25 Nearest Neighbor Algorithms: Voronoi Diagrams and k-d Trees

NEAREST NEIGHBOR ALGORITHMS

Exhaustive k-NN Alg.

Given query point q:
- Scan through all n training pts, computing (squared) distances to q.
- Maintain a max-heap with the k shortest distances seen so far.
  [Whenever you encounter a training point closer to q than the point at the top of the heap, you remove the heap-top point and insert the better point. Obviously you don't need a heap if $k = 1$ or even 5, but if $k = 99$ a heap will substantially speed up keeping track of the kth-shortest distance.]

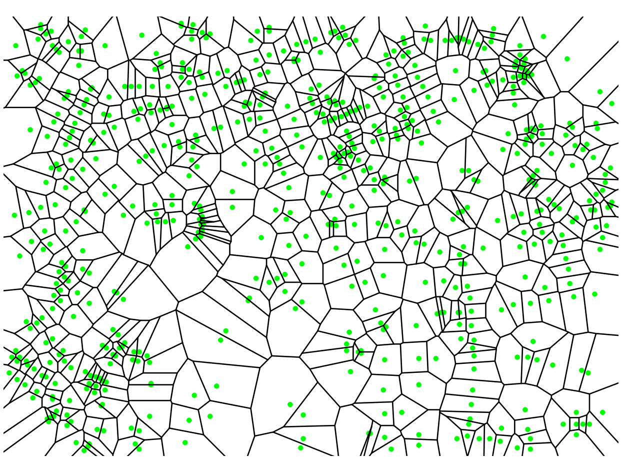
Time to train classifier: 0   [This is the only $O(0)$-time algorithm we'll learn this semester.]
Query time: $O(nd + n \log k)$
  expected $O(nd + k \log n \log k)$ if random pt order
[It's a cute theoretical observation that you can slightly improve the expected running time by randomizing the point order so that only expected $O(k \log n)$ heap operations occur. But in practice I can't recommend it; you'll probably lose more from cache misses than you'll gain from fewer heap operations.]

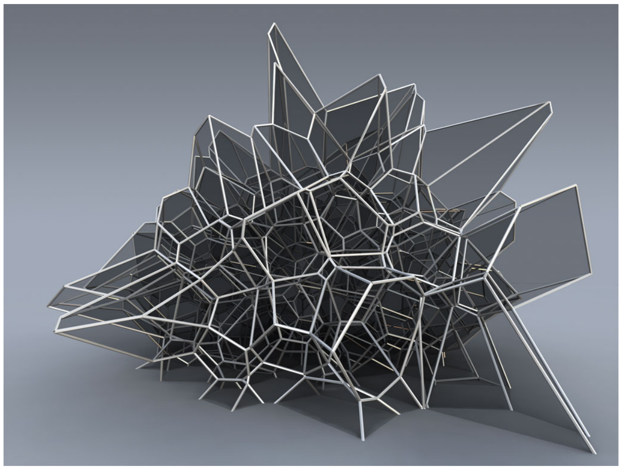
Can we preprocess training pts to obtain sublinear query time?

2–5 dimensions: Voronoi diagrams
Medium dim (up to ~ 30): k-d trees
Large dim: exhaustive k-NN, but can use PCA or random projection
  locality sensitive hashing   [still researchy, not widely adopted]

