Approximate Nearest Neighbors via Point Location Among Balls



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 $(1+\varepsilon)$ - Approximate Nearest Neighbors (ANN)

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Problem statement:

Given q, P, find p such that $d(q, p) \leq (1 + \varepsilon)d(q, P)$ where d(q, P) denotes the smallest distance from q to any other point in P, i.e. distance to its nn



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quadtrees: $(1 + \varepsilon)$ -ANN for bounded spread ring-separator tree: O(n)-ANN shifted quadtrees: $n^{O(1)}$ -ANN

combined: $(1 + \varepsilon)$ -ANN in low dimensions



recap: shifting grids and quadtrees by a random vector bFor a ball B of radius r: the probability that B is not in a single cell of $G^d(b, \Delta)$ is at most $\min\left(\frac{2dr}{\Delta}, 1\right)$.





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For t > 0 holds $\mathbb{P}\left[\mathbb{L}_{b}(p,q) > \log_{2}||p-q||+t\right] \leq \frac{4d}{2^{t}}$. With high probability p and q in same cell at level $\log_{2}||p-q||+c\log n$ (size of cell: $||p-q||n^{c}$)





ANN: today

Approximating a metric space by a hierarchical well-separated tree (HST)

- hierachical well-separated trees
- simple (n-1)-approximation
- fast $n^{O(1)}\text{-approximation in }\mathbb{R}^d$

ANN via point location among balls

- simple construction
- handling a range of radii
- ANN data structure based on HST

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... and next time

point location among approximate balls approximate Voronoi diagrams

Approximating a metric space by a hierarchical well-separated tree (HST)



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metric space M = (X, d):
a set X
a distance function d: X \times X \rightarrow [0, \infty)
?
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$$d(x, y) = 0$$
 iff x=y

- d(x,y) = d(y,x)
- $d(x,z) \leq d(x,y) + d(y,z)$ (triangle inequality)

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metric can be represented as matrix of size $\Theta(n^2)$ metric can be represented as weighted graph G with $d(x, y) = dist_G(x, y)$



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Question: Examples of metric spaces?



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We want:

compact, hierarchical(, approximate) representation





HST: rooted (binary) tree $T \ \mathrm{over} \ P$ with

- label $\Delta_v \geq 0$ for each node $v \in T$
- each leaf u_p uniquely corresponds to a point $p \in P$; $\Delta_u = 0$ for all leaves u.
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example: quadtree with $\Delta_v =$ diameter of cell



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- 1. compute minimum spanning tree
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- 3. build HST bottom-up: add vertex for MST edge with the two merged components as children
- 4. set Δ_v = 0 for leaves
- 5. for v with point set P_v in subtree and MST edge weight $w: \Delta_v := (|P_v| 1) w$



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 $d_T(p,q) := \Delta_{lca(u_p,u_q)}$ is a metric (lca: least common ancestor) metric N t-approximates metric M: $d_M(x,y) \le d_N(x,y) \le t \cdot d_M(x,y)$ simple HST construction: given: metric M = (P, d) as weighted graph 3 1. compute minimum spanning tree 2. sort edges of MST from short to long 3. build HST bottom-up: add vertex for MST edge with the two merged components as children $(I \bullet$ 4. set $\Delta_v = 0$ for leaves

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 $\Delta_{v} = 3d_{M}(a, b)$ $\Delta_{v} = 4d_{M}(b, c)$ $d \bullet c \bullet$

Small Assignment

Construct the HST for this metric space M (weights shown on edges). Is it a t-approximation of M?



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4-approximation



 $d_M \le d_{HST} \le (n-1)d_M$

(0. if u child of $v: \Delta_u \leq \Delta_v$)





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(0. if u child of v: $\Delta_u \leq \Delta_v$) a.) $|P_u| < |P_v|$

b.) edges handled in increasing order by weight





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 $d_M \le d_{HST} \le (n-1)d_M$

(0. if u child of $v: \Delta_u \leq \Delta_v$) 1. $d_{HST} \leq (n-1)d_M$ $x, y \in P, v := lca(u_x, u_y)$. Then $|P_v| - 1 \leq n - 1$ weight(MST edge for v) $\leq d_M(x, y)$





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 $x, y \in P, v := lca(u_x, u_y)$. Then
 $|P_v| - 1 \leq n - 1$
weight(MST edge for v) $\leq d_M(x, y)$
 $\Rightarrow d_{HST}(x, y) = \Delta_v \leq (n-1)d_M(x, y)$
 $1 \cdot 2$





