Data-dependent methods for similarity search in high dimensions

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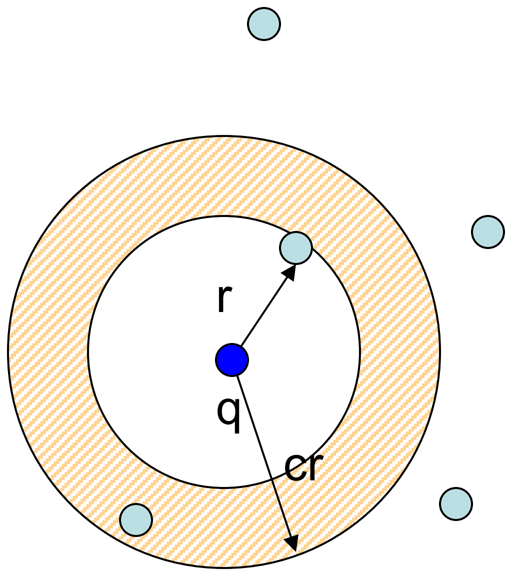
Plan

- On the benefits of using data to design similarity search data structures
- Why it took so long to get it to work (provably, for general high-dimensional pointsets)
- And why this makes realtime computation more difficult

Problem 1: Approximate Near Neighbor

- Given: a set P of n points in a d-dimensional space* and parameters c and r
- Build a data structure which, for any query q:
  - If there is $p \in P$ s.t. $\|q-p\| \leq r$,
  - Then return $p' \in P$ s.t $\|q-p'\| \leq cr$

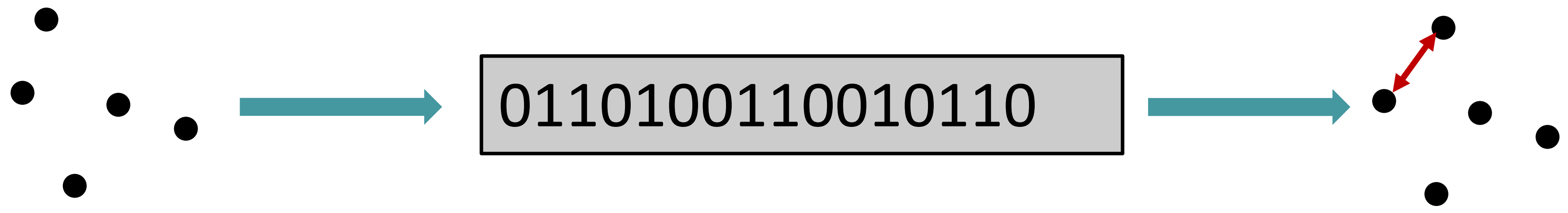
- Why approximate ?
  - Exact algorithm with $n^{1-\beta}$ query time and polynomial preprocessing would violate certain complexity-theoretic conjecture (SETH)
  - Reflected in empirical performance, a.k.a., curse of dimensionality
  - Approximate algorithms are typically faster, in theory and practice



*We assume Euclidean distance in this talk

Problem 2: Approximate Metric Compression

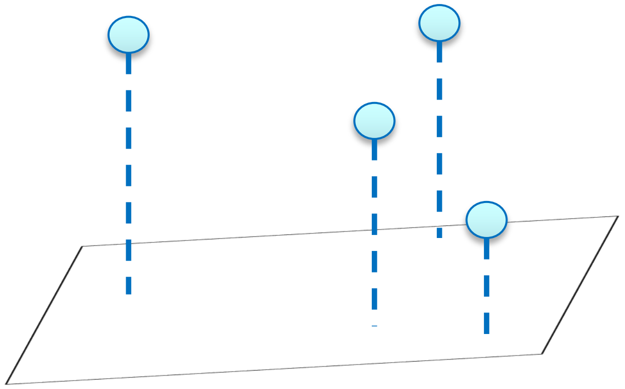
- Given: a set P of n points in a d-dimensional space
- Compress it into as few *bits* as possible
- Estimate pairwise distances within $1+\varepsilon$

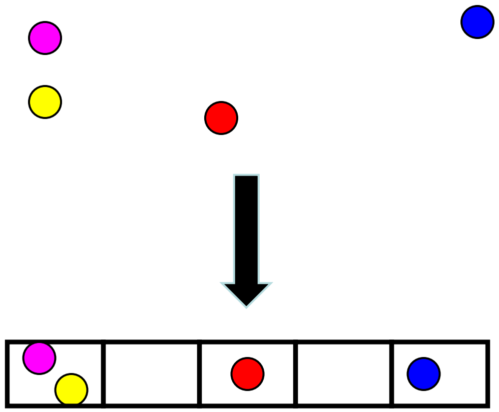


- Exact representation: O(ndB)
  - B=bits of precision; we assume B=O(log n)
- Random projection: $O(n \log(n)/\varepsilon^2 B) = O(n \log(n)^2/\varepsilon^2)$

What do these problems have in common ?

