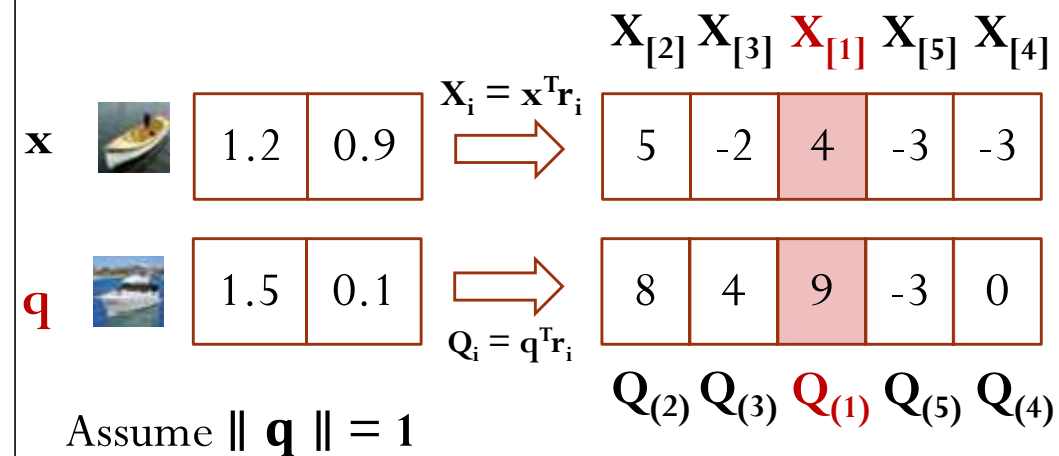
Concomitants of Extreme Order statistics

Random projections: Using \mathbf{D} random vectors $\mathbf{r}_i \sim \mathcal{N}^d(\mathbf{0}, \mathbf{I})$, we have \mathbf{D} bivariate samples (Q_i, X_i) from $\mathcal{N}(\mathbf{0}, \mathbf{0}, 1, \|\mathbf{x}\|, \mathbf{x}^T \mathbf{q})$ where $Q_i = \mathbf{q}^T \mathbf{r}_i$ and $X_i = \mathbf{x}^T \mathbf{r}_i$



Assume $\|\mathbf{q}\| = 1$

Concomitants of Extreme Order statistics



Random projections: Using D random vectors $\mathbf{r}_i \sim N^d(\mathbf{0}, 1)$, we have D bivariate samples (Q_i, X_i) from $N(0, 0, 1, \|\mathbf{x}\|, \mathbf{x}^T \mathbf{q})$ where $Q_i = \mathbf{q}^T \mathbf{r}_i$ and $X_i = \mathbf{x}^T \mathbf{r}_i$

Order statistics: Sort D pairs (Q_i, X_i) by Q -value, we form the order statistics where $Q_{(1)}$ is the first order statistics and $\mathbf{X}_{[1]}$ is the concomitant of the first order statistics.

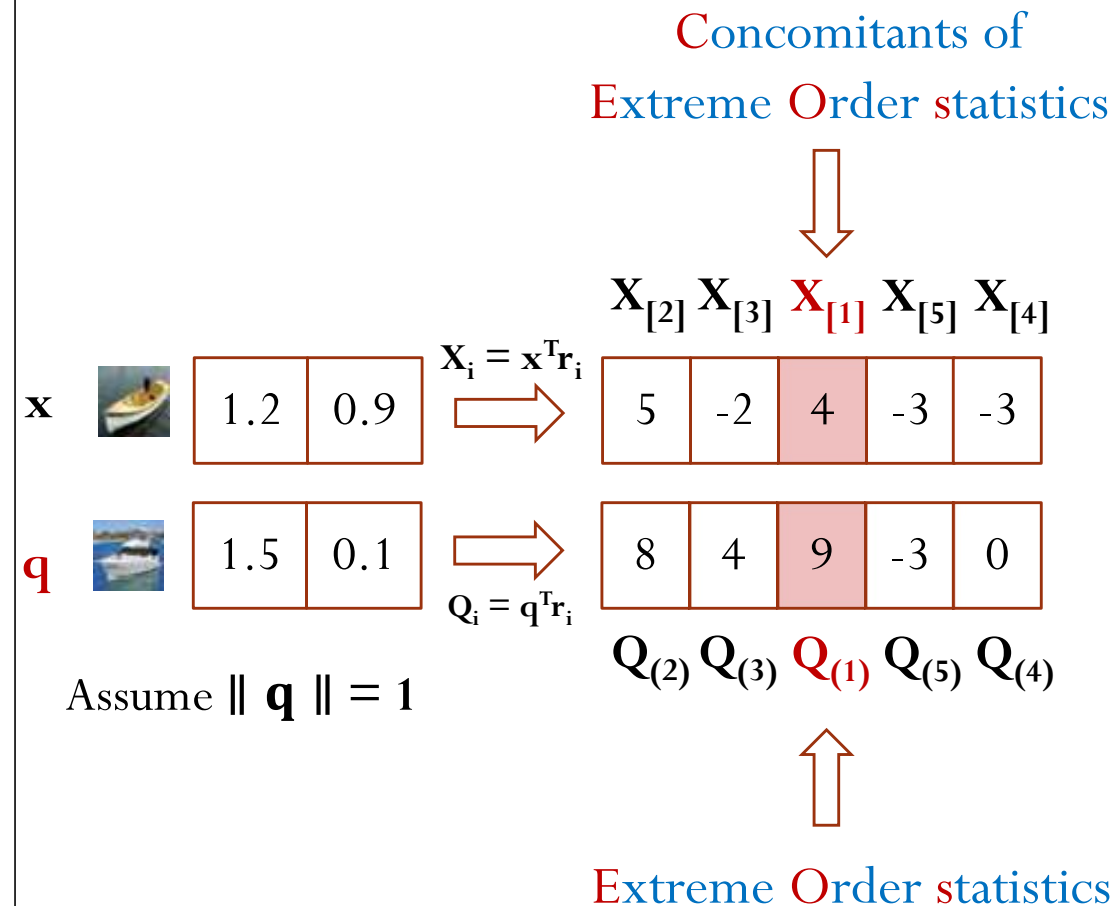
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Random projections: Using D random vectors $\mathbf{r}_i \sim N^d(\mathbf{0}, \mathbf{I})$, we have D bivariate samples (Q_i, X_i) from $N(\mathbf{0}, \mathbf{0}, 1, \|\mathbf{x}\|, \mathbf{x}^T \mathbf{q})$ where $Q_i = \mathbf{q}^T \mathbf{r}_i$ and $X_i = \mathbf{x}^T \mathbf{r}_i$

Order statistics: Sort D pairs (Q_i, X_i) by Q -value, we form the order statistics where $Q_{(1)}$ is the first order statistics and $\mathbf{X}_{[1]}$ is the concomitant of the first order statistics.

Extreme order statistics: When D is sufficiently large, $Q_{(1)}$ is the extreme order statistics and $\mathbf{X}_{[1]}$ is the concomitant of the extreme order statistics.



