FAST APPROXIMATE NEAREST NEIGHBORS WITH AUTOMATIC ALGORITHM CONFIGURATION

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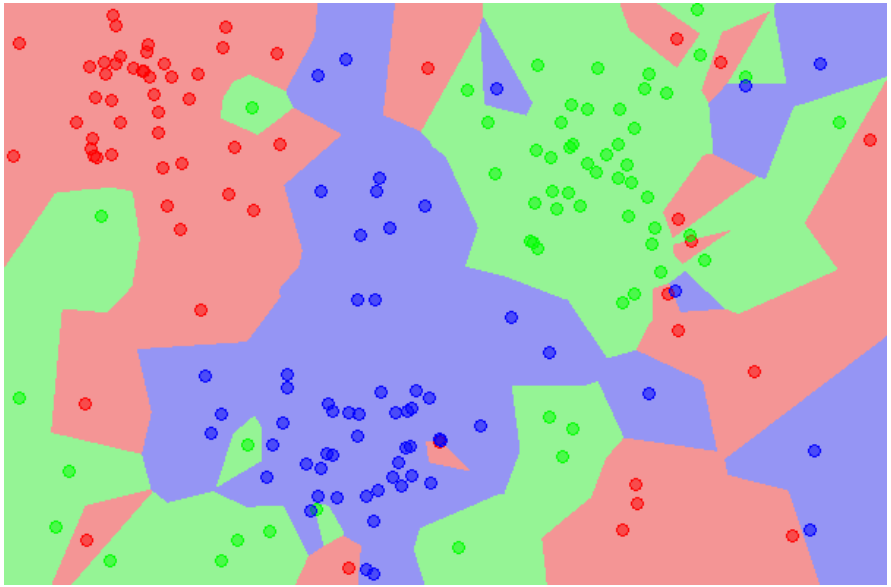
Nearest Neighbors?

Given points $P=\{p_1, \ldots, p_n\}$ in a vector space X,preprocess such that given a query point q in X, we can find the KNN of q in P efficiently.

1-NN example:



http://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm

Why KNN? Applications

SIFT: 128-dimensional feature vector. Find nearest feature vector in DB to match images.

Visual words: Cluster local features into “words” representing regions of an image.

ML: Classifiers

Compression: Best approximations of principal components.

Issues

- Performance of algorithms vary.
  - Dimensionality, internal correlations, dataset size.
- Exact NN not much better than linear search O(Nd) in high dimensions for N scene points, query dimension d.
  - Must turn to approximate NN, sometimes returns non-optimal points.

Contributions

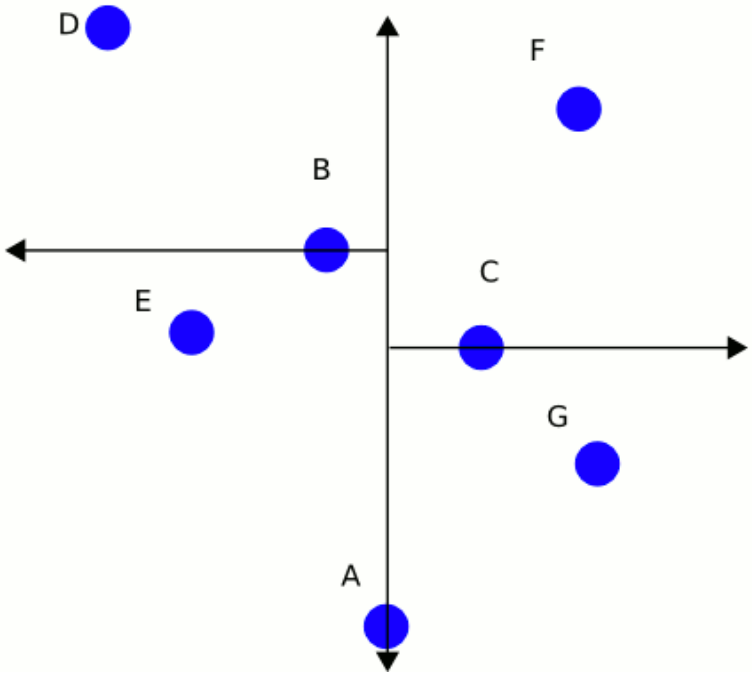
- Determine which algorithm to use given a particular dataset structure.
- Improve the hierarchical k-means algorithm to tree construction time and speed up queries by approximation.