Voronoi Diagrams

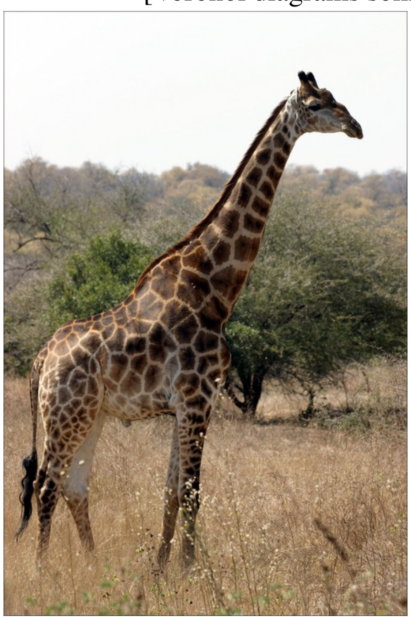
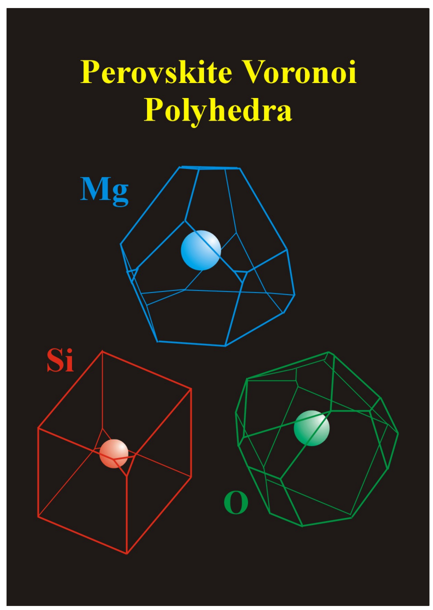
Let X be a point set. The Voronoi cell of $w \in X$ is
Vor $w = \{p \in \mathbb{R}^d : \|p - w\| \leq \|p - v\| \quad \forall v \in X\}$
[A Voronoi cell is always a convex polyhedron or polytope.]
The Voronoi diagram of X is the set of X's Voronoi cells.

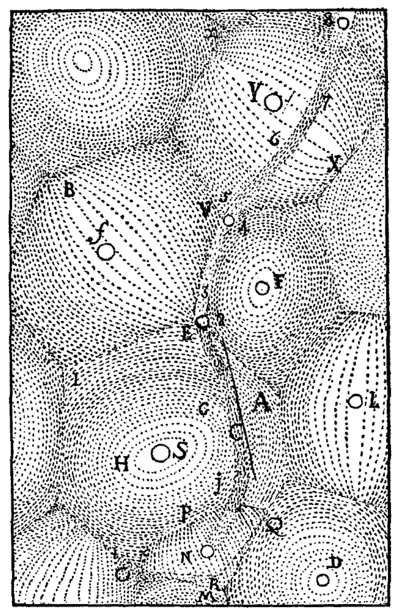





voro.pdf, vormcdonalds.jpg, voronoiGregorEichinger.jpg, saltflat-1.jpg

[Voronoi diagrams sometimes arise in nature (salt flats, giraffe, crystallography).]



giraffe-1.jpg, perovskite.jpg, vortex.pdf

[Believe it or not, the first published Voronoi diagram dates back to 1644, in the book "Principia Philosophiae" by the famous mathematician and philosopher René Descartes. He claimed that the solar system consists of vortices. In each region, matter is revolving around one of the fixed stars (vortex.pdf). His physics was wrong, but his idea of dividing space into polyhedral regions has survived.]

Size (e.g., # of vertices) $\in O(n^{\lceil d/2 \rceil})$
[This upper bound is tight when d is a small constant. As d grows, the tightest asymptotic upper bound is somewhat smaller than this, but the complexity still grows exponentially with d.]
. . . but often in practice it is $O(n)$.
[Here I'm leaving out a constant that may grow exponentially with d.]

Point location: Given query point $q \in \mathbb{R}^d$, find the point $w \in X$ for which $q \in \text{Vor}\ w$.
[We need a second data structure that can perform this search on a Voronoi diagram efficiently.]

2D: $O(n \log n)$ time to compute V.d. and a trapezoidal map for pt location
$O(\log n)$ query time [because of the trapezoidal map]
[That's a pretty great running time compared to the linear query time of exhaustive search.]

*d*D: Use binary space partition tree (BSP tree) for pt location. [Unfortunately, it's difficult to characterize the running time of this strategy, although it is often logarithmic in 3–5 dimensions.]

1-NN only! [A standard Voronoi diagram supports only 1-nearest neighbor queries. If you want the k nearest neighbors, there is something called an order-k Voronoi diagram that has a cell for each possible k nearest neighbors. But nobody uses those, for two reasons. First, the size of an order-k Voronoi diagram is $\Theta(k^2 n)$ in 2D, and worse in higher dimensions. Second, there's no software available to compute one.]

