Flexible Aggregate Similarity Search

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Outline

Introduction and motivation

- Similarity search (aka nearest neighbor search, NN search) is a fundamental tool in retrieving the most relevant data w.r.t. user input in working with massive data: extensively studied.

- However, often time, users may be interested at retrieving objects that are *similar* to *a group Q of query objects*, *instead of just one*.

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- Given an aggregation σ, a similarity/distance function d, a dataset P, and any query group Q:

$$r_p = \sigma\{d(p, Q)\} = \sigma\{d(p, q_1), \ldots, d(p, q_{|Q|})\}, \text{ for any } p$$

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Find $p^* \in P$ having the smallest r_p value ($r_{p^*} = r^*$).

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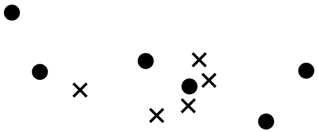

× : group Q of query points

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Figure: Aggregate similarity search in Euclidean space: max and sum.

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agg$=$ max, $p^* = p_3$, $r^* = d(p_3, q_1)$

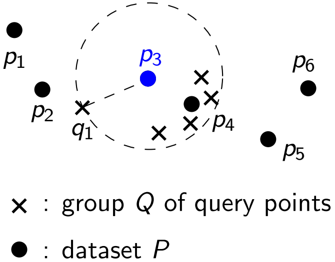


Figure: Aggregate similarity search in Euclidean space: max and sum.

- However, often time, users may be interested at retrieving objects that are *similar* to *a group Q of query objects*, *instead of just one*.

agg=sum, $p^* = p_4$, $r^* = \sum_{q \in Q} d(p_4, q)$

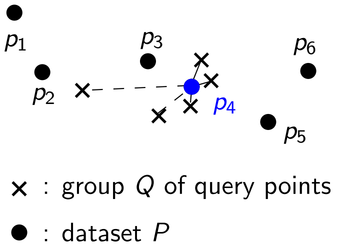


Figure: Aggregate similarity search in Euclidean space: max and sum.

- However, often time, users may be interested at retrieving objects that are *similar* to *a group Q of query objects*, *instead of just one*.
- Aggregate similarity search (ANN) may need to deal with data in high dimensions.

Outline

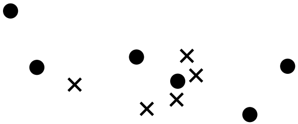
Existing methods for ANN

- R-tree method: branch and bound principle [PSTM04, PTMH05].
- Some other heuristics to further improve the pruning.
- Can be extended to other metric space using M-tree [RBTFT08].
- Limitations:
  - No bound on the query cost.
  - Query cost increases quickly as dataset becomes larger and/or dimension goes higher.

- [PSTM04]: Group Nearest Neighbor Queries. In *ICDE*, 2004.
- [PTMH05]: Aggregate nearest neighbor queries in spatial databases. In *TODS*, 2005.
- [RBTFT08]: A Novel Optimization Approach to Efficiently Process Aggregate Similarity Queries in Metric Access Methods. In *CIKM*, 2008.

Our approach for $\sigma = \max$: AMAX1

- We proposed AMAX1 (TKDE'10):



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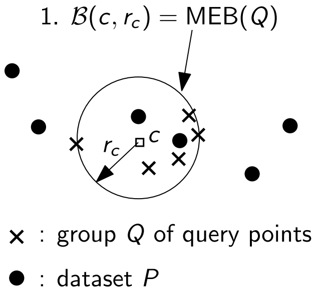
- We proposed AMAX1 (TKDE'10):
  - $\mathcal{B}(c, r_c)$ is a ball centered at c with radius r_c;
  - MEB(Q) is the minimum enclosing ball of a set of points Q;



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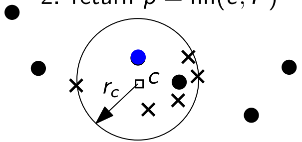
  - $\mathcal{B}(c, r_c)$ is a ball centered at c with radius r_c;
  - MEB(Q) is the minimum enclosing ball of a set of points Q;
  - nn(c, P) is the nearest neighbor of a point c from the dataset P.

1. $\mathcal{B}(c, r_c) = \text{MEB}(Q)$
2. return $p = \text{nn}(c, P)$



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AMAX1 *is a* $\sqrt{2}$*-approximation in any dimension* d *given (exact)* $\mathrm{nn}(c, P)$ *and* $\mathrm{MEB}(Q)$*.*

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Theorem

In any dimension d, given an α-approximate MEB algorithm and an β-approximate NN algorithm, AMAX1 is an $\sqrt{\alpha^2 + \beta^2}$-approximation.

Our approach for $\sigma = \max$: AMAX1

- An algorithm returns (p, r_p) for $\text{ANN}(Q, P)$ is an c-approximation iff $r^* \leq r_p \leq c \cdot r_p$.
- In low dimensions, BBD-tree [AMNSW98] gives $(1+\epsilon)$-approximate NN search; in high dimensions, LSB-tree [TYSK10] gives $(2+\epsilon)$-approximate NN search with high probability; and $(1+\epsilon)-$ MEB algorithm exists even in high dimensions [KMY03].

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- [AMNSW98]: An Optimal Algorithm for Approximate Nearest Neighbor Searching in Fixed Dimensions. In *JACM*, 1998.
- [TYSK10]: Efficient and Accurate Nearest Neighbor and Closest Pair Search in High Dimensional Space. In *TODS*, 2010.
- [KMY03]: Approximate Minimum Enclosing Balls in High Dimensions Using Core-Sets. In *JEA*, 2003

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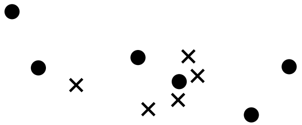

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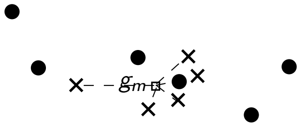

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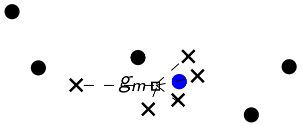

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- Using the Weiszfeld algorithm (iteratively re-weighted least squares), g_m can be computed to an arbitrary precision efficiently.