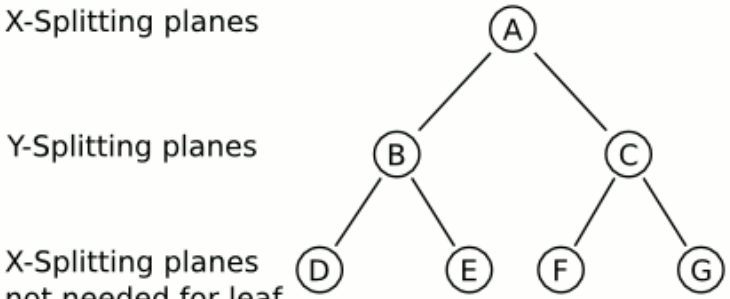
Algorithm 1: KD Tree Search

KD Trees Overview

- “*k*-dimensional trees”
- Split data in half at each level on the axis of greatest variance
- Fast operations for vectors in small dimensions
- In high dimensions, we get *far fewer splits per dimension.*

Visualizing KD Tree Search





http://upload.wikimedia.org/wikipedia/commons/9/9c/KDTree-animation.gif

Early KD Trees (Freidman et al.)

Introduces an optimized kd tree algorithm

- O(N) space
- O(kN log N) tree build time
- O(log N) search

“An algorithm for finding best matches in logarithmic expected time.” Freidman, J. H. et al. (1977)

Early KD Trees (Arya et al.)

Introduces the idea of an ε-approximate nearest neighbor

$\square\ \varepsilon > 0, \square\ \delta \leq d * \text{ceil}[1+6d/\varepsilon]^d$ such that the nearest neighbor can be returned in $O(\delta \log N)$ time

"An optimal algorithm for approximate nearest neighbor searching in fixed dimensions." Arya, S. et al. (1998)

Early KD Trees (Beis & Lowe, 1997)

Achieved a fast approximate nearest neighbor algorithm by fixing the number of leaf nodes examined

Slightly faster than the ε-approximate nearest neighbor method of Arya et al.

Randomized KD Trees

- First implemented by Silpa-Anan & Hartley (2008)
- Faster than traditional KD trees.
- Memory intensive: must build multiple trees for a data set.

Randomized KD Trees (Construction)

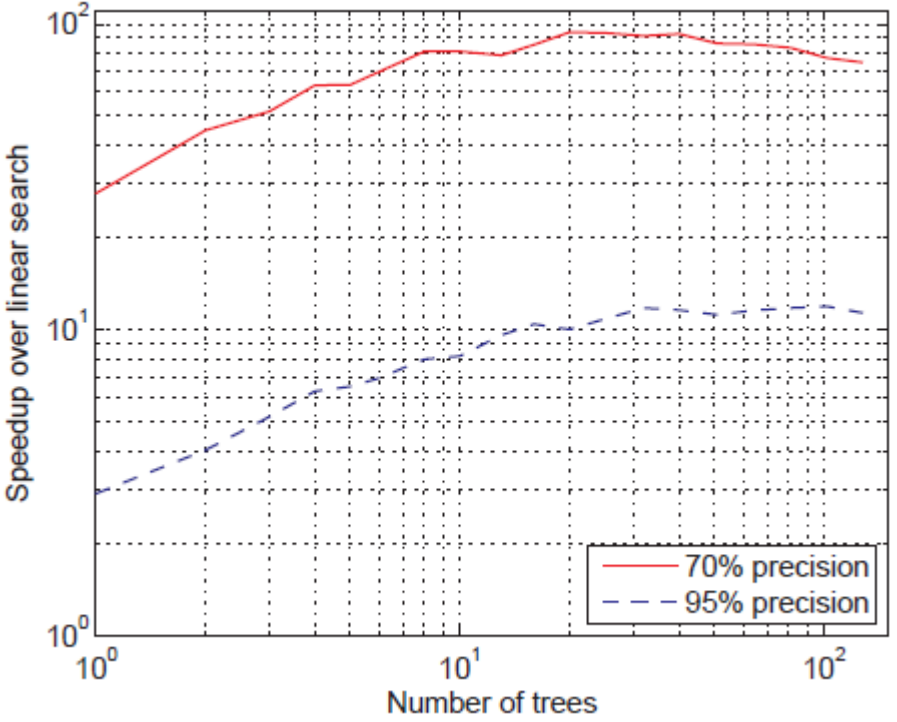
- Multiple trees constructed at once
- One of the top D dimensions of greatest variance randomly selected for each tree
- Data split on that dimension
- D = 5 used for testing
- Varying structure allows each tree search to be independent

Randomized KD Trees

- Single priority queue used to search *m* trees at once; elements ordered by distance from query point
- Fixed number, *n*, of nodes examined (number based on user input search precision)
- On average, *n*/*m* nodes examined per tree
- Best candidates returned