Theory of Concomitants of Extreme Order statistics [DG74]

Concomitants of
Extreme Order statistics



$X_{[2]} X_{[3]} X_{[1]} X_{[5]} X_{[4]}$

$X_i = \mathbf{x}^T \mathbf{r}_i$



5	-2	4	-3	-3
---	----	---	----	----



8	4	9	-3	0
---	---	---	----	---

$Q_i = \mathbf{q}^T \mathbf{r}_i$

$Q_{(2)} Q_{(3)} Q_{(1)} Q_{(5)} Q_{(4)}$



Extreme Order statistics

Extreme order statistics: $Q_{(1)}$ is the maximum variable among D random variables $Q_i = \mathbf{q}^T \mathbf{r}_i \sim N(0, 1)$.

Assume $\|\mathbf{q}\| = 1$

Extreme order statistics:

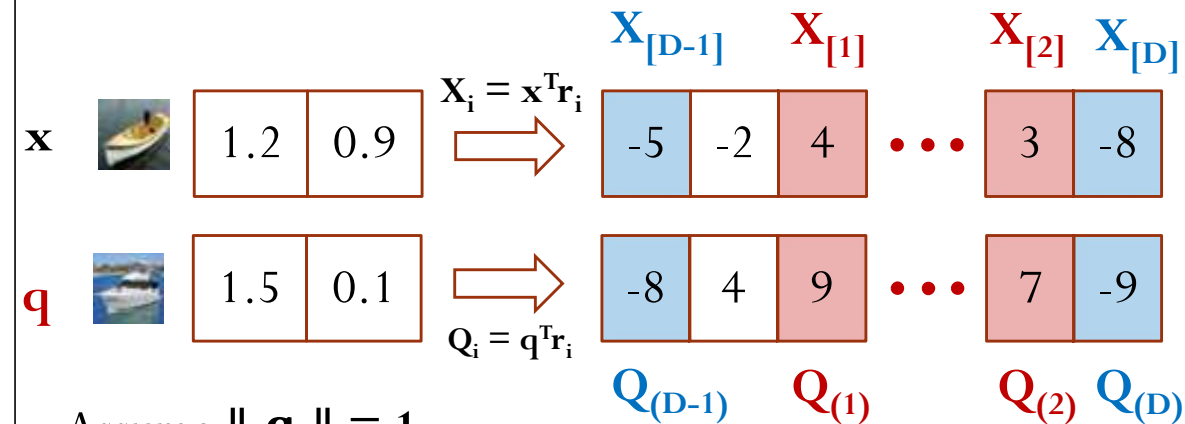
$$E[Q_{(1)}] \approx \sqrt{2\ln(D)}, \text{Var}[Q_{(1)}] \approx 0$$

Concomitant of extreme order statistics:

$$X_{[1]} \sim N(\mathbf{x}^T \mathbf{q} \sqrt{2\ln(D)}, \|\mathbf{x}\|^2 - (\mathbf{x}^T \mathbf{q})^2)$$

Theory of Concomitants of Extreme Order statistics [DG74]

Concomitants of Extreme Order statistics



Top s_0 **maximum** and **minimum** order statistics: $Q_{(i)}$ and $Q_{(D-i+1)}$ where $i = 1, \dots, s_0$

Extreme Order statistics

Extreme order statistics:

$$E[Q_{(i)}] \approx \sqrt{2\ln(D)}$$

$$E[Q_{(D-i+1)}] \approx -\sqrt{2\ln(D)}$$

Concomitant of extreme order statistics:

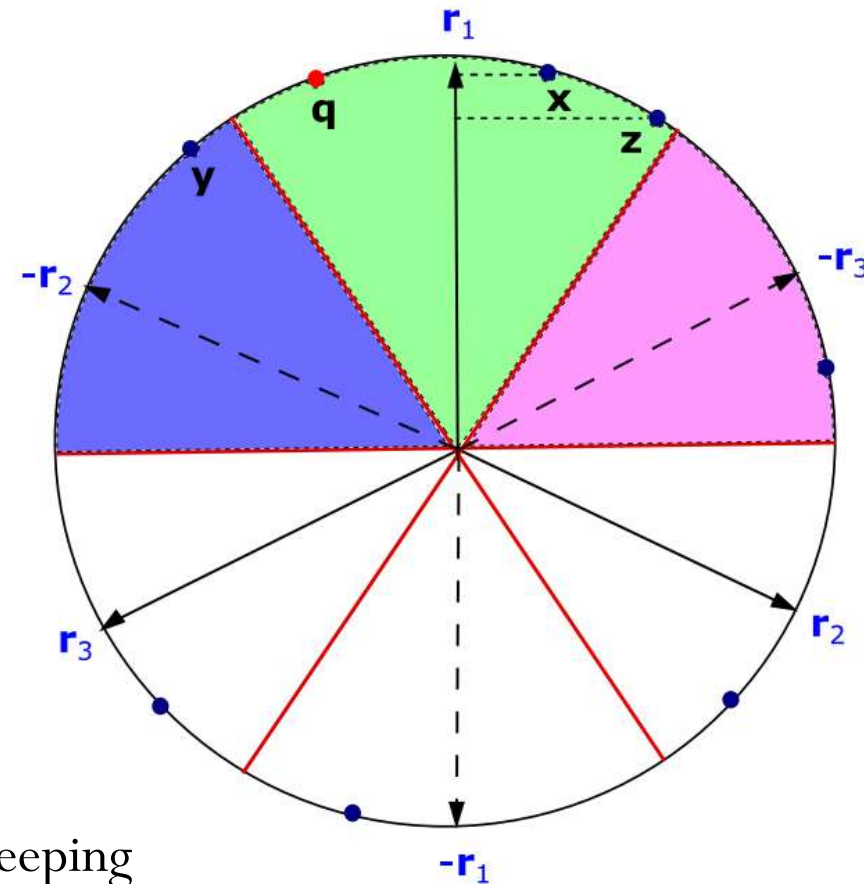
$$X_{[i]} \sim N(\mathbf{x}^T \mathbf{q} \sqrt{2\ln(D)}, \|\mathbf{x}\|^2 - (\mathbf{x}^T \mathbf{q})^2)$$

$$X_{[D-i+1]} \sim N(-\mathbf{x}^T \mathbf{q} \sqrt{2\ln(D)}, \|\mathbf{x}\|^2 - (\mathbf{x}^T \mathbf{q})^2)$$

$X_{[i]}$ and $X_{[D-i+1]}$ are **independent** asymptotically.