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Asum1 *is a* 3*-approximation in any dimension* d *given (exact) geometric median and* $\text{nn}(c, P)$*.*

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Theorem

In any dimension d*, given an* β*-approximate NN algorithm,* $\textsc{Asum1}$ *is an* 3β*-approximation.*

Our approach for $\sigma = \text{sum}$: ASUM1

- Using the Weiszfeld algorithm (iteratively re-weighted least squares), g_m can be computed to an arbitrary precision efficiently.
- Both AMAX1 and ASUM1 can be easily extended to work for kANN search while the bounds are maintained.

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Outline

1. Motivation and Problem Formulation
2. Basic Aggregate Similarity Search
3. Flexible Aggregate Similarity Search
4. Experiments

Definition of flexible aggregate similarity search

- *Flexible aggregate similarity search (*FANN*)*: given support $\phi \in (0, 1]$ and find an object in P that has the best aggregate similarity to (*any*) $\phi|Q|$ query objects (our work in SIGMOD'11).

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$$\sigma = \max,\ \phi = 40\%,\ p^* = p_4,\ r^* = d(p_4, q_3)$$

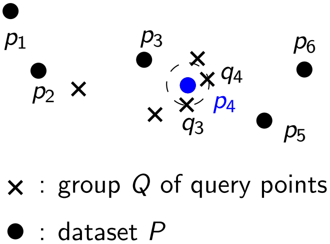

Figure: FANN in Euclidean space: max, $\phi = 0.4$.

Exact methods for FANN

- For $\forall p \in P$, $r_p = \sigma(p, Q^p_\phi)$, where Q^p_ϕ is p's $\phi|Q|$ NNs in Q.

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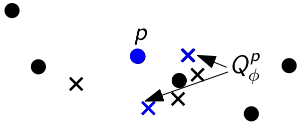
- For $\forall p \in P$, $r_p = \sigma(p, Q_\phi^p)$, where Q_ϕ^p is p's $\phi|Q|$ NNs in Q.

Q_ϕ^p : top $\phi|Q|$ NNs of p in Q



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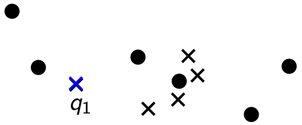
$\phi = 0.4,\ |Q| = 5,\ \phi|Q| = 2$

Exact methods for FANN

- For $\forall p \in P$, $r_p = \sigma(p, Q^p_\phi)$, where Q^p_ϕ is p's $\phi|Q|$ NNs in Q.
- R-tree method, with the branch and bound principle, can still be applied based on this observation.
- In high dimensions, take the brute-force-search (BFS) approach:
  - For each $p \in P$, find out Q^p_ϕ and calculate r_p.

Approximate methods for σ = sum: ASUM



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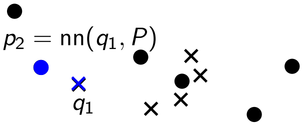

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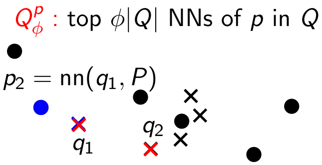

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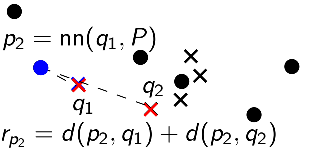

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- Repeat this for every $q_i \in Q$, return the p with the smallest r_p.

Approximation quality of ASUM

Theorem

In any dimension d, given an exact NN algorithm, ASUM *is an 3-approximation.*

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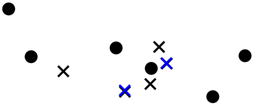
- ASUM still needs $|Q|$ times of NN search in P!

An improvement to ASUM

randomly select a subset of Q!



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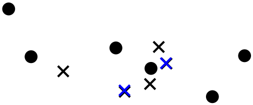

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For any $0 < \varepsilon, \lambda < 1$, *executing* Asum *algorithm only on a random subset of* $f(\phi, \varepsilon, \lambda)$ *points of* Q *returns a* $(3+\varepsilon)$*-approximate answer to* Fann *search in any dimensions with probability at least* $1 - \lambda$, *where*

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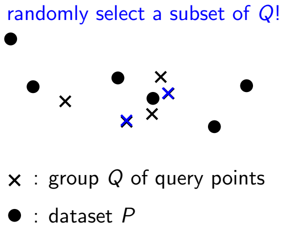

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- For $|Q| = 1000$, $\phi = 0.4$, $\lambda = 10\%$, $\varepsilon = 0.5$, only needs 33 NN search in any dimension.

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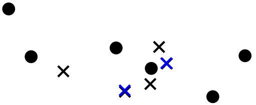

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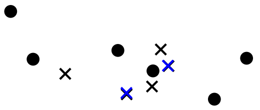

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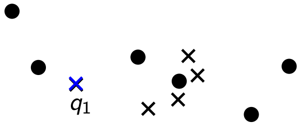
- For $|Q| = 1000$, $\phi = 0.4$, $\lambda = 10\%$, $\varepsilon = 0.5$, only needs 33 NN search in any dimension. (much less in practice, $\frac{1}{\phi}$ is enough!)
- Independent of dimensionality, $|P|$, and $|Q|$!