Randomized KD Trees Efficiency

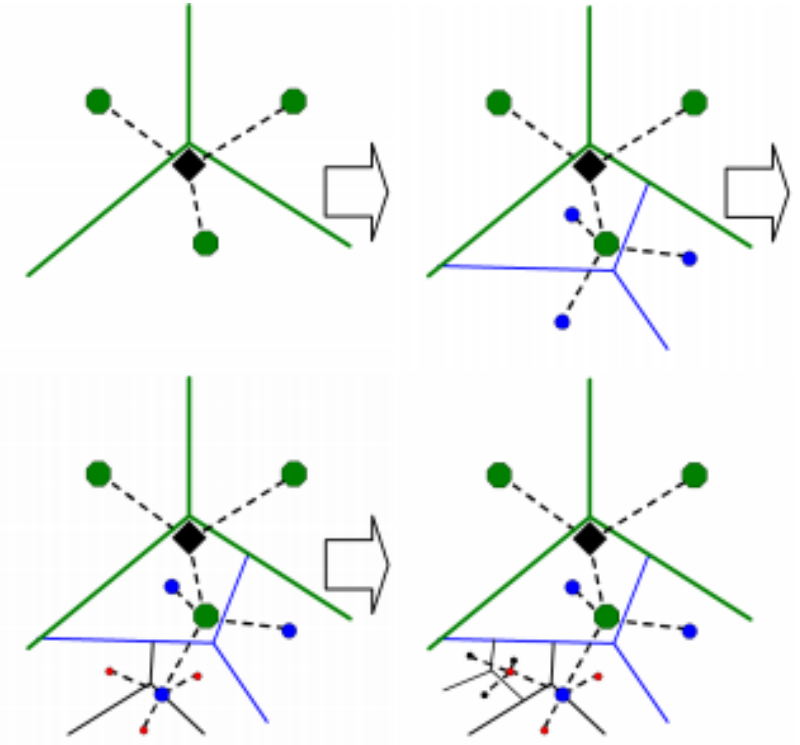
- Performance improves up to $10^{1.3}$ ≈ 20 trees
- 100,000 SIFT features used in test
- Memory overhead increases linearly



Algorithm 2: Hierarchical K-Means

Hierarchical K-Means

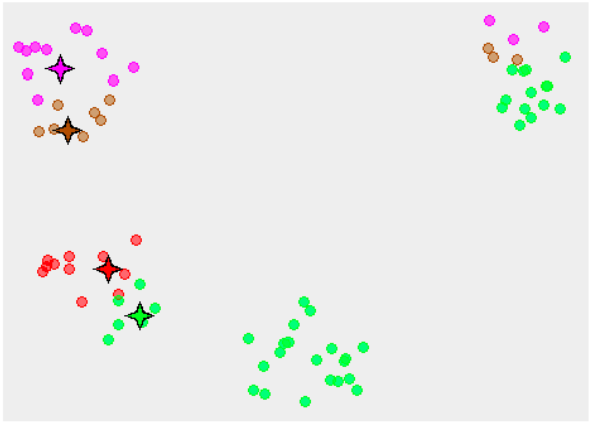
1. Precompute: k-means cluster into K clusters. Then k-means cluster each of these recursively to build a tree.
2. Query: Traverse graph w/ priority queue, limit number of leaf nodes checked.

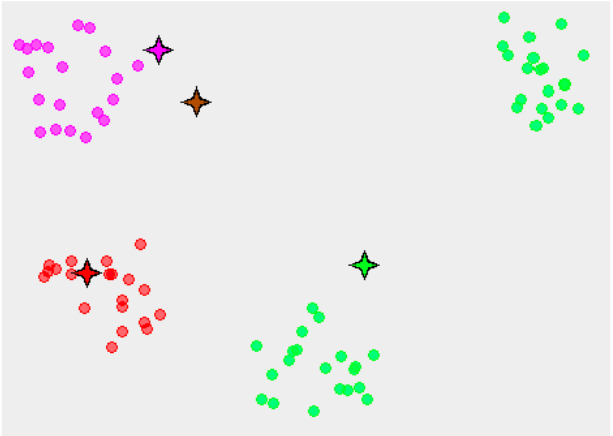


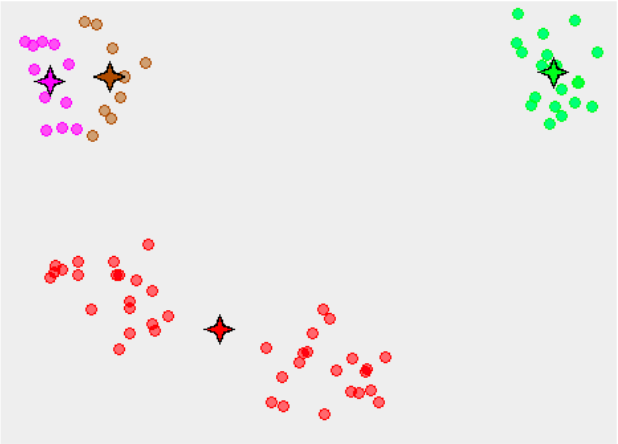
“Scalable recognition with a vocabulary tree”, Nister, Stewenius, 2006