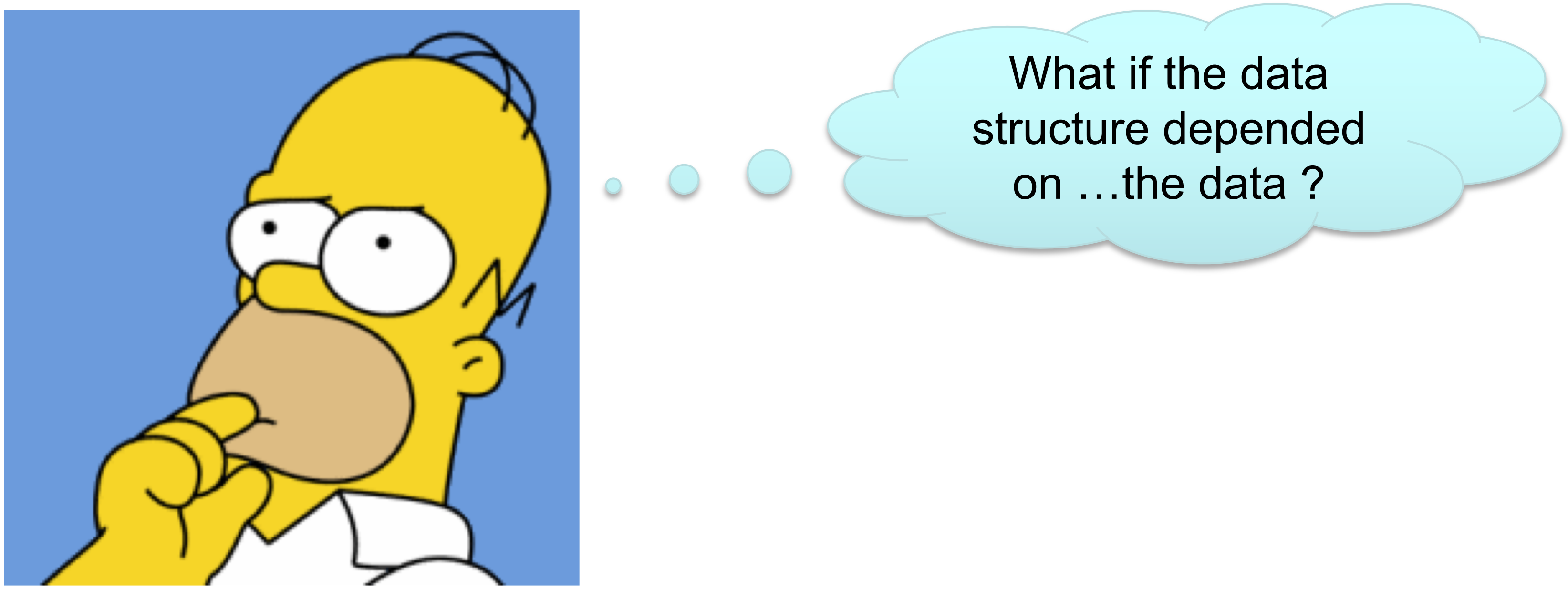
- Until recently, the fastest provable approaches in high d constructed data structures that were essentially oblivious* to the data
  - Random projection
  - Locality-Sensitive Hashing
- Benefits: provable, easy to maintain
  - E.g., for distributed data, no need to coordinate between nodes
- Drawbacks: Less efficient





*Formally, the memory cells accessed to answered queries depend on query q but not on P

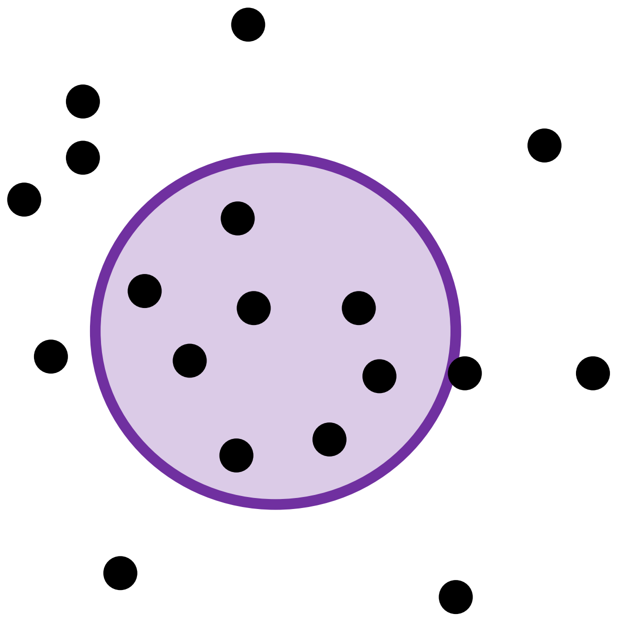
The “idea”



- Why is the answer not obvious ?
- It is often possible to get a data structure that works well when the data *has some structure* (clusters, low-dimensional subspace, i.i.d. from some distribution,etc)
- The tricky part is what to do when the data *does not have* that structure, or any structure in particular

The actual idea

- Every point-set has some structure that can be exploited algorithmically
- Details depend on the context/problem, but at a high level:
  - Either there is dense cluster of small radius, or
  - Points are "spread" out