Approximate methods for $\sigma = \max$: AMAX



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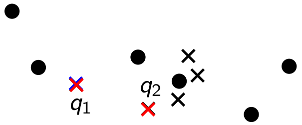
$\phi = 0.4$, $|Q| = 5$, $\phi|Q| = 2$, $\sigma = \max$

Approximate methods for $\sigma = \max$: AMAX

Q_ϕ^q : top $\phi|Q|$ NNs of q in Q, including q



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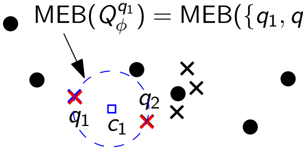

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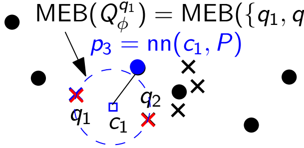

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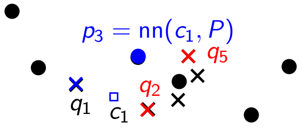

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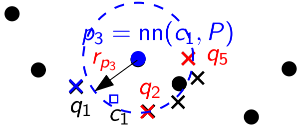

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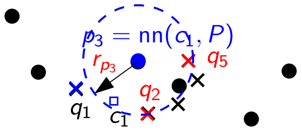

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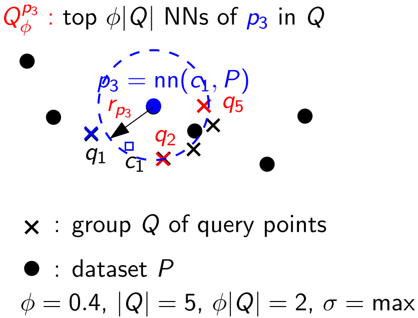

- Repeat this for every $q_i \in Q$, return the p with the smallest r_p.
- Identical to ASUM, except using $p = \text{nn}(c_i, P)$ instead of $p = \text{nn}(q_i, P)$, where c_i is the center of $\text{MEB}(q_i, Q_\phi^{q_i})$.

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In any dimension d, given an exact NN algorithm, AMAX *is an* $(1+2\sqrt{2})$*-approximation.*

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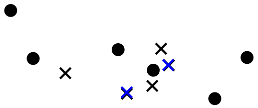
- AMAX still needs $|Q|$ times of MEB and $|Q|$ NN search in P!

An improvement to AMAX

randomly select a subset of Q!



× : group Q of query points

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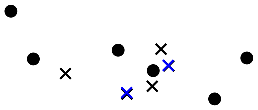

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Theorem

For any $0 < \lambda < 1$, *executing* AMAX *algorithm only on a random subset of* $f(\phi, \lambda)$ *points of* Q *returns a* $(1 + 2\sqrt{2})$*-approximate answer to the* FANN *query with probability at least* $1 - \lambda$ *in any dimensions, where*

$$f(\phi, \lambda) = \frac{\log \lambda}{\log(1 - \phi)} = O(\log(1/\lambda)/\phi).$$

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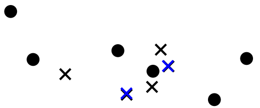

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- For $|Q| = 1000$, $\phi = 0.4$, $\lambda = 10\%$, only needs 5 MEB and NN search in any dimension.

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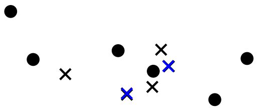

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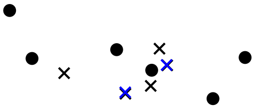

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- For $|Q| = 1000$, $\phi = 0.4$, $\lambda = 10\%$, only needs 5 MEB and NN search in any dimension. (even less in practice, $\frac{1}{\phi}$ is enough!)
- Independent of dimensionality, $|P|$, and $|Q|$!

Other issues

- All algorithms for FANN can be extended to work for top-k FANN.

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- Most algorithms work for any metric space, except AMAX which works for metric space when MEB is properly defined.

Outline

1. Motivation and Problem Formulation
2. Basic Aggregate Similarity Search
3. Flexible Aggregate Similarity Search
4. Experiments

Experiments: setup and datasets

- Experiments are performed in a Linux machine with 4GB of RAM and an Intel Xeon 2GHz CPU.
- Datasets:
  - 2-dimension: Texas (*TX*) points of interest and road-network dataset from the Open Street Map project: 14 million points (we have other 49 states as well).

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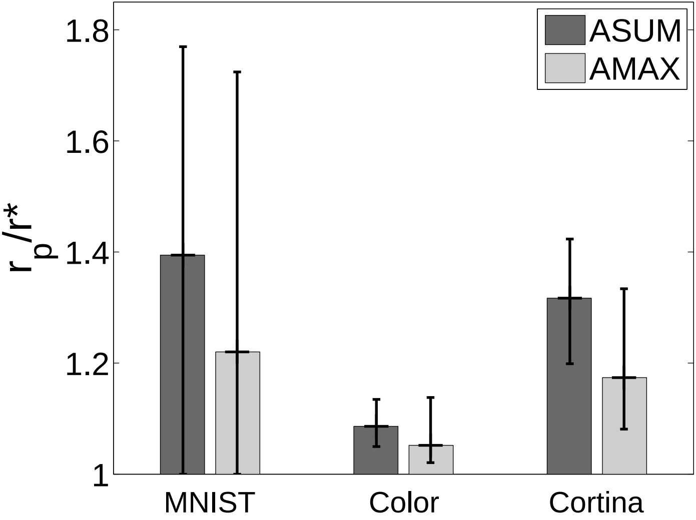
  - High dimensions: datasets from http://kdd.ics.uci.edu/databases/CorelFeatures/CorelFeatures.data.html, http://yann.lecun.com/exdb/mnist/, and http://www.scl.ece.ucsb.edu/datasets/index.htm

dataset	number of points	dimensionality
TX	$14,000,000$	2
RC	synthetic	$2-6$
Color	$68,040$	32
MNIST	$60,000$	50
Cortina	$1,088,864$	74

  - report the average of 40 independent queries, as well as the 5%-95% interval.
  - sampling rate of $\frac{1}{\phi}$ is enough for both Asum and Amax!