Connection to multi-probe Falconn

- Falconn:** If $\mathbf{r}_1 = \arg \max_{\mathbf{r}_i} |\mathbf{q}^\top \mathbf{r}_i|$,
 - Use \mathbf{r}_1 corresponding to $\mathbf{Q}_{(1)}$ as hash value
 - Use $\mathbf{Q}_{(i)}$ and $\mathbf{Q}_{(D-i)}$ as probing buckets where $i = 1, \dots, s_0$
- CEOs:** If $\mathbf{r}_1 = \arg \max_{\mathbf{r}_i} |\mathbf{q}^\top \mathbf{r}_i|$,
 - Use $\mathbf{X}_{[1]} = \mathbf{x}^\top \mathbf{r}_1$ to estimate $\mathbf{x}^\top \mathbf{q}$
 - Use $\mathbf{X}_{[i]}$ and $\mathbf{X}_{[D-i]}$ as estimators of $\mathbf{x}^\top \mathbf{q}$ where $i = 1, \dots, s_0$
- Falconn++ = Falconn + CEOs**



Partition \mathbf{n} points into $2\mathbf{D}$ buckets

Scale each bucket by keeping
 \mathbf{x} with largest $\mathbf{x}^T \mathbf{r}_i$

Falconnn++: A locality-sensitive filtering

- A locality-sensitive filtering (LSF) mechanism:
 - Given a distance function $\mathbf{dist}(\cdot, \cdot)$ and positive values \mathbf{r} , \mathbf{c} , \mathbf{q}_1 , \mathbf{q}_2 where $\mathbf{q}_1 > \mathbf{q}_2$, $\mathbf{c} > 1$. For an $(\mathbf{r}, \mathbf{cr}, \mathbf{p}_1, \mathbf{p}_2)$ -sensitive function \mathbf{h} and \mathbf{x}, \mathbf{y} in $\mathbf{h}(\mathbf{q})$:
 - If $\mathbf{dist}(\mathbf{x}, \mathbf{q}) \leq \mathbf{r}$ then $\Pr [\mathbf{x} \text{ is not filtered}] \geq \mathbf{q}_1$
 - If $\mathbf{dist}(\mathbf{y}, \mathbf{q}) \geq \mathbf{cr}$ then $\Pr [\mathbf{y} \text{ is not filtered}] \leq \mathbf{q}_2$
- Combine LSH and LSF:
 - $\Pr [\mathbf{h}(\mathbf{x}) = \mathbf{h}(\mathbf{q}), \mathbf{x} \text{ is not filtered}] \geq \mathbf{p}_1 \mathbf{q}_1$
 - $\Pr [\mathbf{h}(\mathbf{y}) = \mathbf{h}(\mathbf{q}), \mathbf{y} \text{ is not filtered}] \leq \mathbf{p}_2 \mathbf{q}_2$
- We need $\ln(1/\mathbf{q}_1) / \ln(1/\mathbf{q}_2) \leq \boldsymbol{\rho} \approx 1/\mathbf{c}^2$ to achieve a new exponent $\boldsymbol{\rho}' \leq \boldsymbol{\rho}$

Falconn++

- Asymptotic property of CEOs:

- $\mathbf{X}_{[1]} \sim \mathcal{N}(\mathbf{x}^T \mathbf{q} \sqrt{2 \ln(D)}, \|\mathbf{x}\|^2 - (\mathbf{x}^T \mathbf{q})^2)$
- $\mathbf{Y}_{[1]} \sim \mathcal{N}(\mathbf{y}^T \mathbf{q} \sqrt{2 \ln(D)}, \|\mathbf{y}\|^2 - (\mathbf{y}^T \mathbf{q})^2)$

- Filtering mechanism:

- Define a threshold $\mathbf{t} = (1 - \mathbf{r}^2/2)\sqrt{2 \ln(D)}$. For each bucket corresponding to \mathbf{r}_i , keep any point \mathbf{x} if $\mathbf{x}^T \mathbf{r}_i \geq \mathbf{t}$. Otherwise, discard it.
- Note: $\text{dist}(\mathbf{x}, \mathbf{q}) = \mathbf{r}$, then $\mathbf{x}^T \mathbf{q} = 1 - \mathbf{r}^2/2$

Falconn++'s takeaways

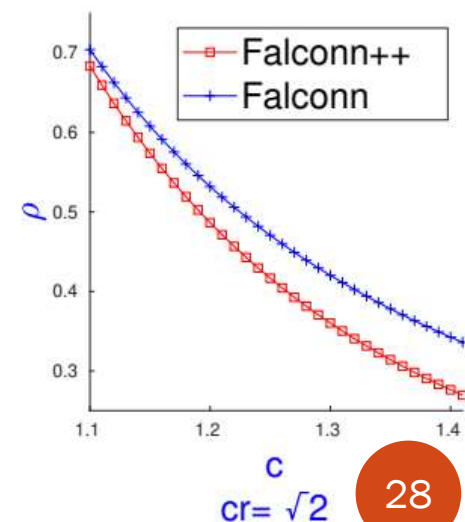
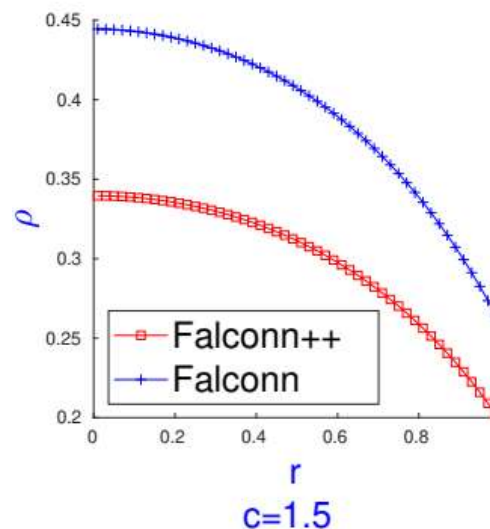
- For sufficiently **large** \mathbf{D} random projections, $c > 1$,

- If $\|\mathbf{x} - \mathbf{q}\| \leq r$, then $\Pr[\mathbf{x} \text{ is not filtered}] \geq q_1 = 1/2$;
- If $\|\mathbf{y} - \mathbf{q}\| \geq cr$, then $\Pr[\mathbf{y} \text{ is not filtered}] \leq q_2 = \frac{1}{\gamma\sqrt{2\pi}} \exp(-\gamma^2/2) < q_1$ where $\gamma = \frac{cr(1-1/c^2)}{\sqrt{4-c^2r^2}} \cdot \sqrt{2 \ln D}$.

- New exponent $\rho' \approx 1/(2c^2 - 2 + 1/c^2)$

$$\rho' = \frac{\ln(1/q_1 p_1)}{\ln(1/q_2 p_2)} \approx \frac{\frac{\ln 2}{\ln D} + \frac{1}{4/r^2 - 1}}{\frac{(1-1/c^2)^2}{4/c^2 r^2 - 1} + \frac{1}{4/c^2 r^2 - 1}}$$

$$\approx \frac{1}{1 + (1 - 1/c^2)^2} \cdot \frac{4/c^2 r^2 - 1}{4/r^2 - 1} \leq \rho.$$



Connection to LSF framework [ALRW17]

- Asymmetric LSF frameworks:

- Apply different filtering conditions on data and query to govern the space-time tradeoff
- Let \mathbf{t}_u and \mathbf{t}_q be two different thresholds.
- Collision: \mathbf{x} and \mathbf{q} pass the filter \mathbf{r}_i with $\Pr[\mathbf{x}^T \mathbf{r}_i \geq \mathbf{t}_u, \mathbf{q}^T \mathbf{r}_i \geq \mathbf{t}_q]$

- Falconn++:

- Use a sufficiently large \mathbf{D} to ensure the asymptotic property of CEOs
- $\mathbf{t}_u = (1 - r^2/2)\sqrt{2\ln(\mathbf{D})}$, $\mathbf{t}_q \approx \sqrt{2\ln(\mathbf{D})}$
- For $\mathbf{p}_2 \mathbf{q}_2 = 1/n$, $\mathbf{D} = O(n^{\rho'})$, Falconn++ yields $O(n^{\rho'})$ query time where $\rho' \approx 1/(2c^2 - 2 + 1/c^2)$ for $r \geq \sqrt{2}$