Problem 1:
Approximate *Near* Neighbor

Basic Data Adaptive Method

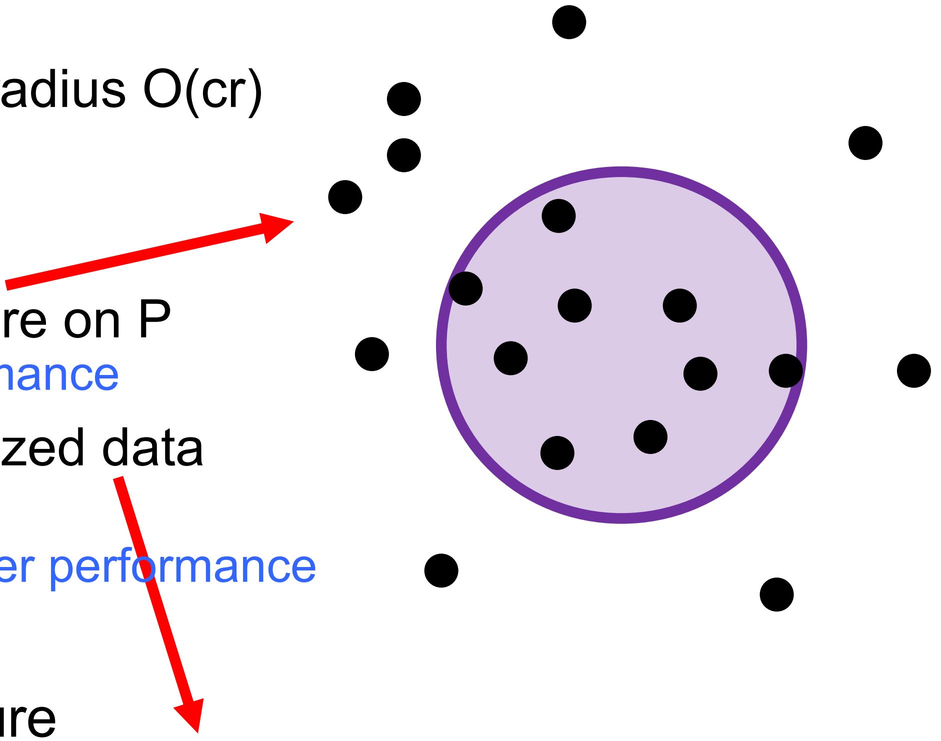
P=input pointset, r=radius, c=approximation

Preprocessing:

1. As long as there is a ball B_i of radius O(cr) containing T points in P
   - P=P-B_i
   - i=i+1
2. Build the basic NN data structure on P
   No dense clusters – better performance
3. For each ball B_i build a specialized data structure for $B_i \cap P$
   Diameter bounded by O(cr) – better performance

Query procedure:

1. Query the main data structure
2. Query all data structures for balls that are “close” to the query



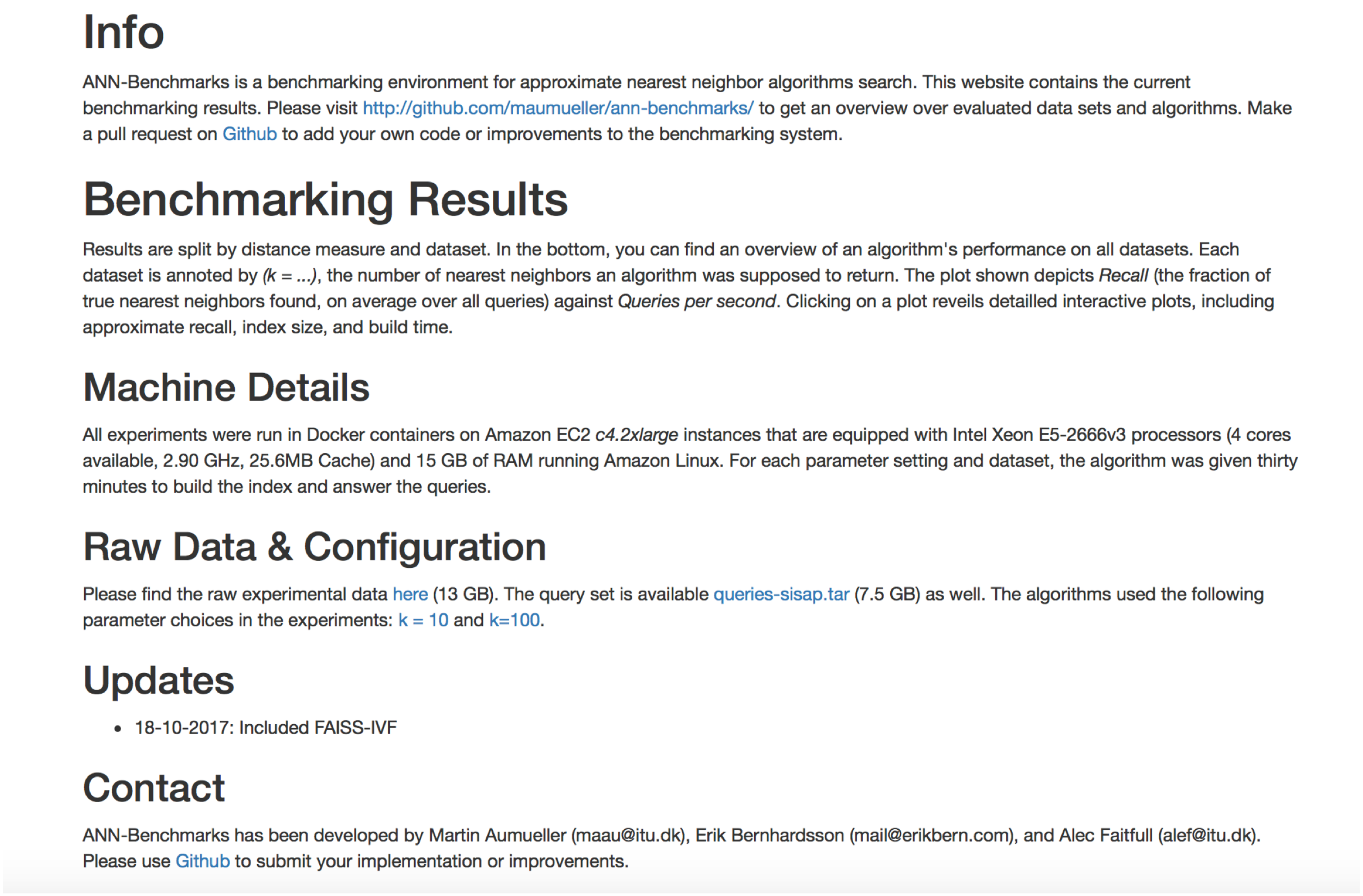
Results

- Theory (c-approximation):

Algorithm	Query Time	Index Space
Data-oblivious LSH(…FOCS'06)	dn^{1/c^2}	n^{1+1/c^2}
Andoni, Indyk, Nguyen, Razenshteyn, SODA'14	$dn^{0.87/c^2 + o(1/c^3)}$	$n^{1+0.87/c^2 + o(1/c^3)}$
Andoni-Razenshteyn, STOC'15	$dn^{1/(2c^2-1)}$	$n^{1+1/(2c^2-1)}$
Andoni et al, SODA'17	tradeoff	

- Practice:
  – Andoni-Indyk-Laarhoven-Razenshteyn-Schmidt (NIPS'15)
  – FALCONN (Razenshteyn-Schmidt)
    - Cross-polytope LSH, plus multi-probe, fast random projections,…

ANN-Benchmarks (third party)



Info

ANN-Benchmarks is a benchmarking environment for approximate nearest neighbor algorithms search. This website contains the current benchmarking results. Please visit http://github.com/maumueller/ann-benchmarks/ to get an overview over evaluated data sets and algorithms. Make a pull request on Github to add your own code or improvements to the benchmarking system.

Benchmarking Results

Results are split by distance measure and dataset. In the bottom, you can find an overview of an algorithm's performance on all datasets. Each dataset is annoted by *(k = ...)*, the number of nearest neighbors an algorithm was supposed to return. The plot shown depicts *Recall* (the fraction of true nearest neighbors found, on average over all queries) against *Queries per second*. Clicking on a plot reveils detailled interactive plots, including approximate recall, index size, and build time.

Machine Details

All experiments were run in Docker containers on Amazon EC2 *c4.2xlarge* instances that are equipped with Intel Xeon E5-2666v3 processors (4 cores available, 2.90 GHz, 25.6MB Cache) and 15 GB of RAM running Amazon Linux. For each parameter setting and dataset, the algorithm was given thirty minutes to build the index and answer the queries.

Raw Data & Configuration

Please find the raw experimental data here (13 GB). The query set is available queries-sisap.tar (7.5 GB) as well. The algorithms used the following parameter choices in the experiments: k = 10 and k=100.

Updates

- 18-10-2017: Included FAISS-IVF

Contact

ANN-Benchmarks has been developed by Martin Aumueller (maau@itu.dk), Erik Bernhardsson (mail@erikbern.com), and Alec Faitfull (alef@itu.dk). Please use Github to submit your implementation or improvements.

ANN-Benchmarks (third party)

