Approximate Nearest Neighbor Search
in high dimensional space

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Higher School of Economics, 2020

- **In session recommendations**

  Given user's u current session $(i_1, i_2, \ldots, i_m)$ in terms of viewd products, goal is to recommend product $i_{m+1} \in I$, where I - large set of items.

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- **Offline evaluation of RecSys**

  Assume we have user's vector representation $\mathbf{u}$, set of user's true relevant items, we would like to compute some $Metric@k$.
  We need to find k items from I with highest similarity score wrt $\mathbf{u}$ (e.g. dot product, cosine similarity).

Motivation
Main Goal

Efficient search of nearest neighbours

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Definition

Given $(\mathcal{X}, \rho)$ *- metric space*[a], $X \subseteq \mathcal{X}$ *- set of* n *points and* $q \in \mathcal{X}$ *- query point, task of Exact k-NN is to find a set* $kNN(q) \subseteq X$ *such that* $|kNN(q)| = k$ *and*

$$\forall x \in kNN(q)\ \forall x' \in X \setminus kNN(q)\ \ \big(\rho(q,x) \leq \rho(q,x')\big)$$

[a] https://en.wikipedia.org/wiki/Metric_space

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Examples of spaces

- $(\mathbb{R}^d, \|\cdot\|_2)$ — Euclidian space
- $\left(\mathbb{R}^d, \arccos \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\| \cdot \|\mathbf{y}\|}\right)$ — $\mathbb{R}^d$ with cosine distance
- ...

Main problems of Exact k-NN

- linear search time complexity of naive solution
- high complexity in high dimensional spaces

Commonly used definitions of the approximate neighbor search

- Search with predefined accuracy

Definition (ε-NN [5])

$$\forall x \in \varepsilon\text{-}NN(q) \ \ (\rho(q,x) \leq (1+\varepsilon)\rho(q,x_k)),$$

where $x_k \in kNN(q)$ - true k-th nearest neighbor of query point q.

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- Search with probability guarantee of finding true k closest points

Definition (ANN)

$$\frac{|ANN(q) \cap kNN(q)|}{k} \geq \delta,$$

i.e. we guarantee that fraction is above a certain threshold $\delta \in [0,1]$.

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We will mainly focus on the latter definition

In terms of speed/guaranties

- Speedup vs Recall plot

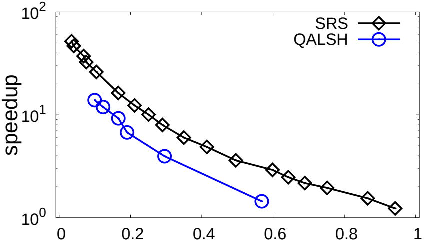

Рис.: Speedup vs Recall

- Recall vs Query time
- Queries per second vs Recall

Other aspects: data structure construction time, footprint size, and scalability

[1] `https://github.com/erikbern/ann-benchmarks`

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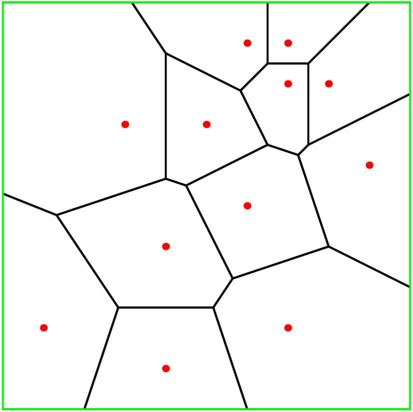
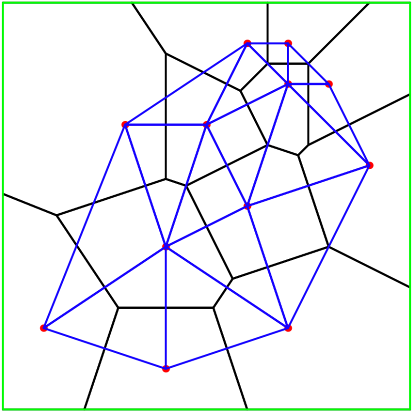