High dimensions: query cost, all datasets



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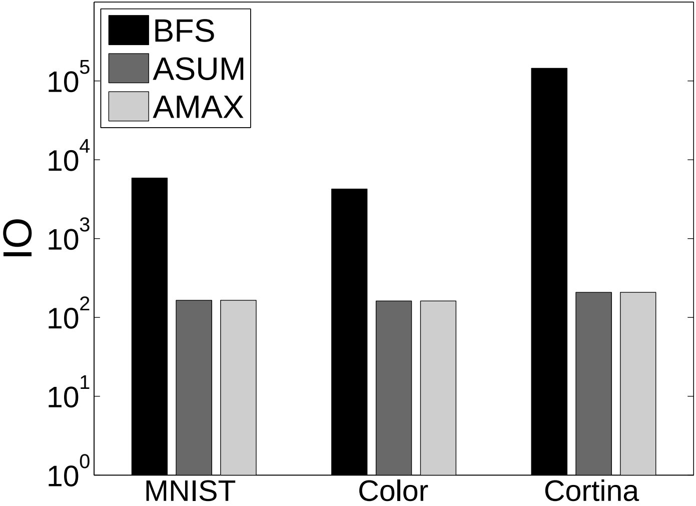
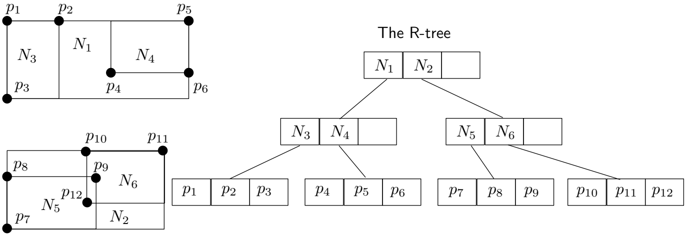


Thank You

Q and A

Existing methods for ANN

- R-tree method: brunch and bound principle [PSTM04, PTMH05].



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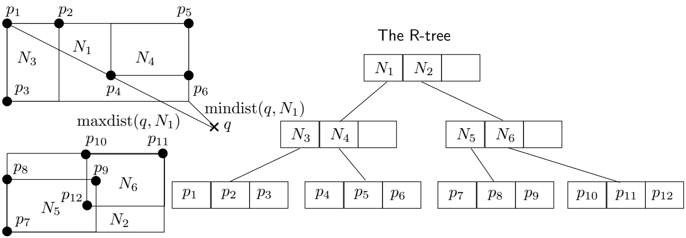
  - For a query point q and a MBR node N_i:

$$\forall p \in N_i, \text{mindist}(q, N_i) \le d(p, q) \le \text{maxdist}(q, N_i).$$



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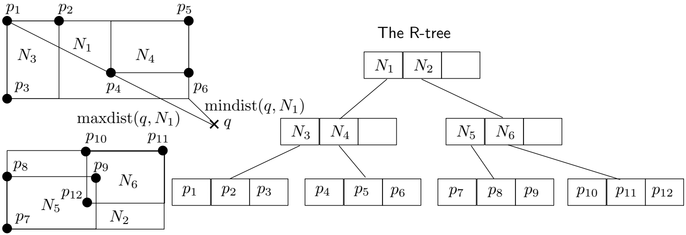

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Existing methods for ANN

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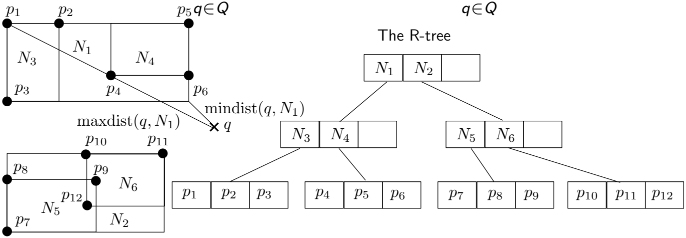

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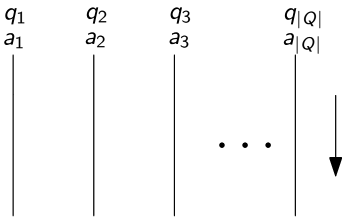

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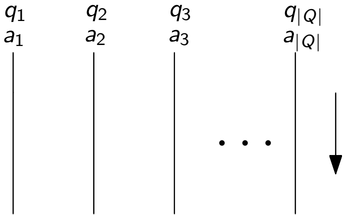

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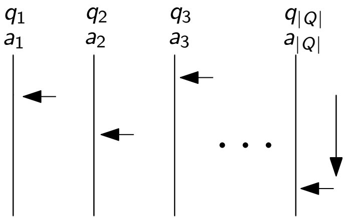

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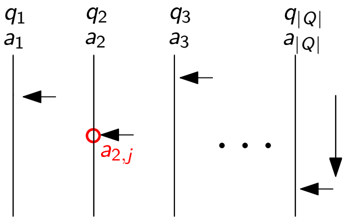

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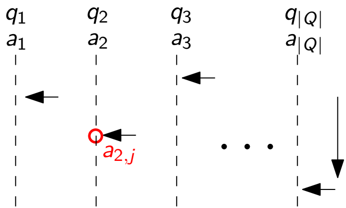

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Symbol	Definition	Default
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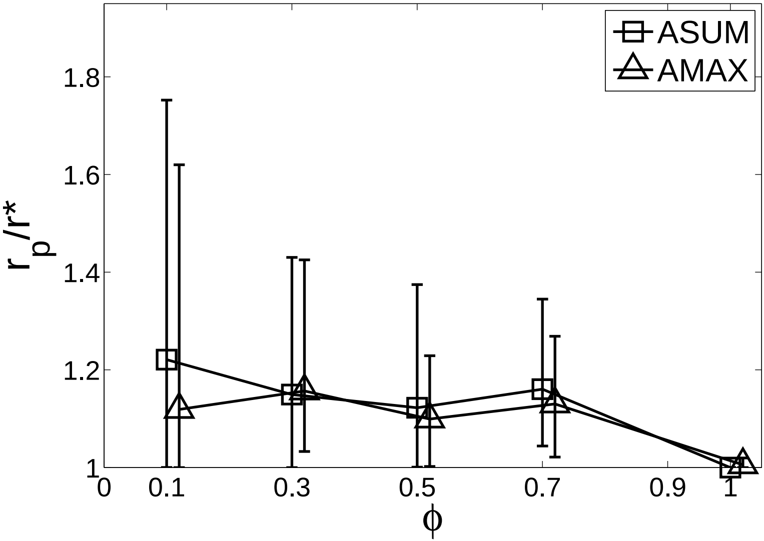