Hierarchical K-Means

Standard K-Means: Lloyd's algorithm.







http://en.wikipedia.org/wiki/K-means_clustering

Hierarchical K-Means

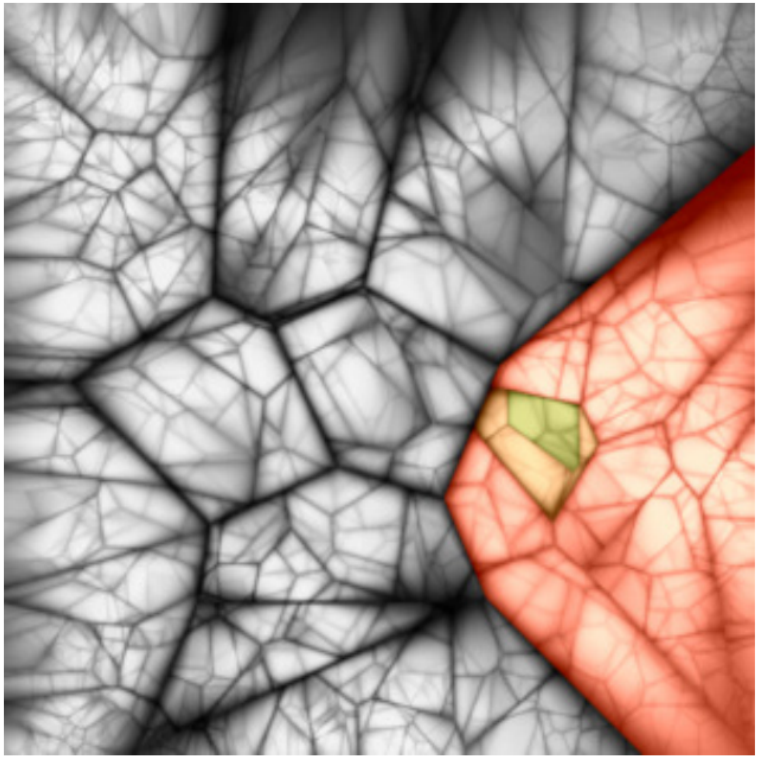
Single level K-means is O(Nkld)** for N data points, k means, I iterations of improvement.

The complexity of K-means tree is then

O(Nkld log(N)) by Master theorem.

** “Efficient clustering and matching for object class recognition,” Leibe et al. 2006

Hierarchical K-Means



Hierarchical k-means tree projected into 2-D. Search depth is labeled from red shallowest to green deepest.

“City Scale Location Recognition” Schindler et al. 2007

Hierarchical K-Means

Improvement: Order of magnitude speedup by using only 7 iterations in each clustering step. 90% of convergence accuracy.

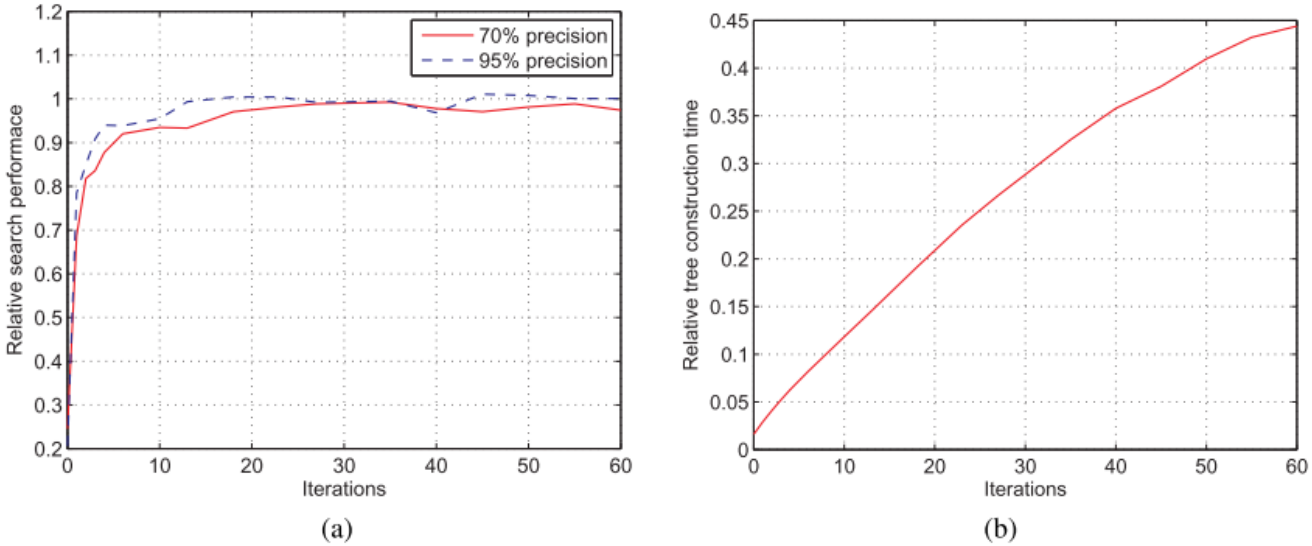


Figure 3: The influence that the number of k-means iterations has on the search time efficiency of the k-means tree (a) and on the tree construction time (b) (100K SIFT features dataset)