Practical implementations

- Data-dependent setting:

- Select a scaling factor $0 < \alpha < 1$ to scale each bucket of size \mathbf{B} to $\alpha \mathbf{B}$
 - Adapt \mathbf{t} to various density
 - Easy to govern the memory footprint (i.e. # points in a table)

- Multi-probe indexing:

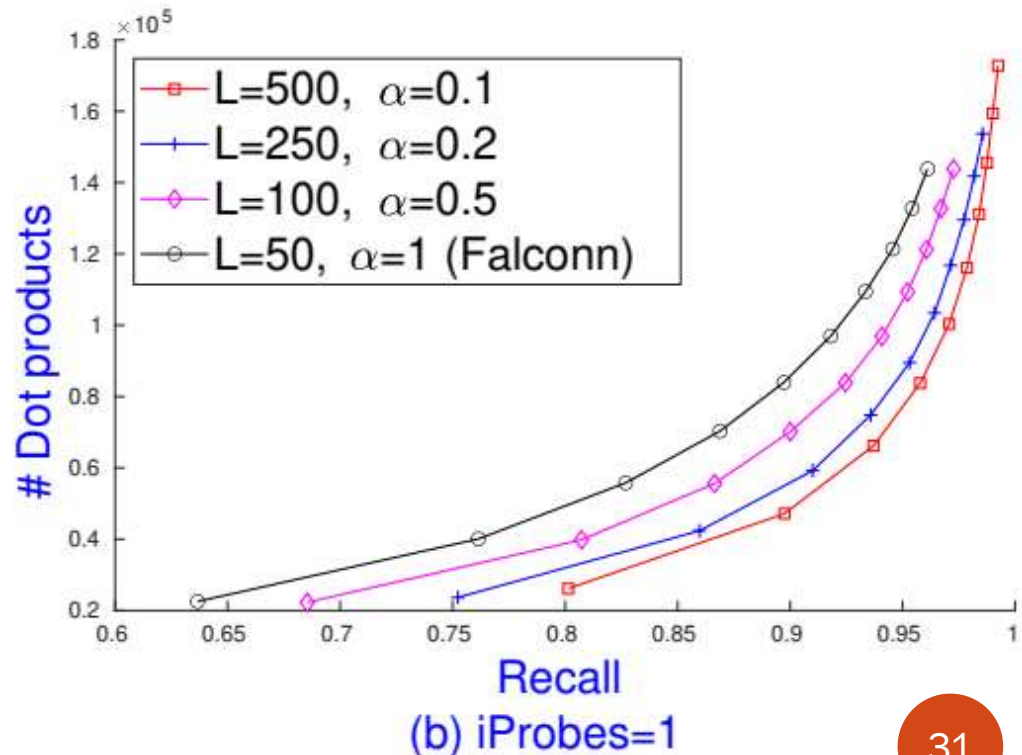
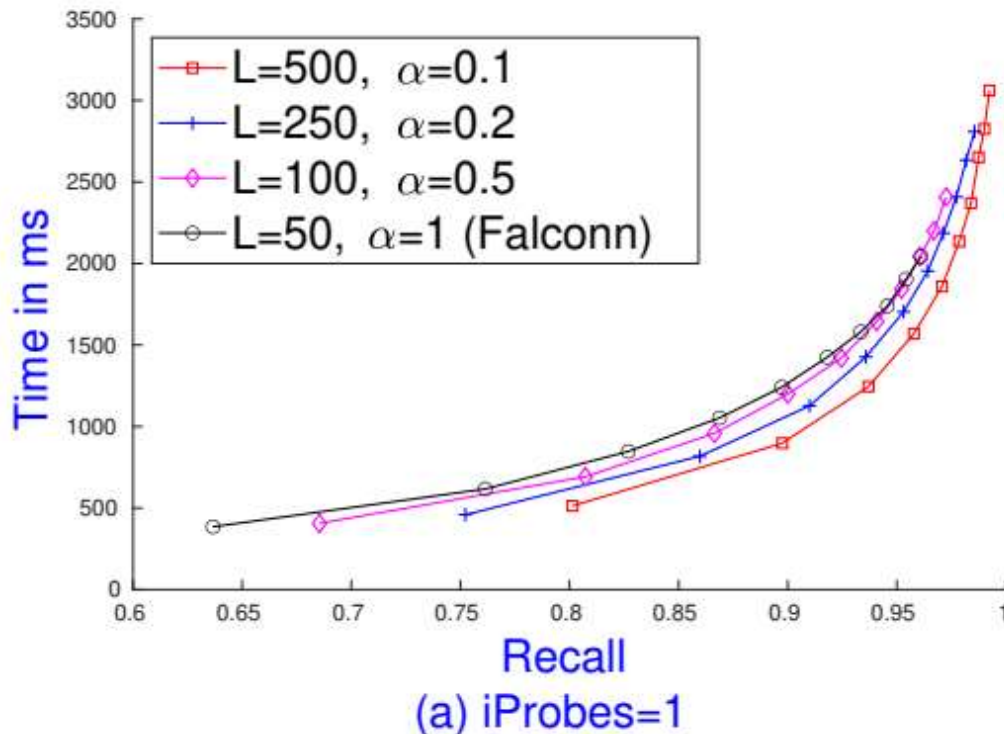
- For each point \mathbf{x} , hash it into $\mathbf{iProbes}$ buckets corresponding the $\mathbf{iProbes}$ closest or furthest random vectors
- Scale each bucket of size \mathbf{B} to $\alpha \mathbf{B} / \mathbf{iProbes}$

- Other heuristics:

- Pseudo-random rotation $\mathbf{HD}_3 \mathbf{HD}_2 \mathbf{HD}_1$ to simulate random projections
- Center the data point \mathbf{X}
- Limit scaling: keep $\max(\mathbf{k}, \alpha \mathbf{B} / \mathbf{iProbes})$ points in a bucket

Falconn++: Scaling bucket

- Experiment on Glove200 with 1.2M points with $k = 20$:
 - $D = 256$, 2 combined LSH functions, each table has $4D^2$ buckets
 - Falconn: $qProbes = \{1000, \dots, 20000\}$, Falconn++: $qProbes/\alpha$