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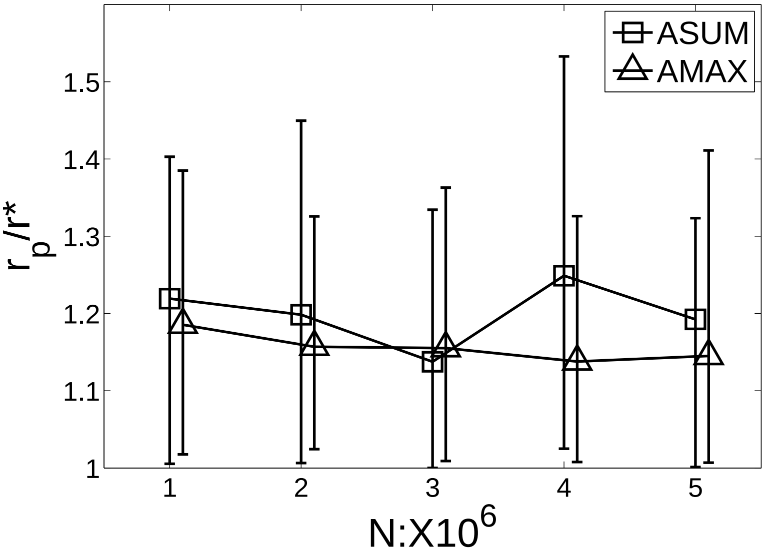
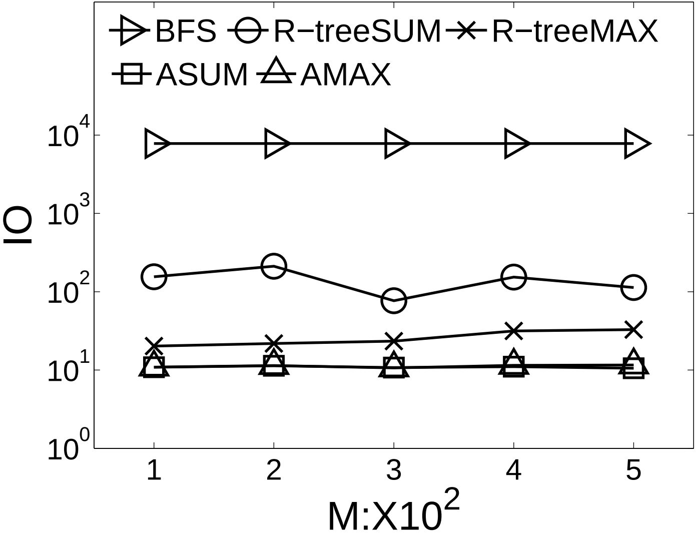


Low dimensions: query cost, vary M



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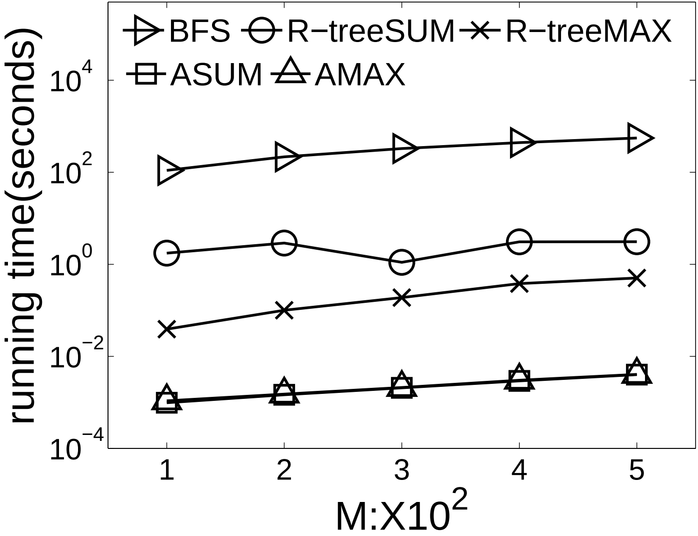

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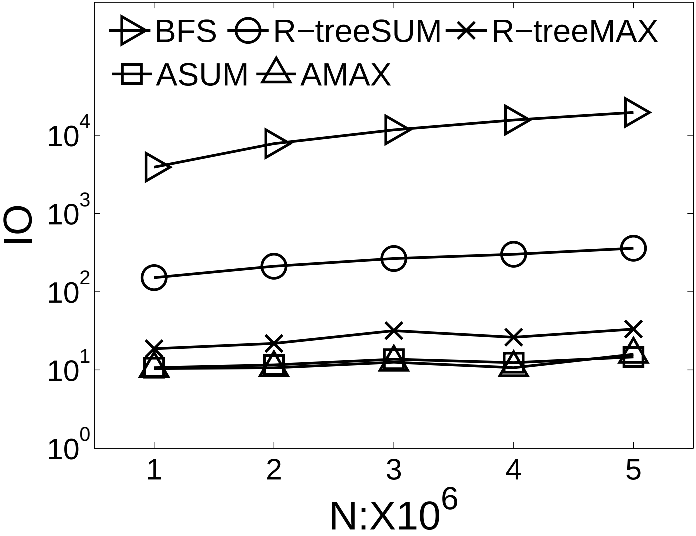