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- 1. $d_{HST} \le (n-1)d_M$
- 2. $d_M \leq d_{HST}$





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 $\begin{aligned} &d_M(x,y) \\ &= \text{weight of shortest path from } x \text{ to } y \text{ in } G \\ &\leq \sum e_i \leq |P_v| \max e_i = \Delta_v \end{aligned}$





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$$d_M(p,q) = ||p-q|| \le \Delta_{lca(u_p,u_q)} = d_{HST}(p,q)$$



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$$d_M(p,q) = \|p-q\| \le \Delta_{lca(u_p,u_q)} = d_{HST}(p,q)$$
$$\le n^{O(1)} \|p-q\| \quad \text{(with high probability)}$$



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Overview

Approximating a metric space by a hierarchical well-separated tree (HST)

- hierachical well-separated trees
- simple (n-1)-approximation
- fast $n^{O(1)}\text{-approximation in }\mathbb{R}^d$

ANN via point location among balls

- simple construction
- handling a range of radii
- ANN data structure based on HST



 $b(p, r) = \{q \mid d(p, q) \leq r\}$ denotes a ball around point p with radius r



q^{o}

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point set P in a metric space $\mathcal M$



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Relation $(1+\varepsilon)\text{-}\text{ANN}$ and PLEB

Gaining some intuition:



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Gaining some intuition:

 $r = d(q, p) \ge d(q, P)$



lacksquare

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Reduction from $(1 + \varepsilon)$ -ANN to Point location among balls

define
$$\mathcal{U}(P,r) = \bigcup_{p \in P} b(p,r)$$

union of balls of radius r





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Lemma: Let $\mathcal{B} = \bigcup_{i=-\infty}^{\infty} \mathcal{U}(P, (1 + \varepsilon)^i)$. For a query q, let p be the center of $\odot_{\mathcal{B}}(q)$. Then p is $(1 + \varepsilon)$ -ANN to q.



Lemma: Let
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We have that $q \in b(s, (1 + \varepsilon)^{i+1})$

It must be that the target ball has a radius $\leq (1 + \varepsilon)^{i+1}$. It cannot be smaller than r, or bigger than $(1 + \varepsilon)^{i+1}$.



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It must be that the target ball has a radius $\leq (1 + \varepsilon)^{i+1}$. It cannot be smaller than r, or bigger than $(1 + \varepsilon)^{i+1}$.

It follows that $||q - p|| \leq radius(\odot_{\mathcal{B}}(q)) \leq (1 + \varepsilon)^{i+1} < (1 + \varepsilon)d(q, P)$



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Observations:

 $\Theta(n^2)$ disks

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(2) need to avoid range dependent on pairs, otherwise

Near neighbor data structure $\mathcal{D}(P,r)$

 \boldsymbol{q} 0

 ${ \bullet }$

Near neighbor data structure $\mathcal{D}(P, r)$ Decides given q, if $d(q, P) \leq r$, or d(q, P) > rIf $d(q, P) \leq r$ it returns a point p s.t. $d(q, p) \leq r$



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A query can be resolved by iteratively checking for each ball in $\mathcal{U}(P,r)$ if it contains q



Near neighbor data structure $\mathcal{D}(P, r)$ Given interval [a, b], Let $\mathcal{N}_i = \mathcal{D}(P, r_i)$ where $r_i = \min((1 + \varepsilon)^i a, b)$ for $i = 0, \dots, M = \lceil \log_{1+\varepsilon}(\frac{b}{a}) \rceil$







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Interval near neighbor data structure $\hat{\mathcal{I}}(P, a, b, \varepsilon)$ Lemma: Given $P, a \leq b$ and $\varepsilon > 0$, one can construct $\hat{\mathcal{I}}(P, a, b, \varepsilon)$ such that: (A) $\hat{\mathcal{I}}$ is made out of $O(\varepsilon^{-1} \log(b/a))$ nn structures, and (B) given a query point q it can decide if:



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number of queries can be achieved by doing a binary search on the radius: $O(\log(\varepsilon^{-1}\log(b/a)))$

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The ANN data structure

Given: set of points P and a t-approximate (B)HST \pmb{H} on P



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recall:

- Each vertex v has a label $\Delta_v \ge 0$.
- $\Delta_v = 0$ if v is a leaf.
- If u is a child of v, then $\Delta_v \geq \Delta_u$
- $\Delta_{lca(u,v)}$ denotes the t-approximated distance between two leaves u and v