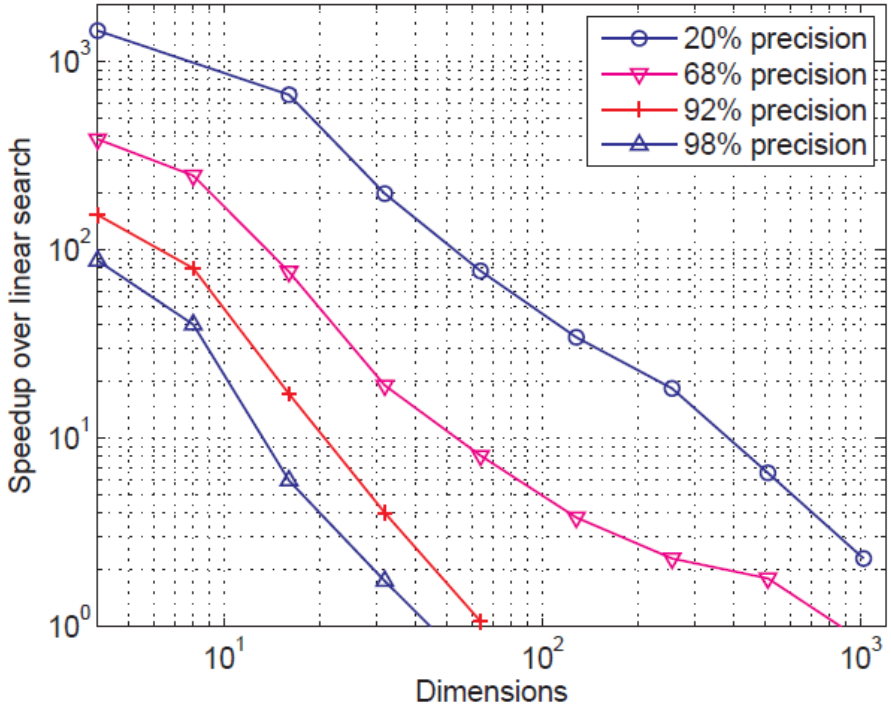
Hierarchical K-Means

Improvement: Best Bin First by distance of cluster center.

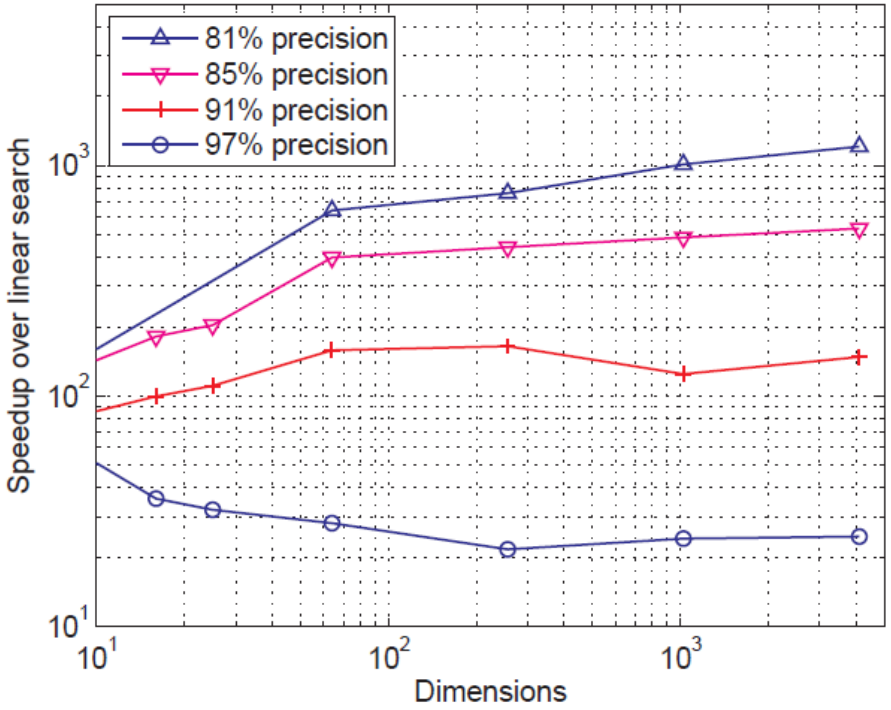
1. Greedily traverse once to a leaf node. Add unexplored branches along path to a priority queue.
2. Restart another greedy traversal from the cluster branch closest to query (can be in the middle of the tree)

Stops after a given number of leaf nodes (points) are checked.