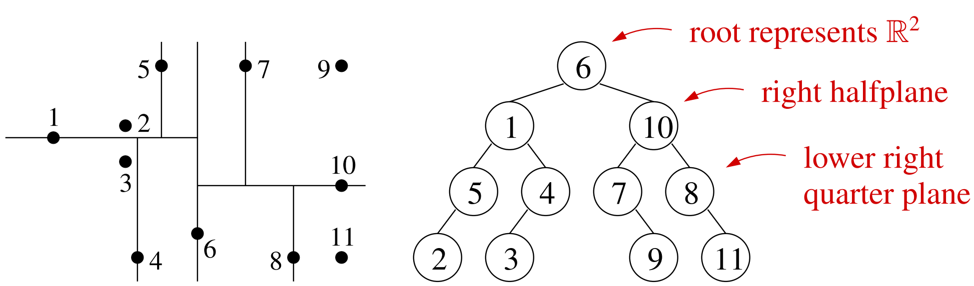
[There are also Voronoi diagrams for other distance metrics, like the ℓ_1 and ℓ_∞ norms.]

[Voronoi diagrams are good for 1-nearest neighbor queries in two dimensions, and maybe up to 5 dimensions, and they're a great concept for understanding the problem of nearest neighbor search. But k-d trees are much simpler and probably faster in 6 or more dimensions.]

k-d Trees

"Decision trees" for NN search. [Just like in a decision tree, each treenode in a k-d tree represents a rectangular box in feature space, and we split a box by choosing a splitting feature and a splitting value belonging to a training point in the box. But we use different criteria for choosing splits.] Differences:

– Choose splitting feature w/greatest width: feature i in $\max_{i,j,k}(X_{ji} - X_{ki})$.
  [With nearest neighbor search, we don't care about the entropy. Instead, what we want is that if we draw a sphere around the query point, it won't intersect very many boxes of the decision tree. So it helps if the boxes are nearly cubical, rather than long and thin.]
  Cheap alternative: rotate through the features. [We split on the first feature at depth 1, the second feature at depth 2, and so on. This builds the tree faster, by a factor of $O(d)$.]
– Choose splitting value: median point for feature i; OR midpoint $\frac{X_{ji}+X_{ki}}{2}$.
  Median guarantees $\lfloor \log_2 n \rfloor$ tree depth; $O(nd \log n)$ tree-building time.
  [. . . or just $O(n \log n)$ time if you rotate through the features. An alternative to the median is splitting at the box center, which improves the aspect ratios of the boxes, but it could unbalance your tree. A compromise strategy is to alternate between medians at odd depths and centers at even depths, which also guarantees an $O(\log n)$ depth.]
– Each internal node stores a training point. [. . . that lies in the node's box. Usually the splitting point.]
  [Some k-d tree implementations have points only at the leaves, but it's better to have points in internal nodes too, so when we search the tree, we often stop searching earlier.]

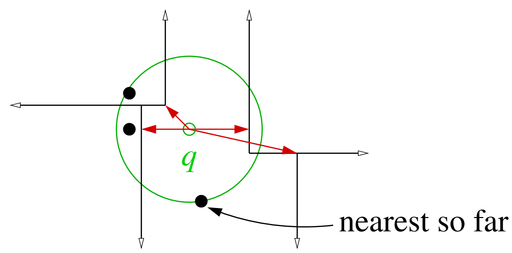


[Draw this by hand. kdtreestructure.pdf]

[Once the tree is built, the classification algorithm is different too. Most importantly, you usually have to visit multiple leaves of the tree to find the nearest neighbor. We sometimes use an approximate nearest neighbor algorithm to save time, instead of demanding the exact nearest neighbor.]

Goal: given query pt q, find a training pt w such that $\|q - w\| \leq (1 + \epsilon) \|q - s\|$,
where s is the closest training pt.
$\epsilon = 0 \Rightarrow$ exact NN; $\epsilon > 0 \Rightarrow$ approximate NN.

Query alg. maintains:
- Nearest neighbor found so far (or k nearest). goes down ↓
- Binary min-heap of unexplored subtrees, keyed by distance from q. goes up ↑



[Draw this by hand. kdtreequery.pdf] [A query in progress.]

[Each subtree represents an axis-aligned box. The query tries to avoid searching most of the boxes/subtrees by searching the boxes close to q first. We measure the distance from q to a box and use it as a key for the subtree in the heap. The search stops when the distance from q to the kth-nearest neighbor found so far $\leq$ the distance from q to the nearest unexplored box (times $1 + \epsilon$). For example, in the figure above, the query never visits the box at far lower right, because it doesn't intersect the circle.]