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- $\Delta_{lca(u,v)}$ denotes the t-approximated distance between two leaves u and v
- Each vertex v has a representative leaf repr_v .
- $\operatorname{repr}_u \in \{\operatorname{repr}_v \mid v \text{ is a child of } u\}$



Given: set of points P and a t-approximate (B)HST ${\pmb H}$ on P

Recursively build search tree T (top-down):



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$$r_{v} = \frac{\Delta(u^{v})}{4t} \text{ and } R_{v} = \mu \Delta(u^{v})$$
$$\mu = O(\varepsilon^{-1} \log n)$$

 $\hat{\mathcal{I}}_v$ can be used to determine search path in T



S

S





subtle:

 S_{out} contains rep_{u_v} but no other points of S_L and S_R .







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- $d(q, P^v) \in (r_v, R_v]$: Then the query finds a $(1 + \varepsilon/4)$ -ANN point $s \in P^v$ and returns it as the answer to the query
- $d(q, P^v) > \mathbf{R}_v$:

Then the search continues recursively in v_{out}



Correctness

Lemma: The point returned by the data structure is a $(1 + \varepsilon)$ -ANN to the query point q in P.

Proof (sketch, case 1): $d(q, P^v) \leq r_v$; recurse into subtree with returned point p.

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Proof (sketch, case 1):

 $d(q, P^v) \leq r_v$; recurse into subtree with returned point p. We need to show that the algorithm recurses into a subtree which contains a $(1 + \varepsilon)$ -ANN point. If the algorithm continues to v_L , we have that $d(P_L^v, P^v \setminus P_L^v) \geq \Delta(u^v)/t$. For $q_L = nn(q, P_L^v)$, by the triangle inequality we have that

$$d(q, P_v \setminus P_L^v) \ge d(q_L, P^v \setminus P_L^v) - d(q, q_L) \ge \frac{\Delta(u^v)}{t} - \frac{\Delta(u^v)}{$$

$$r_{v} > \frac{\Delta(u^{v})}{2t} > r_{v}$$
$$= \frac{\Delta(u^{v})}{4t}$$

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Let $U(n_v)$ be the number of balls used in $\hat{\mathcal{I}}_v$, we have $\mu = O(\varepsilon^{-1} \log n)$ and $\hat{\mathcal{I}}(P, a, b, \varepsilon)$ is made out of $O(\frac{n}{\varepsilon} \log(b/a))$ balls (previous slide).

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$$U(n_v) = O(\frac{n_v}{\varepsilon} \log \frac{R_v}{r_v}) = O(\frac{n_v}{\varepsilon} \log(\frac{t\log}{\varepsilon}))$$

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For the total number of balls, we get the recurrence $B(n) = U(n) + B(n_L) + B(n_R) + B(n_{out})$ (we have $n_L, n_R, n_{out} \le n/2 + 1$ and $B(n_L) + B(n_R) + B(n_R)$ This results in $B(2n) = O(\varepsilon^{-1}n\log n\log(\varepsilon^{-1}t\log n)) = O((n+1))$

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count each occurrence of point as repr. (overall 2n)

$$p_{out})=n$$
). $n/arepsilon)\log^2n)$

Number of Queries

Lemma: For $t = n^{O(1)}$, the ANN-query algorithm performs $O(\log(n/\varepsilon))$ near neighbor queries

Proof (sketch):

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Lemma: For $t = n^{O(1)}$, the ANN-query algorithm performs $O(\log(n/\varepsilon))$ near neighbor queries

Proof (sketch):

For every internal node v on the search path π in T corresponds to a situation where $d(q, P) \leq r_v$ or $d(q, P) > R_v$, which can be decided by two nearest neighbor queries.

In the final node u in π , the search algorithm resolves the query using $O\left(\log \frac{\log R_v/r_v}{\varepsilon}\right)$ $= O(\log(1/\varepsilon) + \log\log n)$ near neighbor queries.

Since the depth of the tree is $O(\log n)$, the total number of queries becomes $O(\log n + \log(1/\varepsilon) + \log \log n) = O(\log n/\varepsilon).$

Summary

Approximating a metric space by a hierarchical well-separated tree (HST)

- hierachical well-separated trees
- simple (n-1)-approximation
- fast $n^{O(1)}\text{-approximation}$ in \mathbb{R}^d

ANN via point location among balls

- simple construction
- handling a range of radii
- ANN data structure based on HST

... and next time

point location among approximate balls approximate Voronoi diagrams