Data Dimensionality

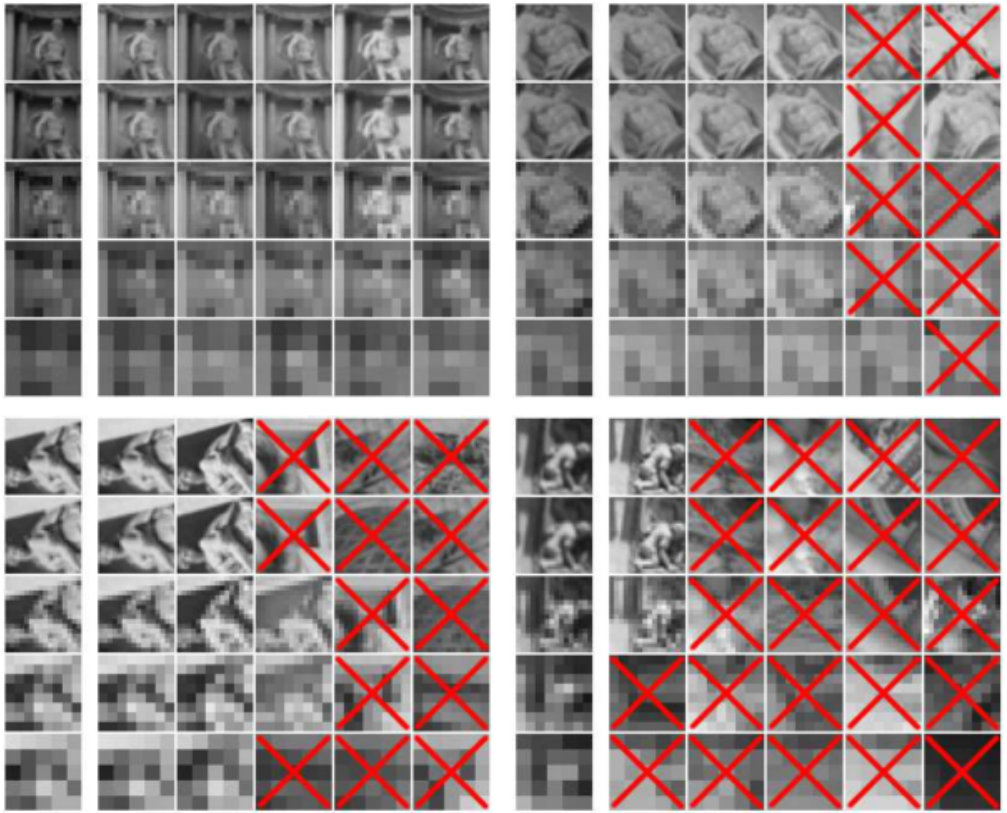


(a) Random vectors



(b) Image patches

Data Dimensionality



Queries on Trevi Fountain patch data set with different patch sizes. Demonstrates that even for high dimensional data (64x64 = 4096 dimensions in a patch) that similarity in a small number of dimensions provides strong enough evidence to determine overall patch similarity.

Choosing an Algorithm

Data features:

- Correlations between dimensions.
- Size of data set.

Algorithm features:

- Number of kd-trees.
- Branching factor of k-means.
- Number of iterations in k-means clustering step.

Choosing an Algorithm

$$cost = \frac{s + w_b b}{(s + w_b b)_{\text{opt}}} + w_m m$$

s -- search time

b -- tree build time

w_b -- build time weight

$m = m_t/m_d$ -- ratio of tree memory to raw data

w_m -- tree memory weight

Choosing an Algorithm

$$cost = \frac{s + w_b b}{(s + w_b b)_{\text{opt}}} + w_m m$$

$(s + w_b b)_{opt}$ -- optimal time cost if memory doesn't matter.

Computed during following optimization process.

Choosing an Algorithm

For a given data set, compute cost for:

- {1,4,8,16,32} kd trees
- {16,32,64,128,256} k-means branching factor.
- {1,5,10,15} k-means clustering iterations