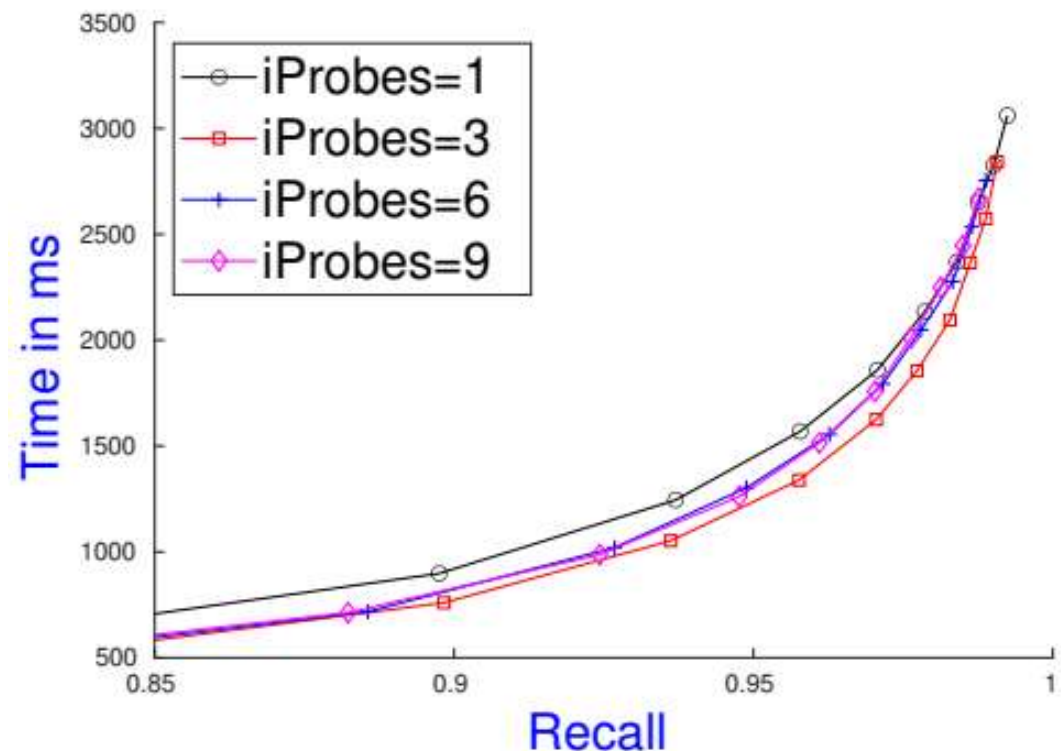
Falconn++: Multi-probe indexing

- Observation:

- Overfitting: Large **iProbes** degrades performance
- **iProbes = 2D** is as similar as theoretical LSF framework

- Setting iProbes:

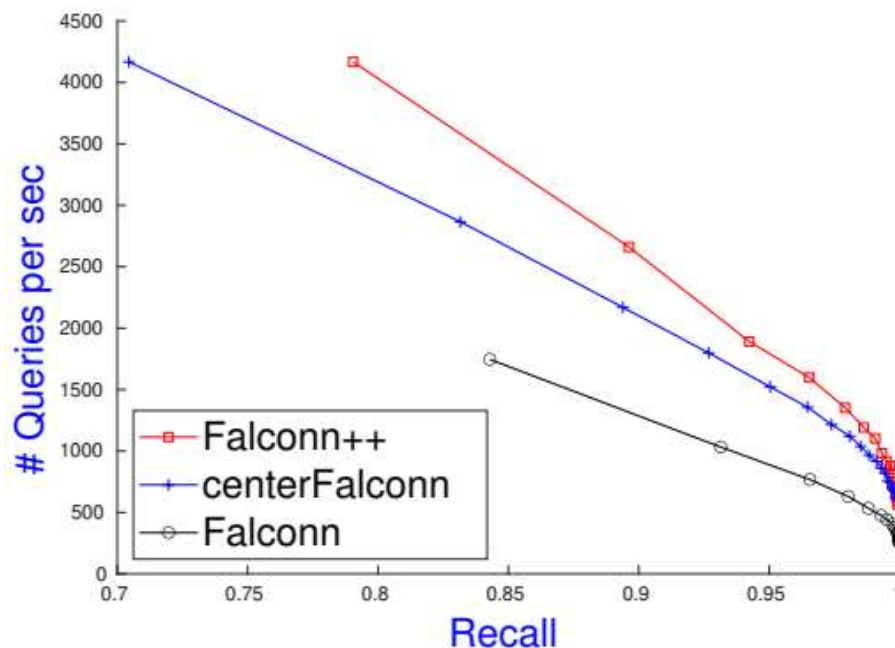
- $k \approx n \cdot \text{iProbes} / 4D^2$
- Each bucket has roughly $k=20$ points, especially sparse buckets
- **iProbes = 3**: $1.2M \cdot 3 / 2^{18} = 16$



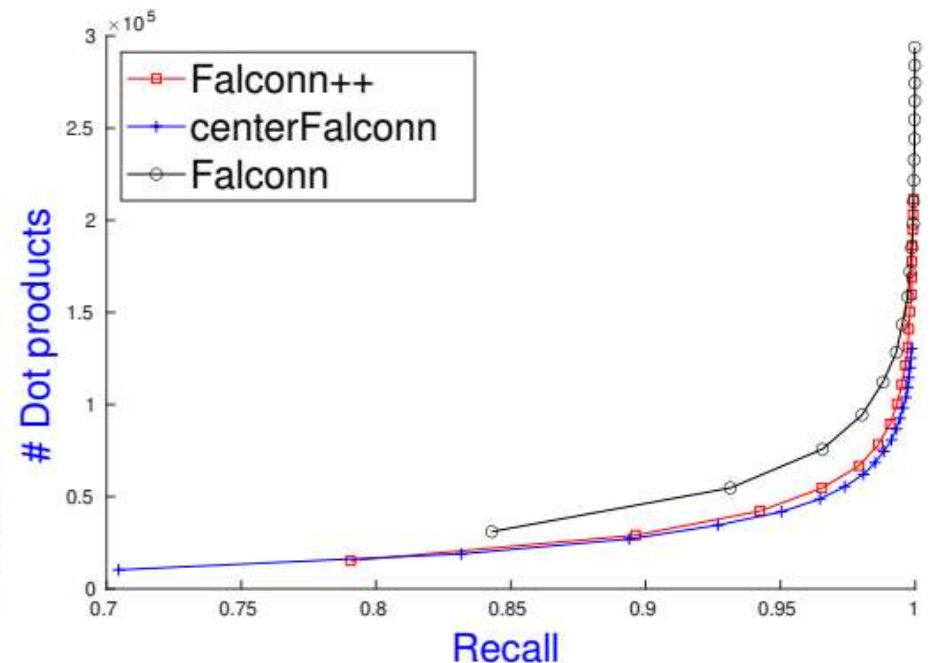
Recall
(c) $L=500$, $\alpha=0.1$
Glove200, $k = 20$

Falconn++: Centering data

- Experiment on Glove200 with $k = 20$:
 - $D = 256$, 2 combined LSH functions, $4D^2$ buckets/table, $L = 500$
 - Falconn++: $\alpha = 0.1$, iProbes = 3, qProbes/ α