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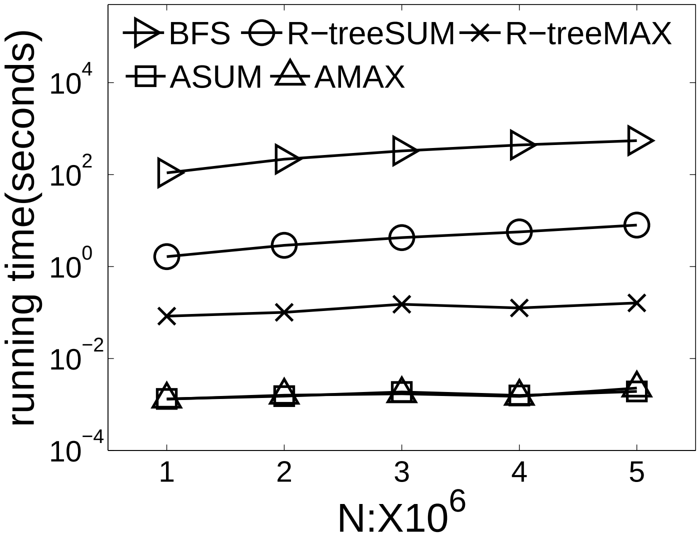
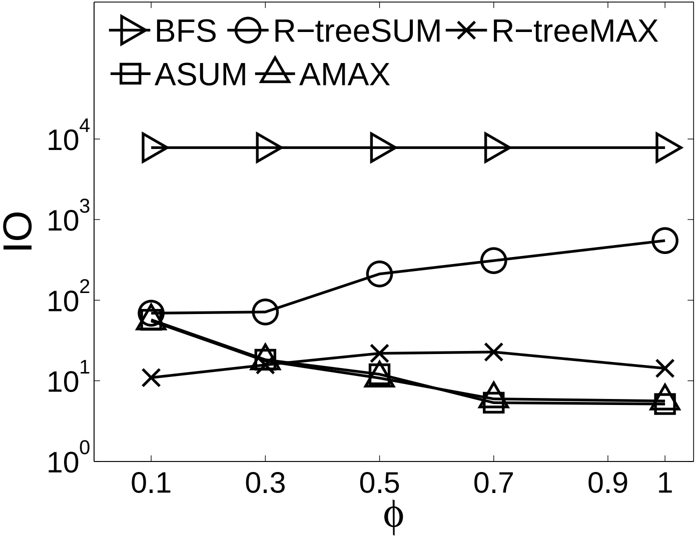


Low dimensions: query cost, vary ϕ



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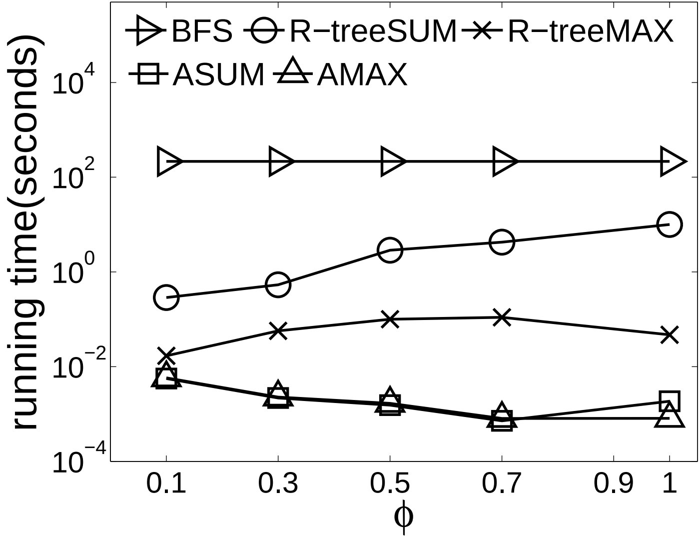
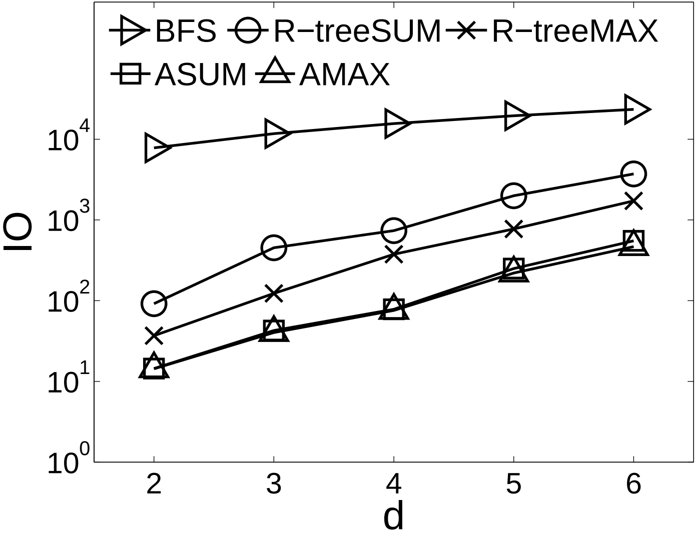


Low dimensions: query cost, vary *d*



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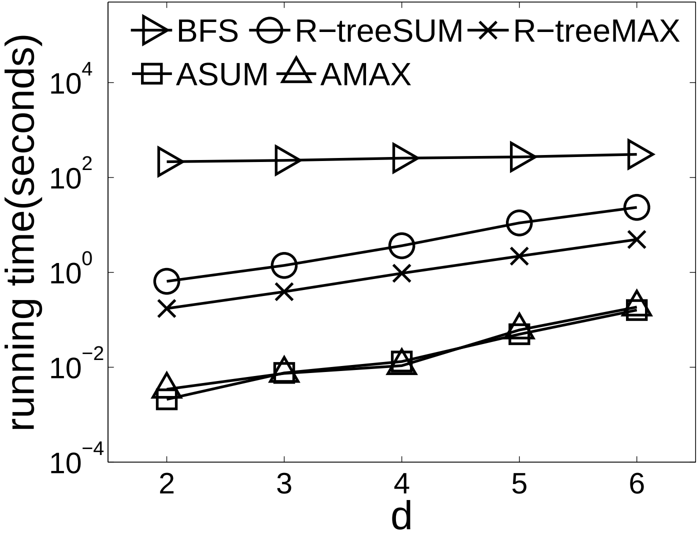
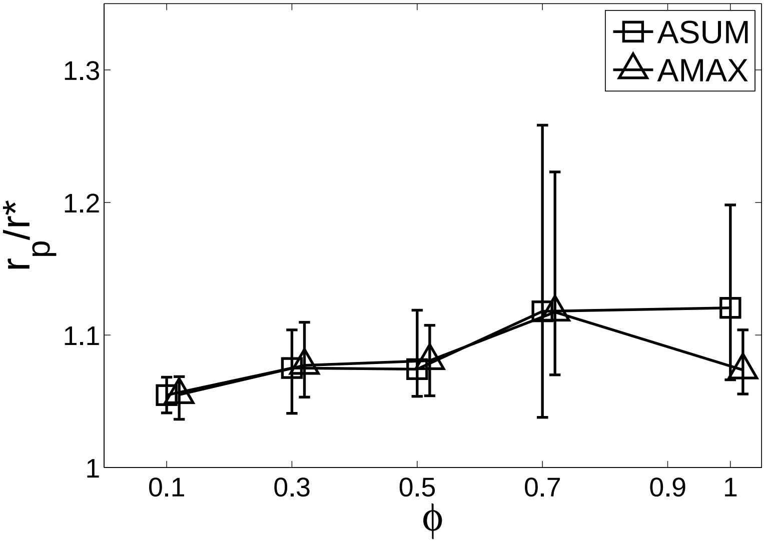