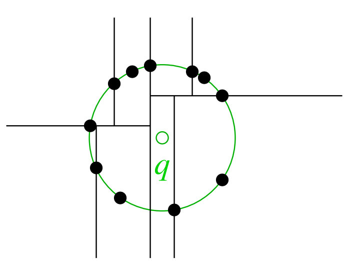
Alg. for 1-NN query:

$Q \leftarrow$ heap containing root node with key zero
$r \leftarrow \infty$
while Q not empty and $(1 + \epsilon) \cdot \text{minkey}(Q) < r$
  $B \leftarrow \text{removemin}(Q)$
  $w \leftarrow B$'s training point
  $r \leftarrow \min\{r, \text{dist}(q, w)\}$ [For speed, store square of r instead.]
  $B', B'' \leftarrow$ child boxes of B
  if $(1 + \epsilon) \cdot \text{dist}(q, B') < r$ then insert$(Q, B', \text{dist}(q, B'))$ [The key for B' is $\text{dist}(q, B')$]
  if $(1 + \epsilon) \cdot \text{dist}(q, B'') < r$ then insert$(Q, B'', \text{dist}(q, B''))$
return point that determined r

For k-NN, replace "r" with a max-heap holding the k nearest neighbors.

Works with any ℓ_p norm for $p \in [1, \infty]$. [k-d trees are not limited to the Euclidean (ℓ_2) norm.]

Why ϵ-approximate NN?



[Draw this by hand. kdtreeproblem.pdf] [A worst-case exact NN query.]

[In the worst case, we may have to visit every node in the *k*-d tree to find the exact nearest neighbor. In that case, the *k*-d tree is slower than simple exhaustive search. This is an example where an *approximate* nearest neighbor search can be much faster. In practice, settling for an approximate nearest neighbor sometimes improves the speed by a factor of 10 or even 100, because you don't need to look at most of the tree to do a query. This is especially true in high dimensions—remember that in high-dimensional space, the nearest point often isn't much closer than a *lot* of other points.]

Software: ANN (U. Maryland), FLANN (U. British Columbia), GeRaF (U. Athens) [random forests!]

Example: im2gps

[I want to emphasize the fact that exhaustive nearest neighbor search really is one of the first classifiers you should try in practice, even if it seems too simple. So here's an example of a modern research paper that uses 1-NN and 120-NN search to solve a problem.]

Paper by James Hays and [our own] Prof. Alexei Efros.
[Goal: given a query photograph, determine where on the planet the photo was taken. Called geolocalization. They evaluated both 1-NN and 120-NN. What they did not do, however, is treat each photograph as one long vector. That's okay for tiny digits, but too expensive for millions of travel photographs. Instead, they reduced each photo to a small descriptor made up of a variety of features that extract the essence of each photo.]
[Show slides (im2gps.pdf). Sorry, images not included here. http://graphics.cs.cmu.edu/projects/im2gps/]

[Bottom line: With 120-NN, their most sophisticated implementation came within 64 km of the correct location about 50% of the time.]

RELATED CLASSES [if you like machine learning, consider these courses in 2024–25]

CS 180/280A (fall): Computer Vision/Photography
CS 182/282A (spring): Deep Neural Networks
EECS 127 (both), 227AT (spring), 227BT (fall): Numerical Optimization [a core part of ML]
[It's hard to overemphasize the importance of numerical optimization to machine learning, as well as other CS fields like graphics, theory, and scientific computing.]
EECS 126 (both): Random Processes [Markov chains, expectation maximization, PageRank]
EE C106A/B (fall/spring?): Intro to Robotics [dynamics, control, sensing]
Math 110: Linear Algebra [but the real gold is in Math 221]
Math 221 (fall): Matrix Computations [how to solve linear systems, compute SVDs, eigenvectors, etc.]
CS C281B (spring): Learning & Decision Making
CS C267 (spring): Scientific Computing [parallelization, practical matrix algebra, some graph partitioning]
CS C280 (spring): Computer Vision
CS 288 (fall): Natural Language Processing
CS 294-43 (spring): Visual & Language Models (Darrell)
CS 294-150 (spring): ML & Biology (Listgarten)
CS 294-158 (spring): Deep Unsupervised Learning (Abbeel)
CS 294-162 (fall): ML Systems (Gonzalez/Zaharia)
CS 294-256 (spring): ML for Hardware Design (Wawrzynek)
CS 294-258 (spring): Models of Language (Suhr)
VS 265: Neural Computation