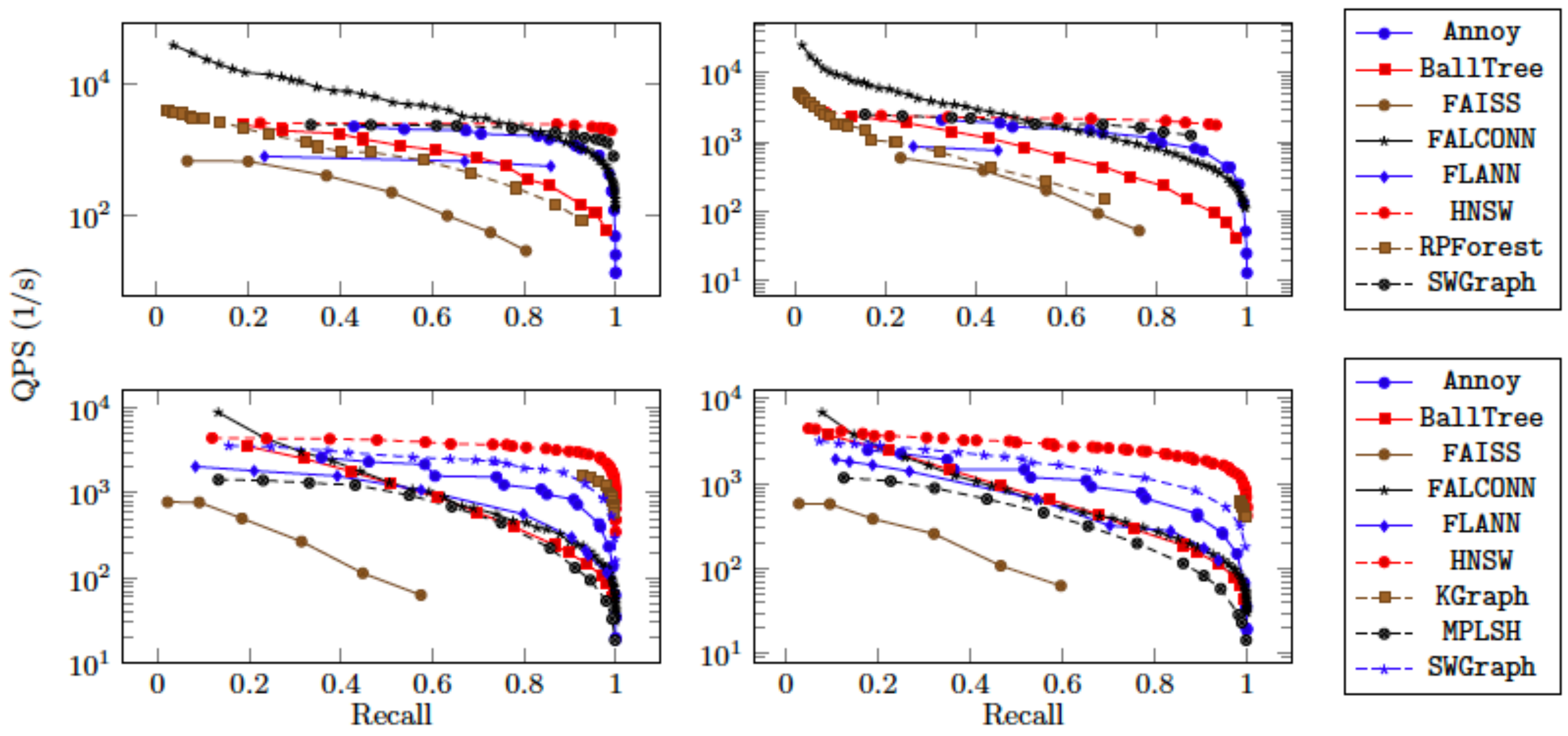


Fig. 4. Recall-QPS (1/s) tradeoff - up and to the right is better. Top: GLOVE, bottom: SIFT; left: 10-NN, right: 100-NN.

Aumuller, Bernhardsson, Faithfull, SISAP’17

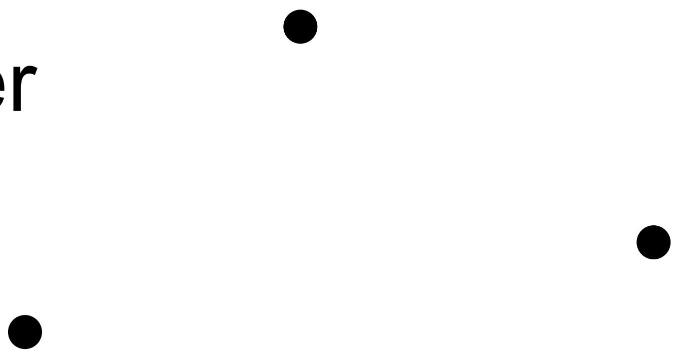
Problem 2:
Metric compression

Metric compression

Approach	Bound	Reference	Note
No compression	$O(nd \log n)$		
Random projection	$O\left(\frac{n \log^2 n}{\varepsilon^2}\right)$	Johnson-Lindenstrauss 1984	
Hierarchical clustering	$O\left(\frac{n \log n \log 1/\varepsilon}{\varepsilon^2}\right)$	Indyk-Wagner, SODA'17	Near-optimal
Hierarchical clustering++	$O\left(\frac{n \log n}{\varepsilon^2}\right)$	Indyk-Wagner, 2018	Optimal
Quad tree with pruning	$\left(\frac{n \log n \left(\log 1/\varepsilon + \log\log n\right)}{\varepsilon^2}\right)$	Indyk-Razenshteyn-Wagner, NIPS'17	Practical

Intuition

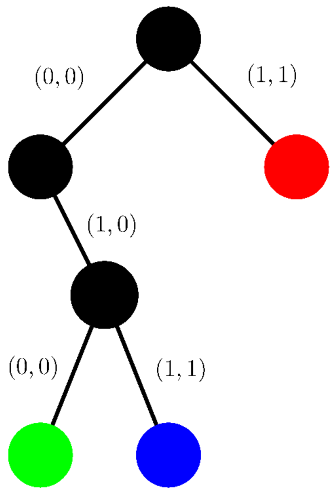
(multilevel vector quantization)