High dimensions: approximation quality



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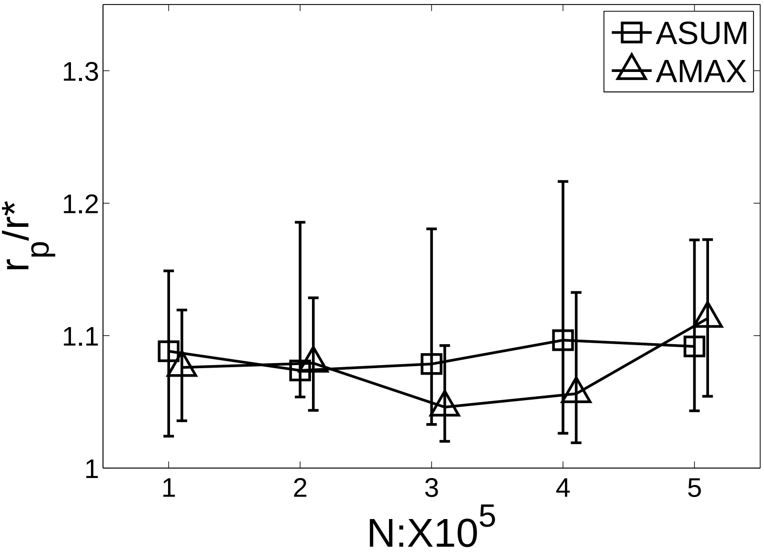

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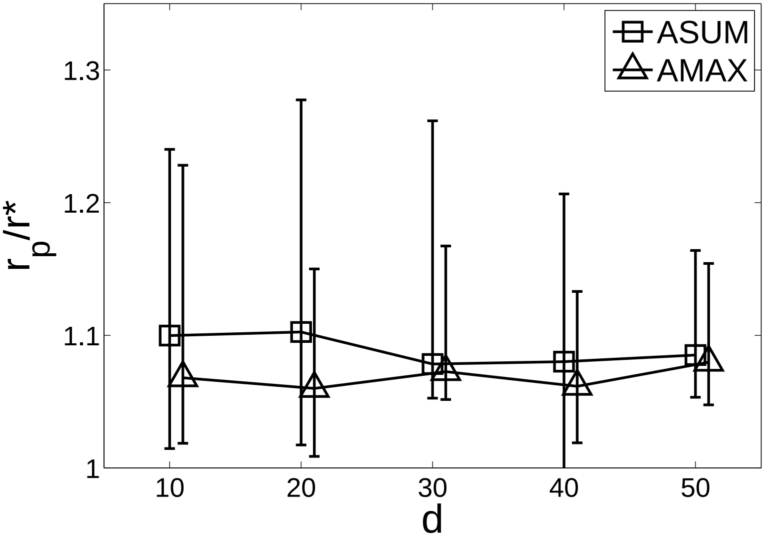
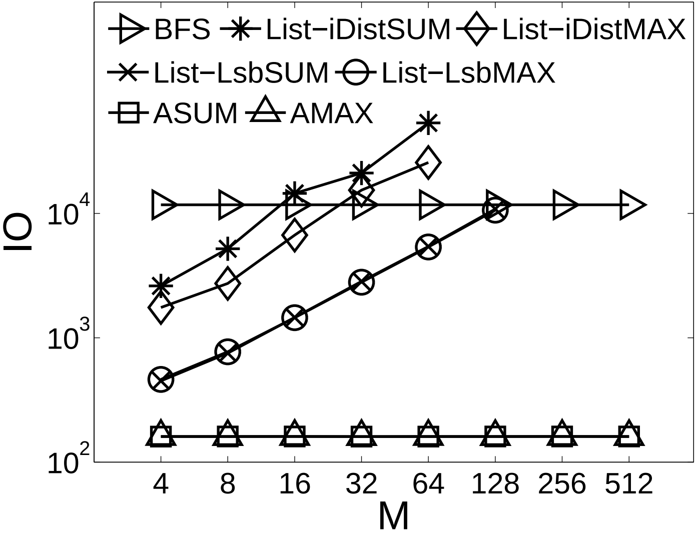


High dimensions: query cost, vary M



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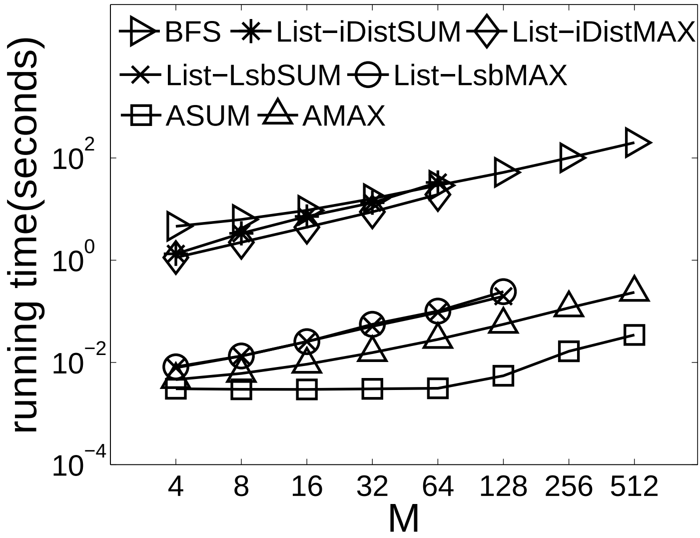
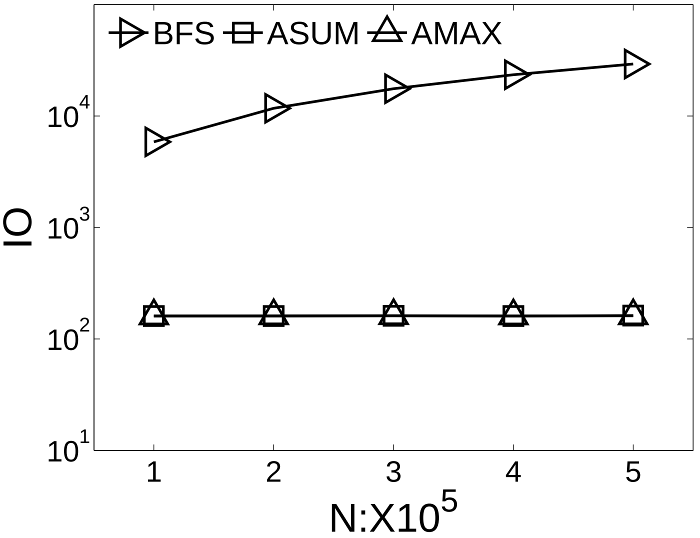