Consider set of points $X = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\} \subseteq \mathbb{R}^2$. With every point $\mathbf{x}_i$ associated region $R(\mathbf{x}_i)$ such that $\forall \mathbf{x} \in R(\mathbf{x}_i)\ \forall j \neq i\ (\|\mathbf{x} - \mathbf{x}_i\|_2 < \|\mathbf{x} - \mathbf{x}_j\|_2)$

[2] `https://en.wikipedia.org/wiki/Voronoi_diagram`

Dual graph for a Voronoi diagram (Delaunay Graph)[3]



Graph $G = \langle V, E \rangle$, where $V = X$ and $(u, v) \in E$ iff $R(u)$ and $R(v)$ are neighbours

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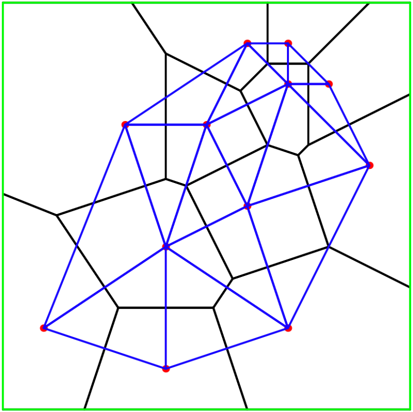

Graph $G = \langle V, E \rangle$, where $V = X$ and $(u, v) \in E$ iff $R(u)$ and $R(v)$ are neighbours

Algorithm 2.2 Greedy_Search$(q, v_{\text{entry_point}})$

$v_{cur} \leftarrow v_{\text{entry\_point}}$
$\delta_{\min} \leftarrow \rho(q, v_{cur})$; $\quad v_{next} \leftarrow NIL$
for all $u \in N(v_{cur})$ **do**
    $\delta \leftarrow \rho(q, u)$
    if $\delta < \delta_{\min}$ **then**
        $\delta_{\min} \leftarrow \delta$
        $v_{next} \leftarrow u$
if $v_{next} = NIL$ **then**
    return v_{cur}
return Greedy_Search(q, v_{next})

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Properties of Greedy Search in Delaunay Graph

- *GS will always find true nearest neighbour to query point*
- *Result could be generilized to other metric spaces*
- *GS could be linear in the worst case*

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Definition (Navigatable Small World)

Graphs with $\mathcal{O}(\log^{\alpha} n)$ scalability ($\alpha \geq 1$) of the GS algorithm are called navigable small world graphs

- Build graph G that approximates Delaunay Graph and has NSW property
- Greedy search for ANN (with ability to choose search accuracy)
- GS time complexity $\mathcal{O}(\log^2 n)$ (avg. node degree multiplied by avg. path length)

[4] `https://github.com/nmslib/nmslib`

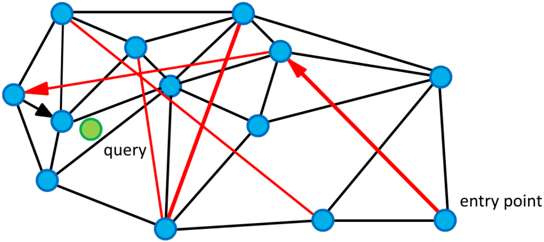

Рис.: Vertices are the data in metric space, black edges are the approximation of the Delaunay graph, and red edges are long range links for logarithmic scaling. Arrows show a sample path of the greedy algorithm from the entry point to the query (shown green)

Algorithm 2.3 k-NNSearch(q, m, k)

$tempRes \leftarrow \emptyset; candidates \leftarrow \emptyset; visited \leftarrow \emptyset; result \leftarrow \emptyset$ ▷ empty TreeSets
for $i = 1, \dots, m$ **do**
    put random entry point in candidates
    $tempRes \leftarrow \emptyset$
    loop
        get element c closest from candidates to q
        remove c from candidates
        if c is further than k-th element from result **then**
            break
        for all $e \in N(c)$ **do**
            if $e \notin visited$ **then**
                add e to visited, candidates, tempRes
    add objects from tempRes to result
return best k elements from result

Algorithm 2.4 Insert(x, f, w)

$N_x \leftarrow k$-NNSearch(x, w, f)
for all $u \in N_x$ **do**
  $N(x) \leftarrow N(x) \cup \{u\}$
  $N(u) \leftarrow N(u) \cup \{x\}$