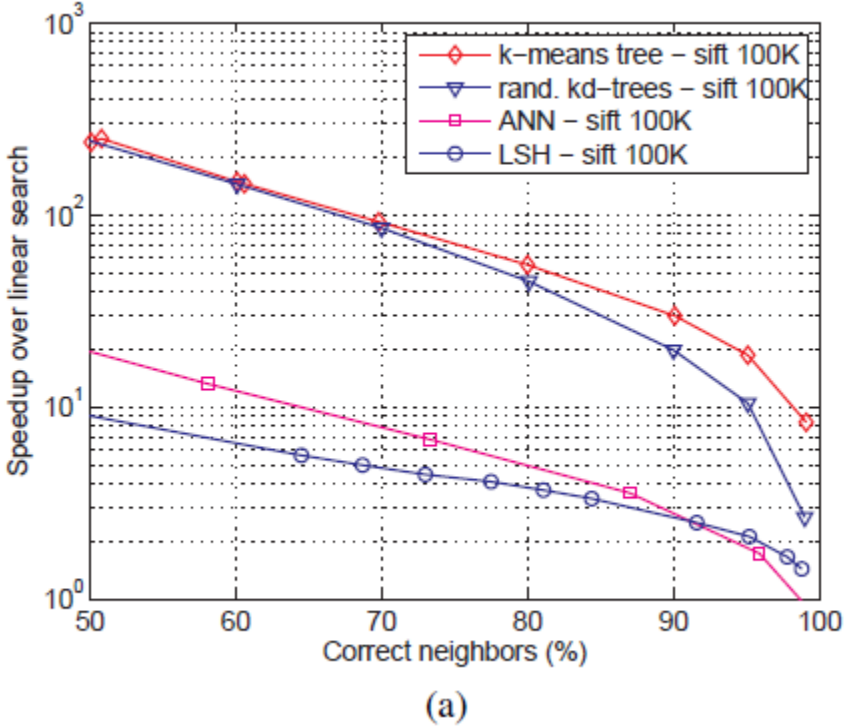
May check 1/10 of the data set and still be close to optimum.

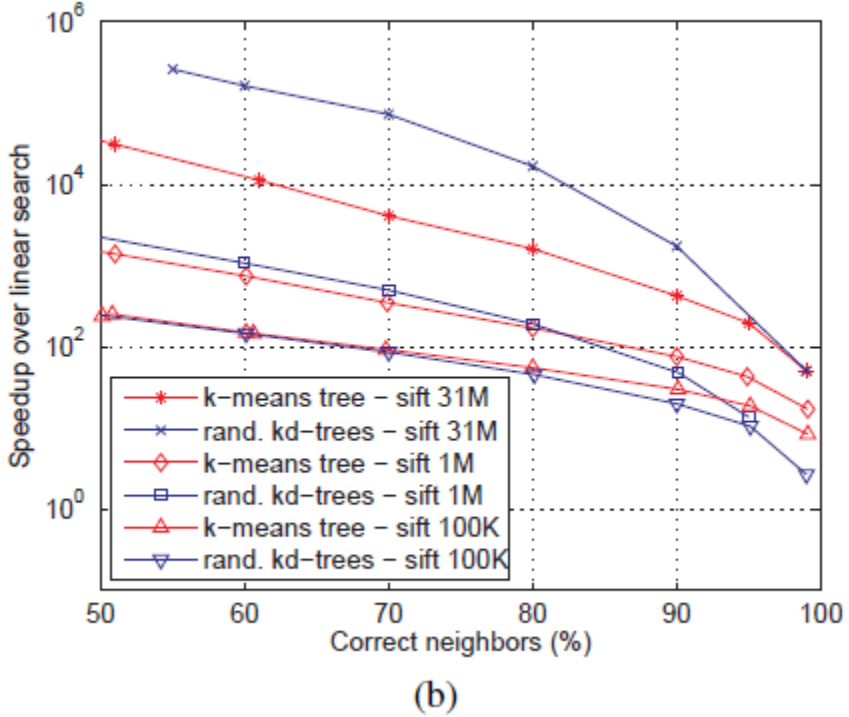
Choosing an Algorithm

Optimize using simplex locally after finding the best option from the previous step.

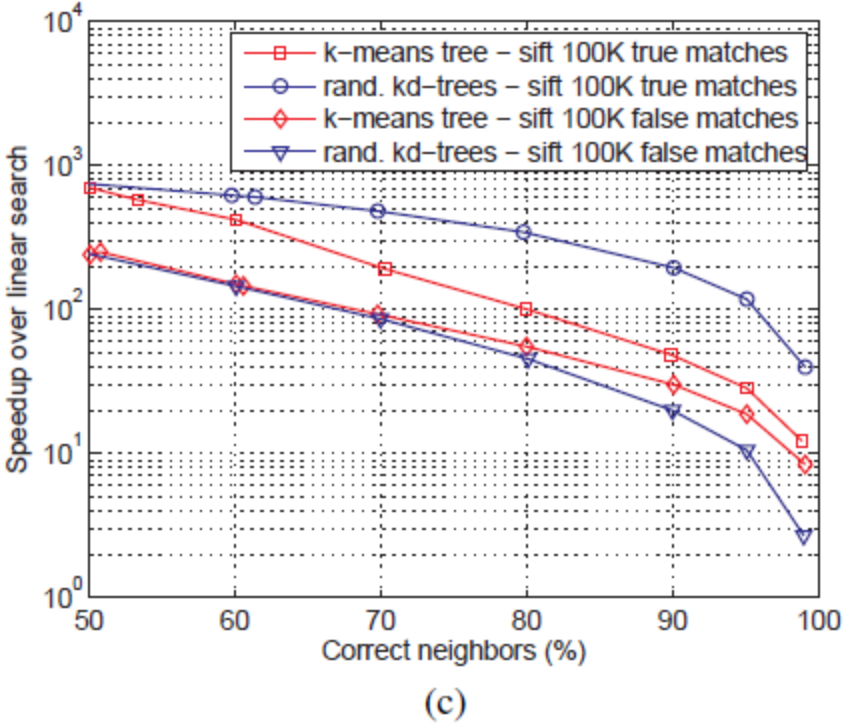
Expensive to optimize, but results for each type of dataset can simply be stored.