High dimensions: query cost, vary N



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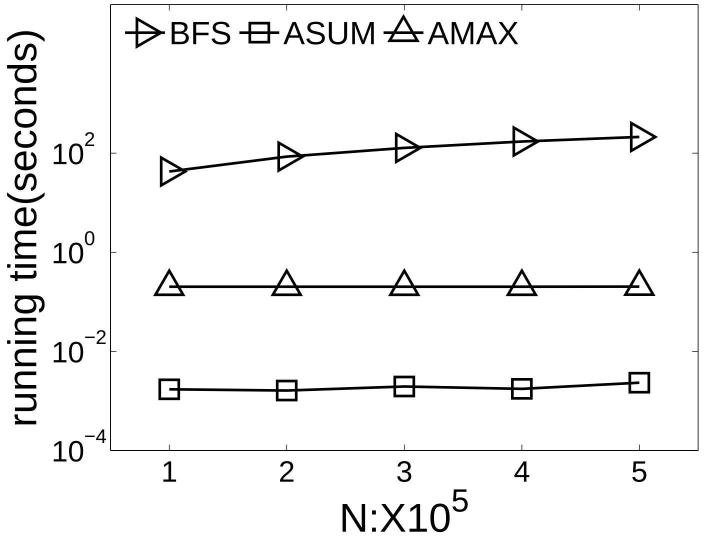

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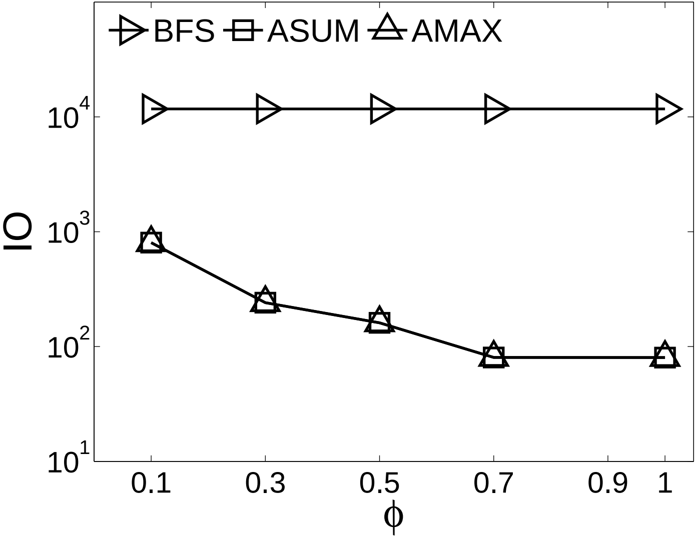

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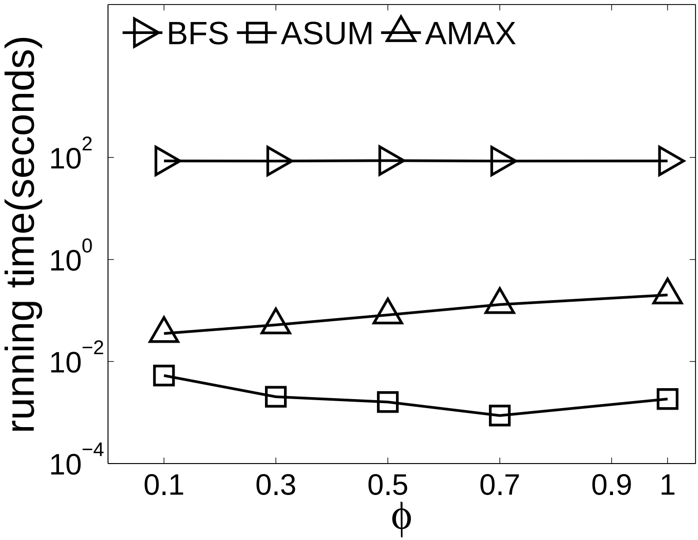
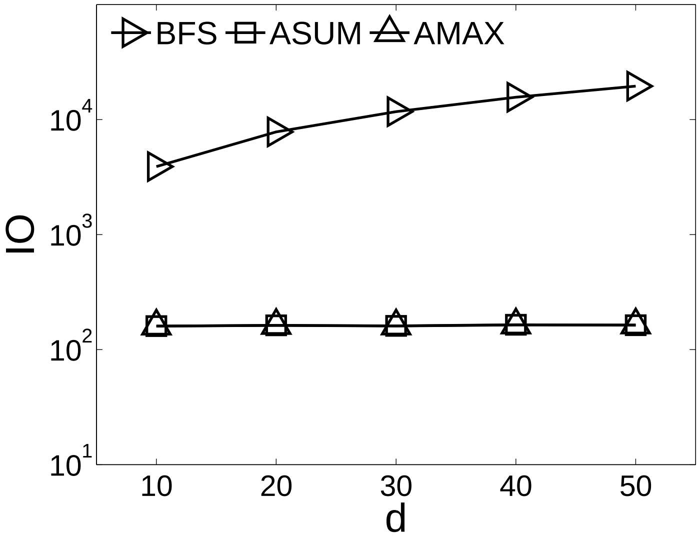


High dimensions: query cost, vary d



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