(a) Speed-recall tradeoff



(b) # Dot products-recall tradeoff

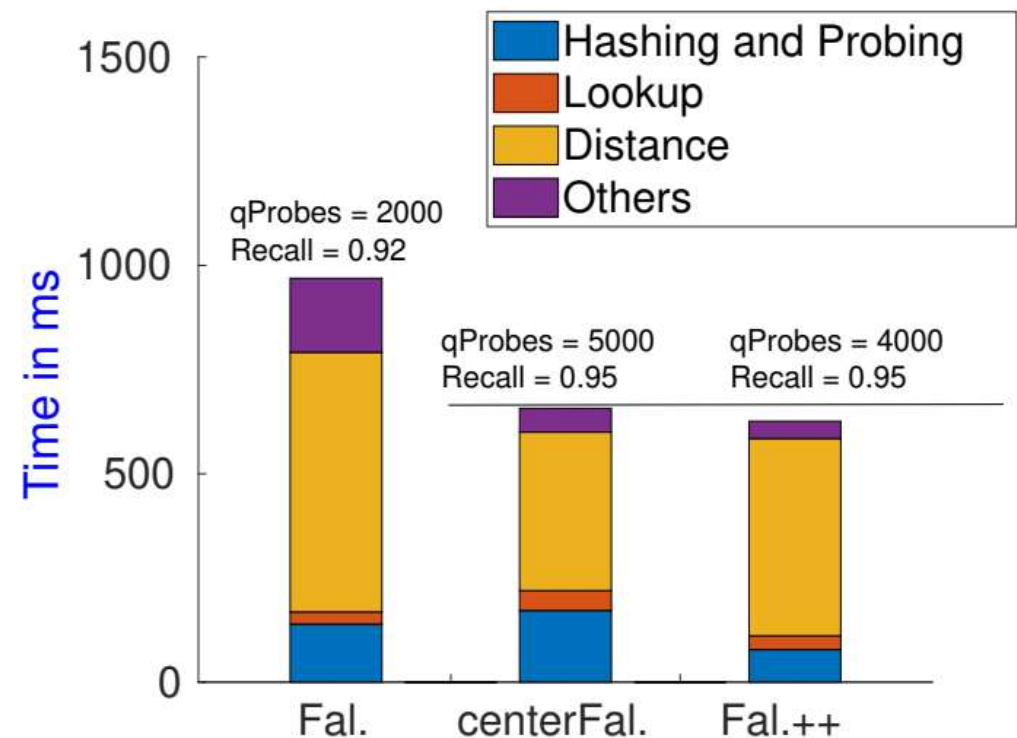
Falconn++: Limit scaling & centering

- Observations:

- After centering, buckets are more balanced.
- With $\alpha = 0.1$, $iProbes = 3$, and keep $\max(k, \alpha B / iProbes)$ points, # points/table $\approx 2.42 n$
- Less $qProbes$ and hash evaluation time than Falconn

- Future improvement:

- SimHash signatures to reduce distance computation time

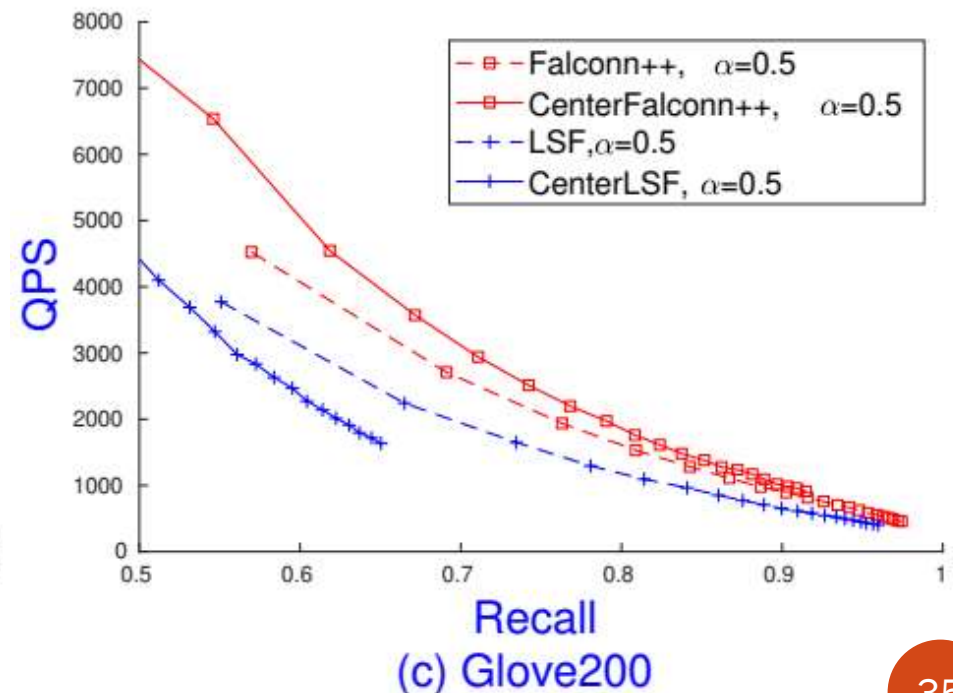
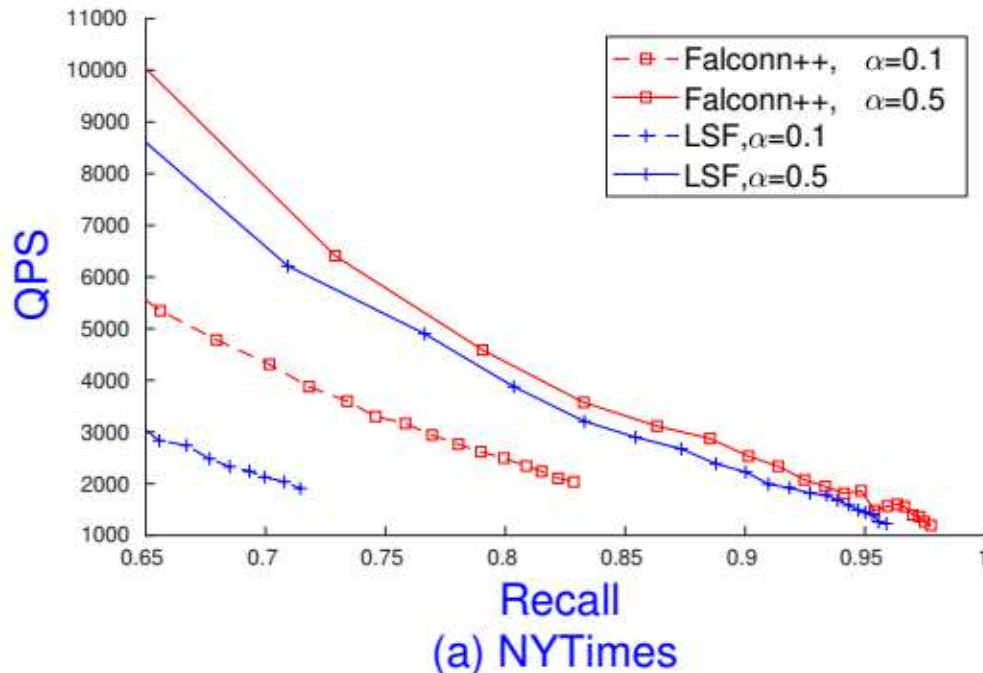