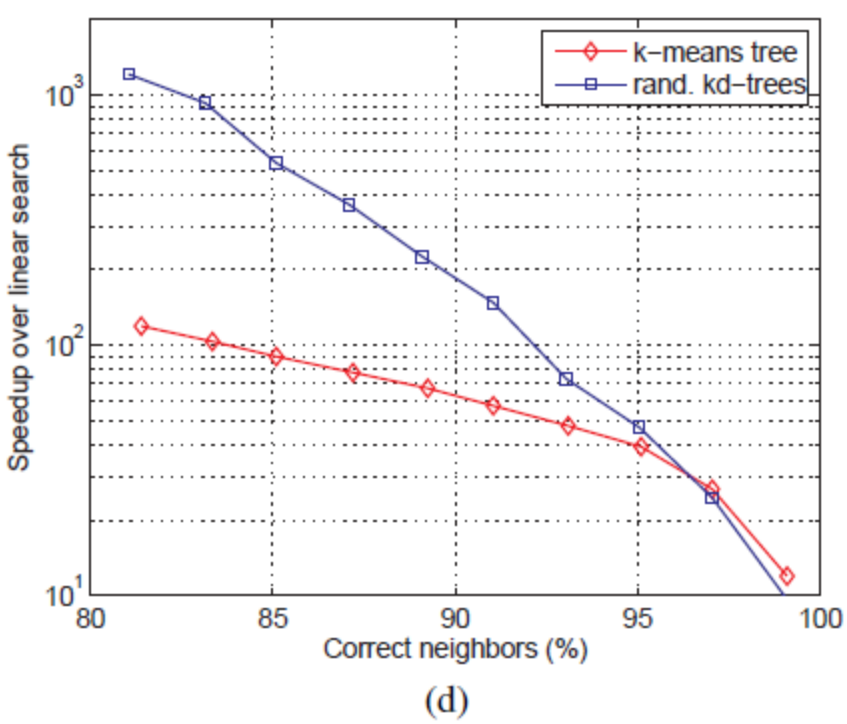
Results


k−means tree − sift 100K
rand. kd−trees − sift 100K
ANN − sift 100K
LSH − sift 100K
Speedup over linear search
Correct neighbors (%)
(a)


k−means tree − sift 31M
rand. kd−trees − sift 31M
k−means tree − sift 1M
rand. kd−trees − sift 1M
k−means tree − sift 100K
rand. kd−trees − sift 100K
Speedup over linear search
Correct neighbors (%)
(b)

Results


k−means tree − sift 100K true matches
rand. kd−trees − sift 100K true matches
k−means tree − sift 100K false matches
rand. kd−trees − sift 100K false matches
Speedup over linear search
Correct neighbors (%)
(c)


k−means tree
rand. kd−trees
Speedup over linear search
Correct neighbors (%)
(d)

Results

$Pr.(\%)$	w_b	w_m	Algorithm	Dist. Error	Search Speedup	Memory Used	Build Time
60%	0	0	k-means, 16, 15	0.096	181.10	0.51	0.58
	0	1	k-means, 32, 10	0.058	180.9	0.37	0.56
	0.01	0	k-means, 16, 5	0.077	163.25	0.50	0.26
	0.01	1	kd-tree, 4	0.041	109.50	0.26	0.12
	1	0	kd-tree,1	0.044	56.87	0.07	0.03
	*	∞	kd-tree,1	0.044	56.87	0.07	0.03
90%	0	0	k-means, 128, 10	0.008	31.67	0.18	1.82
	0	1	k-means, 128, 15	0.007	30.53	0.18	2.32
	0.01	0	k-means, 32, 5	0.011	29.47	0.36	0.35
	1	0	k-means, 16, 1	0.016	21.59	0.48	0.10
	1	1	kd-tree,1	0.005	5.05	0.07	0.03
	*	∞	kd-tree,1	0.005	5.05	0.07	0.03

In Conclusion

- Improved hierarchical k-means tree search algorithm
- Identification of two best nearest neighbor search algorithms for any data set
- Automatic choice of algorithm and optimal parameters
- Algorithms contained in public domain library