Emperical study showed that graph G constructed with this inserting procedure is a good Delaunay approximation and has NSW property

m

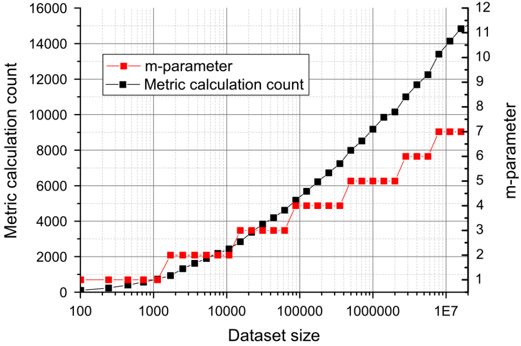

Рис.: Distance calculations and the value of m to get a 0.999 recall versus the size of the dataset for $d = 20$. The metric calculation count has $C \log^2 n$ complexity scaling.

w for optimal recall changes slowly (logarithmically) with the dataset size

f $3d$ where d - dimensionality of space (good value for high recall)

Hierarchical Navigable Small World[5] [10]

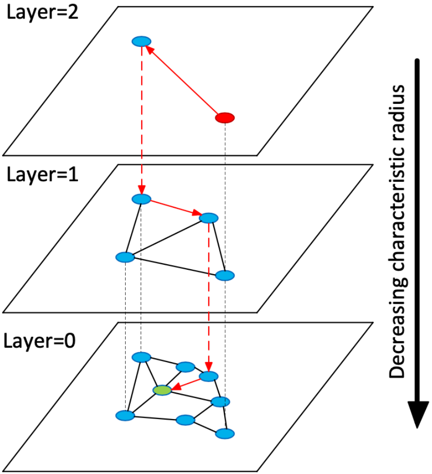

Рис.: Illustration of the Hierarchical NSW idea. The search starts from an element from the top layer (shown red). Red arrows show direction of the greedy algorithm from the entry point to the query (shown green)

[5] https://github.com/nmslib/nmslib

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Given $(\mathcal{X}, \rho)$ - metric space, set of object $X \subseteq \mathcal{X}$ and a hash function $h: \mathcal{X} \to [m]$.

LSH property

Similar items have larger probability to be mapped to the same bucket than dissimilar items.

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To find $ANN(q)$ we need to exemine bucket of object q

Definition

A family $\mathcal{H}$ of hash functions is called (d_1, d_2, p_1, p_2)-sensitive ($d_1 < d_2$) if for any $x, y \in \mathcal{X}$

- *if* $\rho(x, y) \leq d_1 \quad \Rightarrow \quad \mathbb{P}\{h(x) = h(y)\} \geq p_1$
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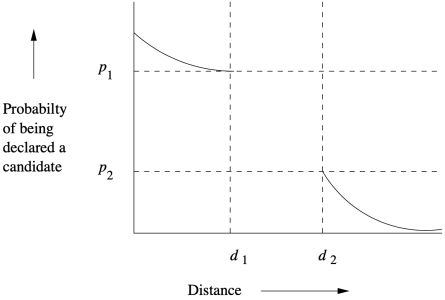

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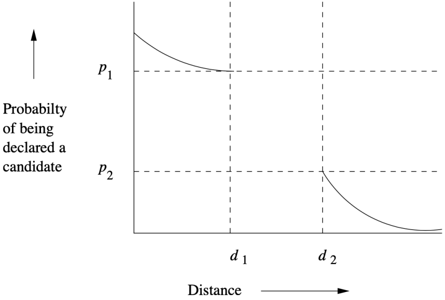

It is possible to drive p_1 and p_2 apart while keeping d_1 and d_2 fixed

- Given family $\mathcal{H}$ we can construct family $\mathcal{H}'$ in a following way
  1. Select $h_1, h_2, \ldots, h_r \sim_{\text{i.i.d}} \mathcal{H}$,
  2. New hash function $h(x) = [h_1(x), h_2(x), \ldots, h_r(x)] \in \mathcal{H}'$
  3. $\forall x, y \in \mathcal{X}$

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Remark

AND-construction lowers all probabilities, but if we choose $\mathcal{H}$ and r judiciously, we can make the small probability p_2 get very close to 0, while the higher probability p_1 stays significantly away from 0.