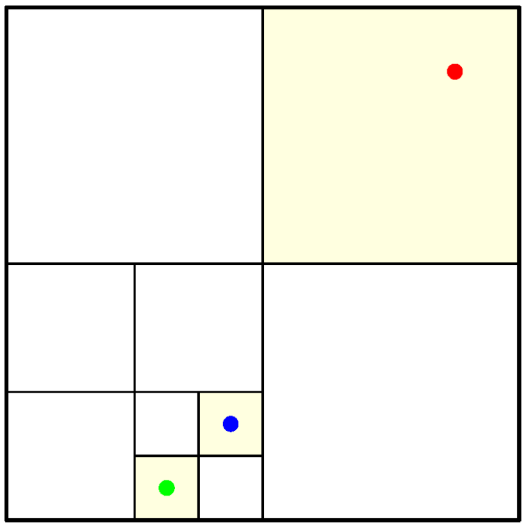


- Either there is dense cluster of small radius
  - Store cluster center and displacements from it
- Or points are “spread”
  - Only few distance scales to worry about
  - $O\left(\frac{\log n}{\varepsilon^2}\right)$ bits per point per scale

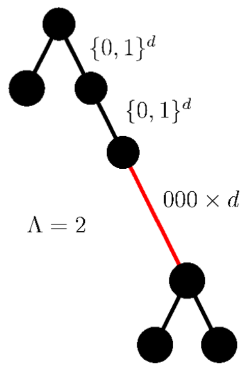
Quad tree

- Quad tree in R^d
- Can be seen as a binary expansion in each dimension
- Need $\Theta(\log n)$ levels
- $\Theta(nd \log n) = \Theta\left(\frac{n \log^2 n}{\varepsilon^2}\right)$ bits total – no improvement yet





Pruning



- Compress paths of degree-2 nodes of length $> \Lambda$
- Leave only the first Λ edges
- Decompress the remainder into zeros
- The total size is

$$O(nd\Lambda) = O\left(\frac{n\Lambda \cdot \log n}{\varepsilon^2}\right)$$

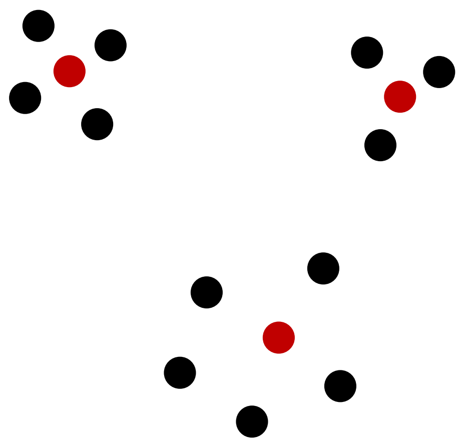
- Set $\Lambda = O(\log\log n + \log(1/\varepsilon))$

Experiments: baselines

- We compare the new algorithm (QuadSketch) with two baselines:
  - Grid-based compression (round every coordinate)
  - Product Quantization (PQ) **[Jegou, Douze, Schmid 2009]**
    - Good in practice (and popular)
    - No theoretical guarantees (for arbitrary data sets)

PQ: k-means

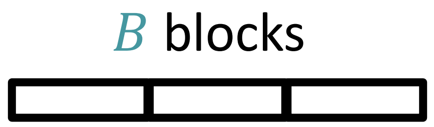
- A way to cluster a dataset
- Find k centers $c_1, c_2, \ldots, c_k$
- Minimize $\sum_i \|p_i - c_{u_i}\|_2^2$, where
  - c_{u_i} is the center closest to p_i
- NP-hard, good approximation algorithms
- Can be used as a sketch
  - Replace points by their centers ($\log k$ bits)
- Estimate: $\|c_q - c_s\|_2$
- Problem: **too many centers**



PQ: blocks

- Introduced in Jegou-Douze-Schmid'09
- Partition a vector in B blocks
- Project a dataset on each block, and find k-means in each
- Sketch of $B \log k$ bits (k^B landmarks as opposed to k)
- Estimation:
  - One-time cost $O(dk)$
  - Plus $O(B)$ per point