(c) Query time components

Glove200, $k = 20$

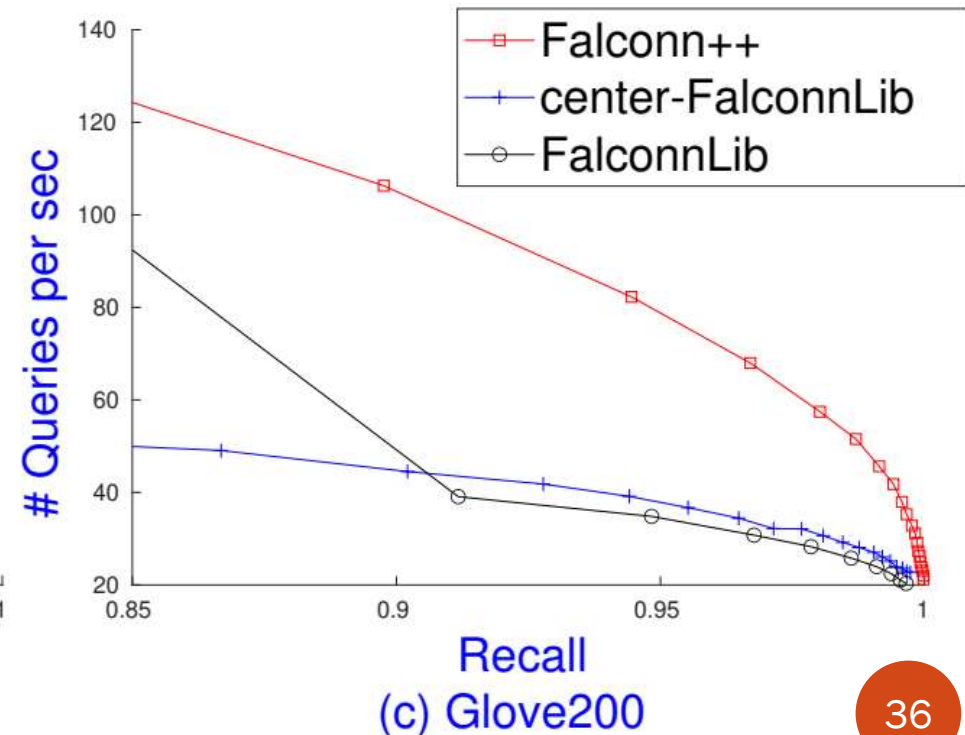
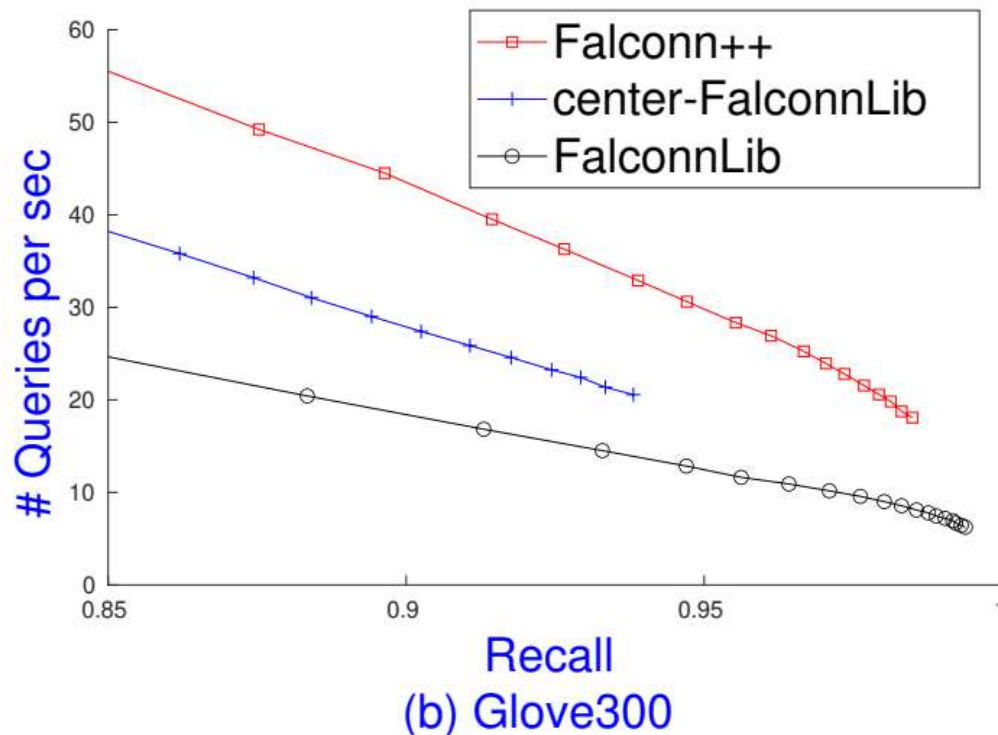
Falconn++ vs. Theoretical LSF

- **LSF**: Select \mathbf{t}_u s.t. $\Pr [\mathbf{x}^\top \mathbf{r}_i \geq t_u]^2 = \alpha/4D^2$
 - Falconn++: No limit scaling, only centering
 - **iProbes = 1, $\mathbf{D} = \{128, 256\}$, $\mathbf{L} = 100$** , 2 combined LSH/LSF functions



Falconn++ vs. FalconnLib

- Glove300 and Glove200 with **k = 20** and **1 thread**:
 - **L = 500**, **D = 256**, **$\alpha = 0.1$** , **iProbes = {1, 3}**, **4D² buckets/table**
 - Falconn: **L = 50** (Glove300), **L = 1210** (Glove200)



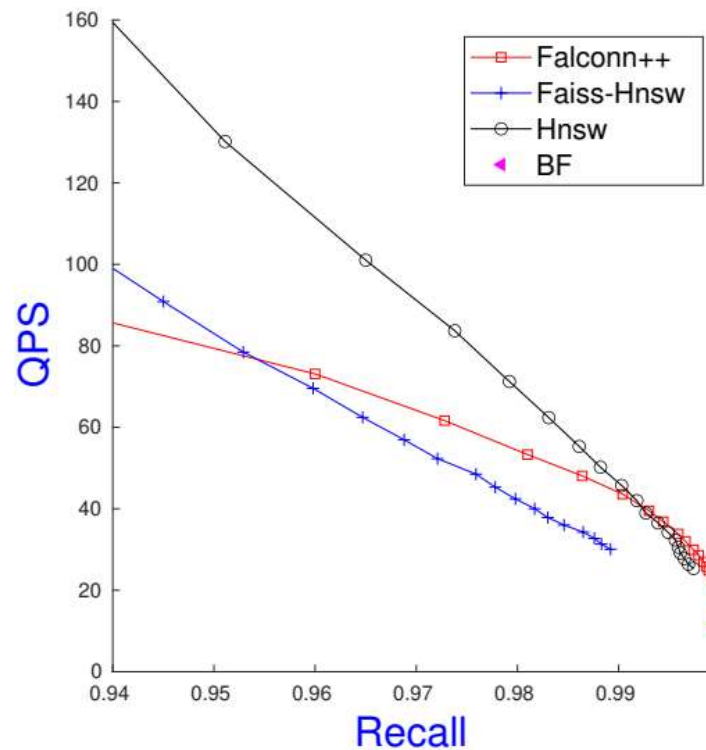
Falconn++ vs Hnsw

- Parameter settings:

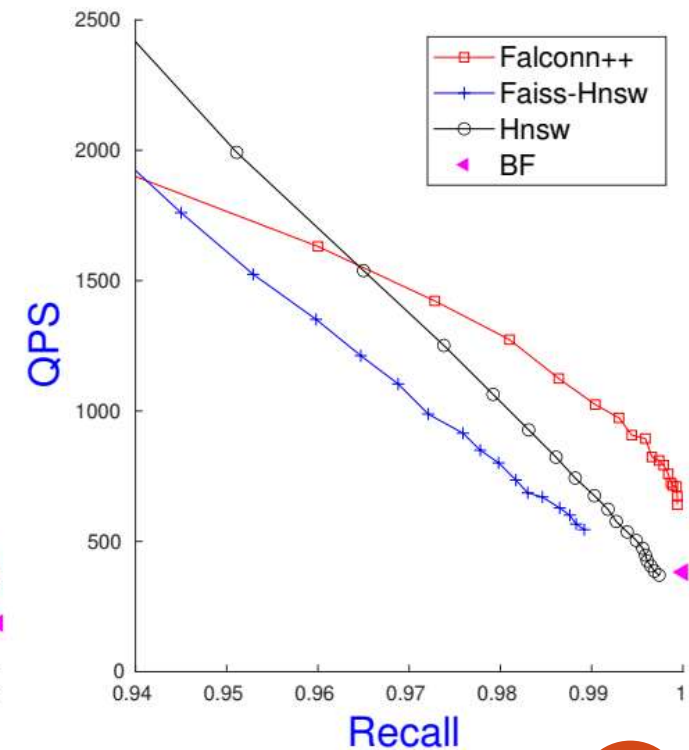
- Hnsw: **ef-index** = 200, **M** = 512, vary **ef-query**
- Falconn++: **D** = 256, **L** = 350, **α** = 0.01, **iProbes** = 3, vary **qProbes**

Indexing

Space: **5.4GB**
Hnsw: **13.7 mins**
Falconn++: **1.1 mins**



(c) Glove200, 1 thread

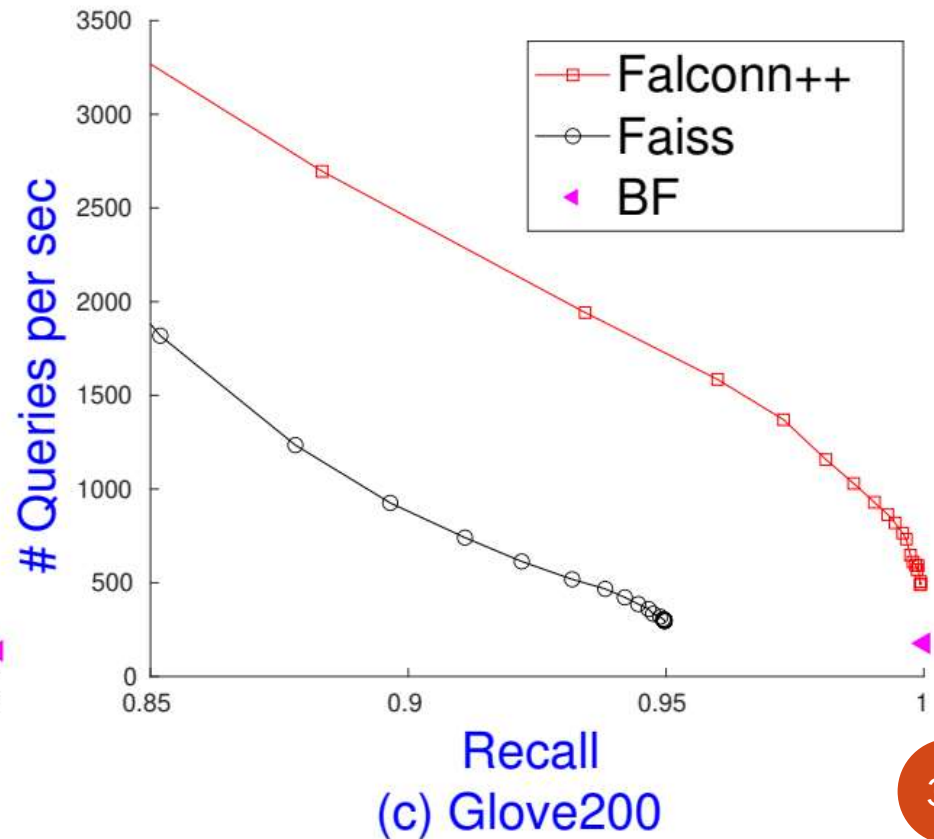
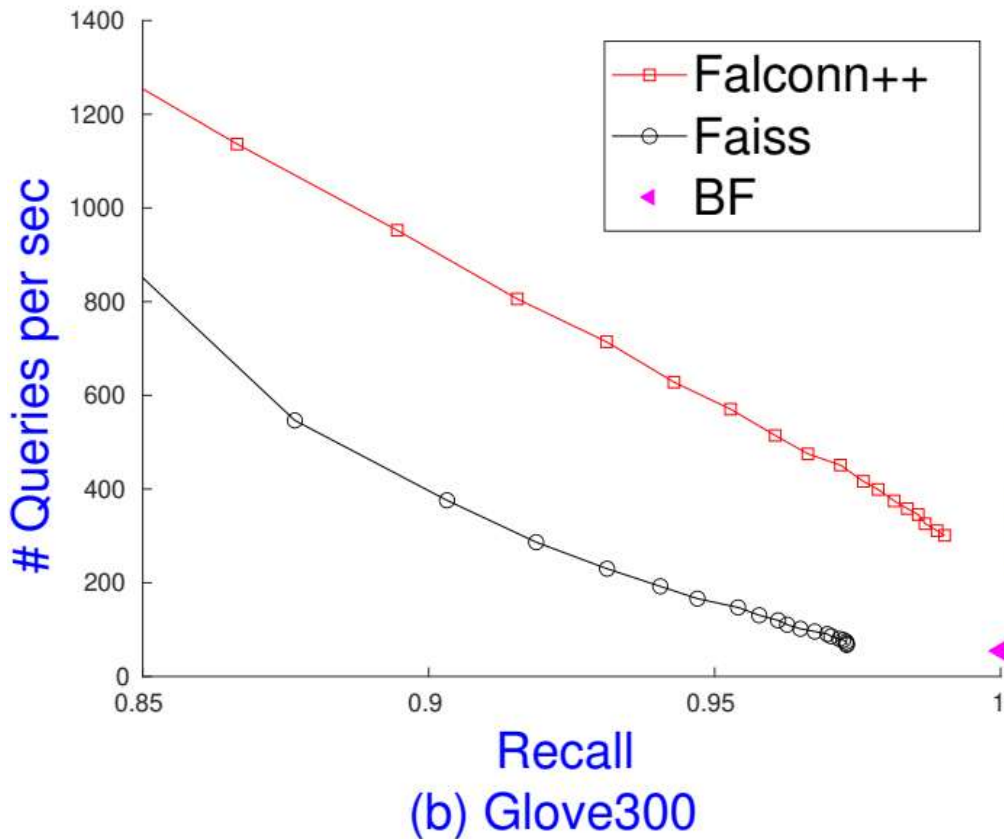


(d) Glove200, 64 thread

Falconn++ vs Faiss

- Parameter settings:

- Faiss: $m = 256$, $nlist=1000$, 8 bits/centroid, vary probe
- Falconn++: $D = 256$, $L = 350$, $\alpha = 0.01$, $iProbes = 3$, vary $qProbes$



Open problem

- Practical LSH & LSF pattern:
 - Existing for Euclidean distance with $\rho = 1/c^2$
- Characterize # random projections \mathbf{D}
- Characterize the scaling factor α