- Given family $\mathcal{H}$ we can construct family $\mathcal{H}'$ in a following way
  1. Select $h_1, h_2, \ldots, h_b \sim_{\text{i.i.d}} \mathcal{H}$,
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- OR-construction turns (d_1, d_2, p_1, p_2)-sensitive family $\mathcal{H}$ into $(d_1, d_2, 1-(1-p_1)^b, 1-(1-p_2)^b)$-sensitive family $\mathcal{H}'$

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Remark

OR-construction makes all probabilities rise, but by choosing $\mathcal{H}$ and b judiciously, we can make the larger probability approach 1 while the smaller probability remains bounded away from 1.

- There are different kinds of LSH families for different distances or similarities
- We can cascade AND- and OR-constructions in any order to make the low probability close to 0 and the high probability close to 1

- Consider $(\mathbb{R}^n, \theta)$, where $\theta(\mathbf{x}, \mathbf{y}) = \arccos \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\| \cdot \|\mathbf{y}\|}$ - space with cosine distance

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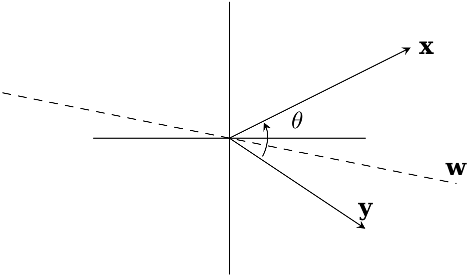
- $\mathbf{w}$ - random hyperplane through the origin



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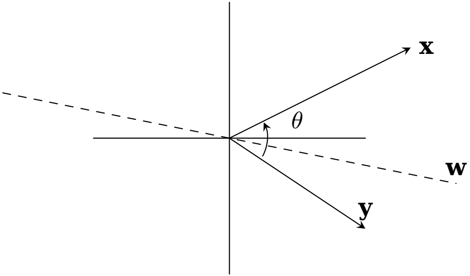

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- Set of such random hyperplanes defines $(d_1, d_2, 1 - \frac{d_1}{180}, 1 - \frac{d_2}{180})$ - sensitive family $\mathcal{H}$

LSH families examples

Min-hash [6]

- Consider $(2^{\mathcal{U}}, J)$, where $\mathcal{U}$ - finite set of m elements and $J(S,S') = 1 - \frac{|S \cap S'|}{|S \cup S'|}$ - set of sets with Jaccard distance
- $\pi : [m] \to [m]$ - random permutation
- $h_\pi(S) = \min\limits_{x \in S} \pi(x)$ - *minhash* function
- It is easily shown that $\mathbb{P}\{h(S) = h(S')\} = 1 - J(S,S')$

Resume

- The LSH scheme has very nice theoretic properties
- However, as the hash functions are data-independent, the practical performance is not as good as expected in certain applications

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Property

Distance computation using the hash values is efficient and well approximates the original distance ρ

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This strategy exploits two advantages of hash codes:

- distance using hash codes can be efficiently computed and the cost is much smaller than that of the computation in the input space
- the size of the hash codes is much smaller than the input features and hence can be loaded into memory

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Learning to hash task: learning a hash function, $y = h_\theta(\mathbf{x})$, such that the NNS in the V space is efficient and the result is an effective approximation of the true NNS result in the $\mathcal{X}$ space.

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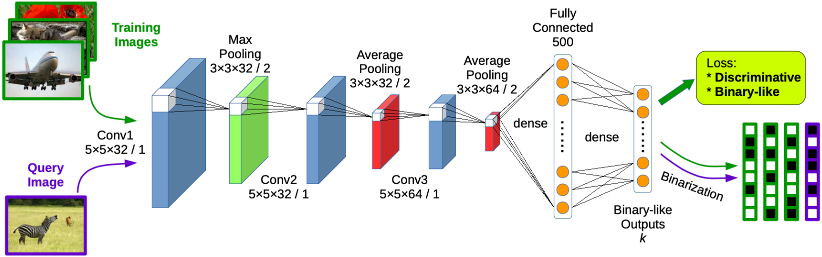
- Optimization criterion

Hash function $h \colon \Omega \to \{+1, -1\}^k$, where Ω - RGB space:



Training data:

- Set of image pairs along with label: $\{(I_{i,1}, I_{i,2}, y_i)\}_{i=1}^{N}$, where $y_i = \mathbb{1}\{I_{i,1}$ not similar to $I_{i,2}\}$

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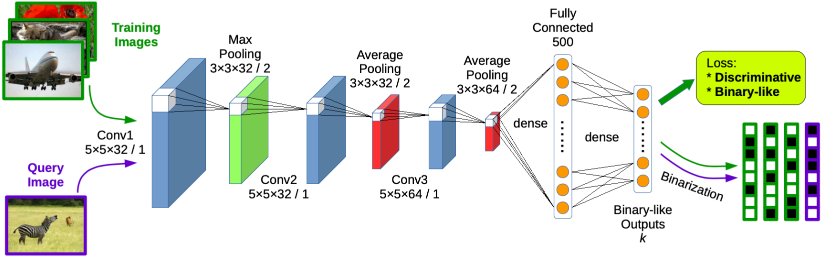

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Similarity measure: $D_h(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^k \mathbb{1}\{\mathbf{x}_i \neq \mathbf{y}_i\}$ - Hamming distance

Main idea: codes of similar images should be as close as possible, while the codes of dissimilar images being far away

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- Loss wrt the pair of images $I_1, I_2 \in \Omega$

$$L(\mathbf{b}_1, \mathbf{b}_2, y) = \frac{1}{2}(1-y)D_h(\mathbf{b}_1, \mathbf{b}_2) + \frac{1}{2}y \ \max\{m - D_h(\mathbf{b}_1, \mathbf{b}_2), 0\},$$

  where $\mathbf{b}_i = h(I_i) \in \{+1, -1\}^k$ - network output and $m > 0$ - margin threshold parameter.

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- Optimization criterion

$$\mathcal{L} = \sum_{i=1}^{N} L(\mathbf{b}_{i,1}, \mathbf{b}_{i,2}, y_i) \ \rightarrow \ \min$$

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- Loss wrt the pair of images $I_1, I_2 \in \Omega$

$$L(\mathbf{b}_1, \mathbf{b}_2, y) = \frac{1}{2}(1-y)D_h(\mathbf{b}_1, \mathbf{b}_2) + \frac{1}{2}y\ \max\{m - D_h(\mathbf{b}_1, \mathbf{b}_2), 0\},$$

  where $\mathbf{b}_i = h(I_i) \in \{+1, -1\}^k$ - network output and $m > 0$ - margin threshold parameter.
- Optimization criterion

$$\mathcal{L} = \sum_{i=1}^{N} L(\mathbf{b}_{i,1}, \mathbf{b}_{i,2}, y_i) \ \rightarrow\ \min$$

it is infeasible to directly optimize $\mathcal{L}$

Relaxed loss function

$$
\begin{aligned}
L(\mathbf{b}_1, \mathbf{b}_2, y) = &\frac{1}{2}(1-y)\|\mathbf{b}_1 - \mathbf{b}_2\|_2^2 \\
&+ \frac{1}{2}y\ \max\{m - \|\mathbf{b}_1 - \mathbf{b}_2\|_2^2, 0\} \\
&+ \underbrace{\alpha(\||\mathbf{b}_1| - \mathbf{1}\|_1 + \||\mathbf{b}_2| - \mathbf{1}\|_1)}_{\text{regularizer to replace the binary constraints}}
\end{aligned}
$$

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Annoy[6] [2, 7]

Very simple idea. Go directly to `https://bit.ly/2YsuEb1` to see details

[6] `https://github.com/spotify/annoy`

FAISS[7] [4]

[7] `https://github.com/facebookresearch/faiss`

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Resume

1. There are many different solutions to ANN problem which can be categorized into
   - Neighbourhood-based
   - Hashing-based (LSH, Learning to Hash)
   - Space Partitioning-based
2. Commonly used benchmark[8] for ANN methods evaluation

[8] `https://github.com/erikbern/ann-benchmarks`

Recommendations

1. When there are sufficient computing resources HNSW is the best choice for ANNS on high dimensional data
2. Annoy is also a very good choice
3. If there are avaliable GPU then FAISS is a good choice

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