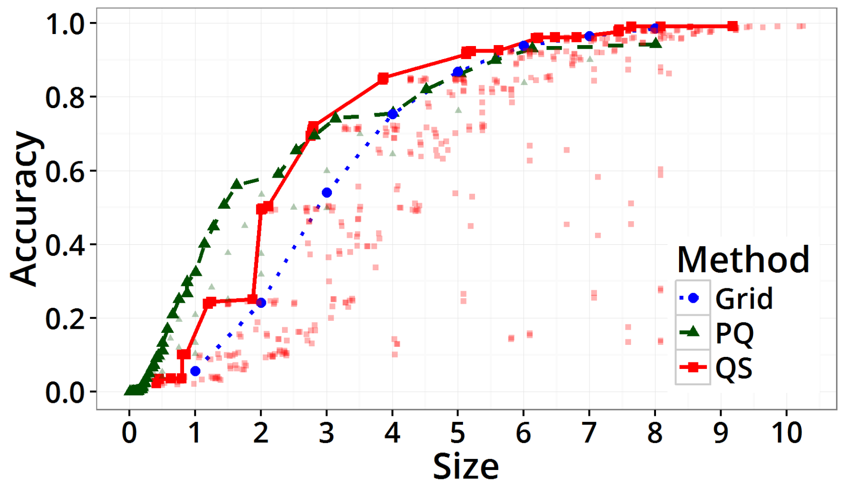
- We add the same trick to Quadsketch

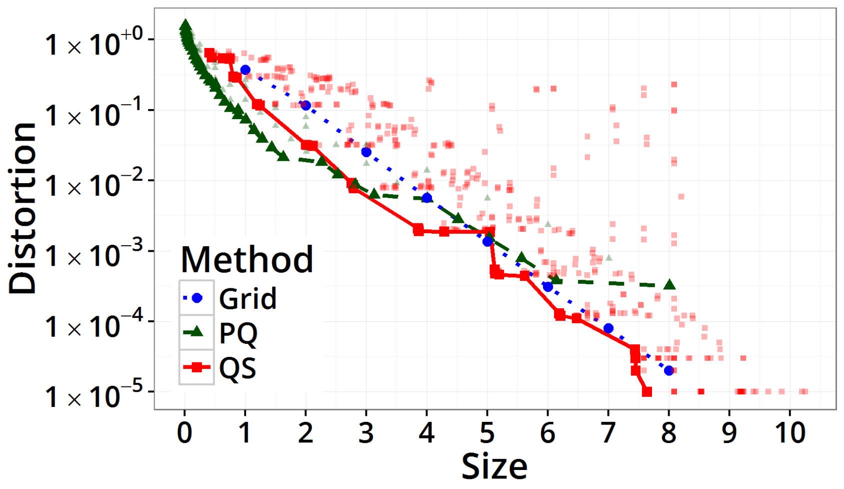


Experiments: protocol and datasets

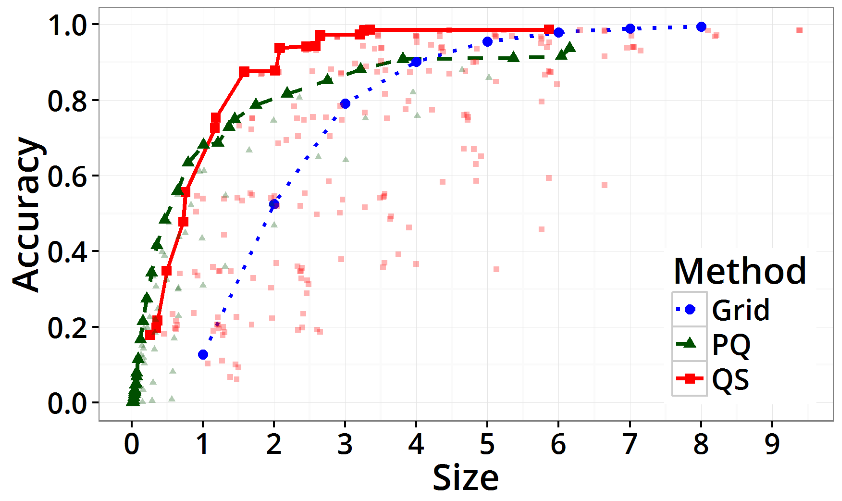
- We look at:
  - 1-NN accuracy
  - Distortion of 1-NN
- Datasets:
  - **SIFT1M** (1M points, 128 dimensions)
  - **MNIST** (60K points, 784 dimensions)
  - **Taxi** (9K points, 48 dimensions)
  - **Diagonal** (synthetic, 10K points, 128 dimensions)

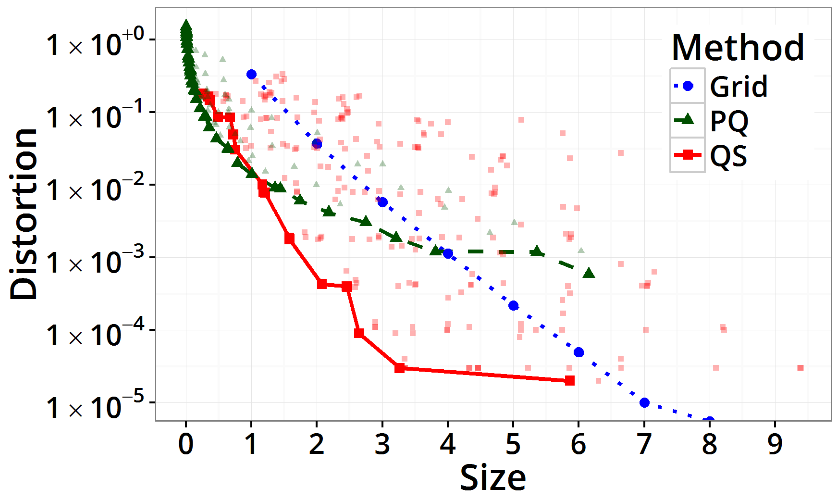
Results: SIFT1M



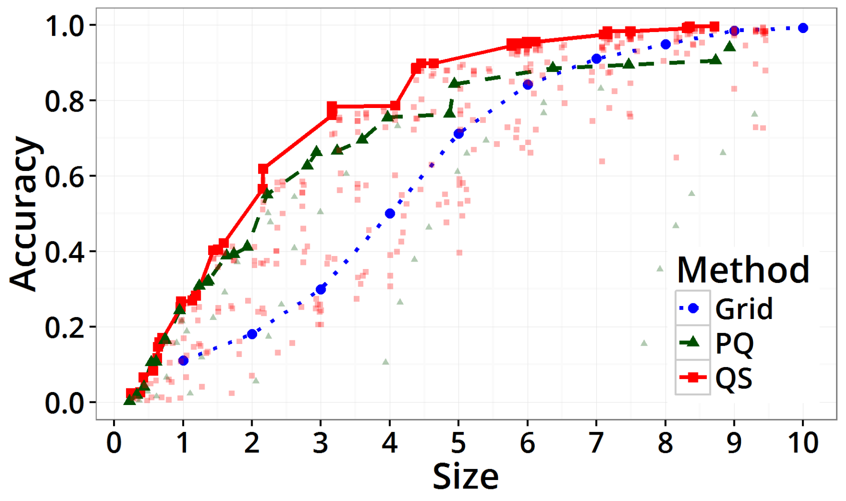


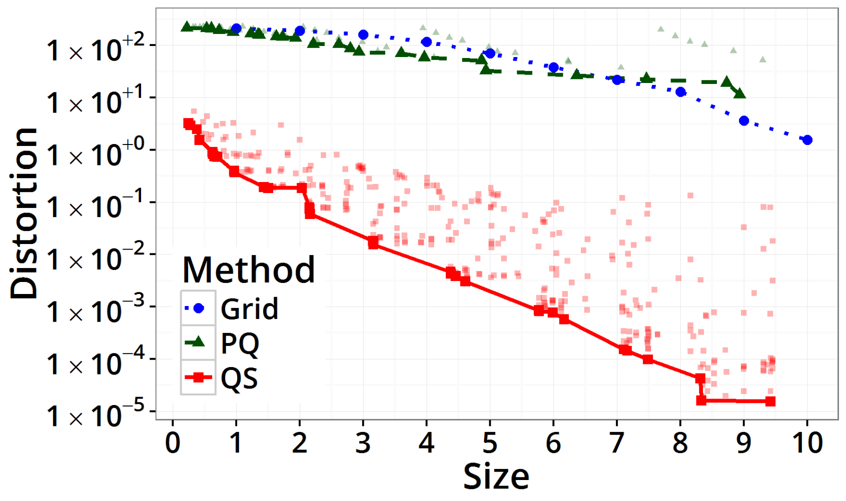
Results: MNIST



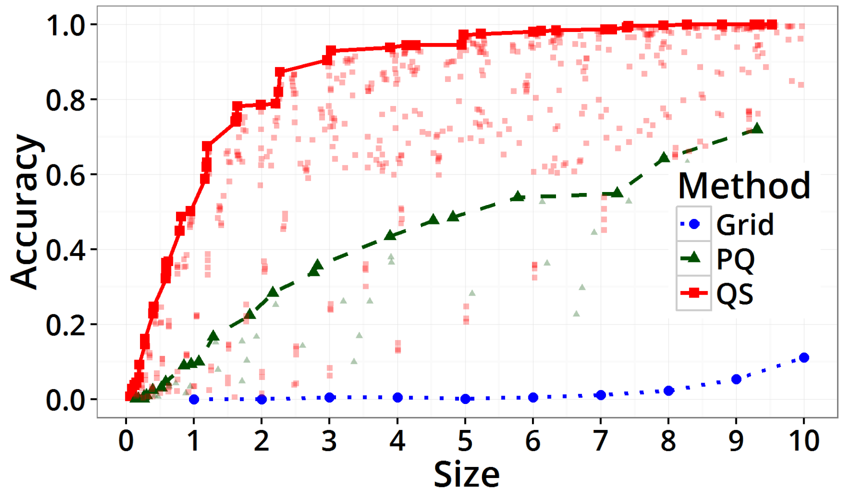


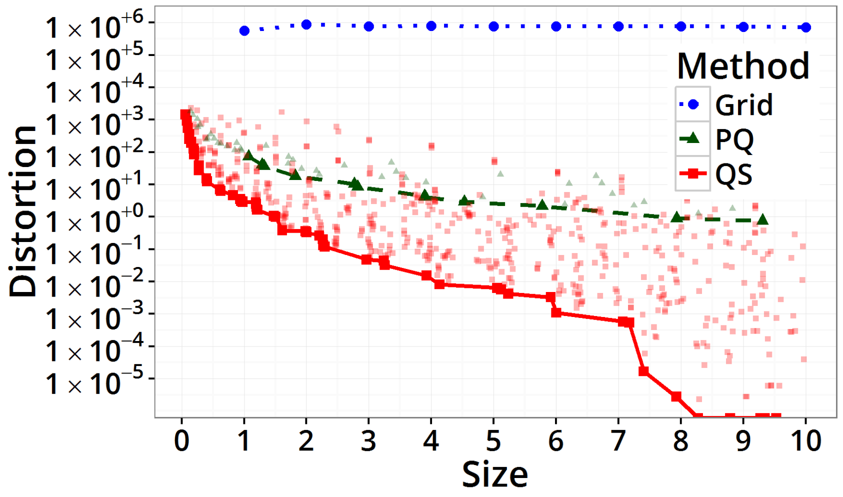
Results: Taxi





Results: Diagonal





Conclusions

- Data helps designing data structures (duh…)
- ..provably, for general high-dimensional pointsets
- Code:
  - FALCONN: https://github.com/FALCONN-LIB/FALCONN
  - Quadsketch: https://github.com/talwagner/quadsketch
- Open problem: make these data structures dynamic (a.k.a. "real-time")