COMS 4771 Lecture 3

1. Nearest neighbor classification.

Nearest neighbor classification

THE OPTIMAL CLASSIFIER

Let $(X, Y) \sim P$.
The classifier $f \colon \mathcal{X} \to \mathcal{Y}$ with the smallest prediction error

$$\operatorname{err}(f) = \Pr[f(X) \neq Y]$$

is the **Bayes classifier**

$$f^{\star}(x) = \operatorname*{arg\,max}_{y \in \mathcal{Y}} \Pr\Big[Y = y \,\Big|\, X = x\Big].$$

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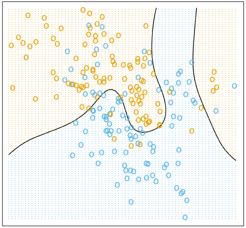
- **Last lecture**: use "generative" models to approximate $\Pr[Y = y | X = x]$.
- **This lecture**: directly approximate the **decision boundaries** of $f^\star$.

discriminative model



Text

Nearest neighbor (NN) classifier

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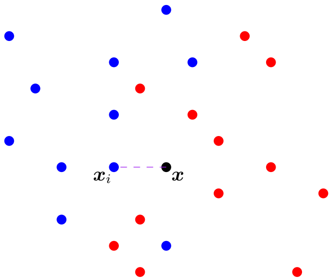
On input $\boldsymbol{x}$,

1. Let $\boldsymbol{x}_i$ be the point among $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$ that is closest to $\boldsymbol{x}$.
2. Return y_i.



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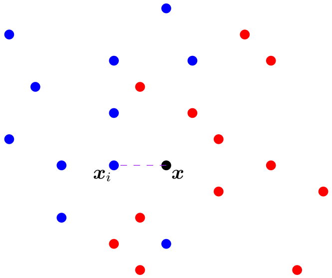

Question: how should we measure distance between points in $\mathcal{X}$?

A default choice of distance for data in $\mathbb{R}^d$:

$$\text{Euclidean } (\ell_2) \text{ distance}: \quad \|\boldsymbol{u} - \boldsymbol{v}\|_2 := \sqrt{\sum_{i=1}^{d} (u_i - v_i)^2}.$$

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But there are many other (and often better) options ...

Example: OCR with NN classifier

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- **Observation**: First mistake (correct label is '2') might've been avoided by looking at three nearest neighbors (whose labels are '8', '2', '2') . . .

test point three nearest neighbors

k-NEAREST NEIGHBORS CLASSIFIER

Given **training data** $(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_n, y_n) \in \mathcal{X} \times \mathcal{Y}$, construct $\hat{f}_k \colon \mathcal{X} \to \mathcal{Y}$ as follows:

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(Break ties in both steps arbitrarily.)

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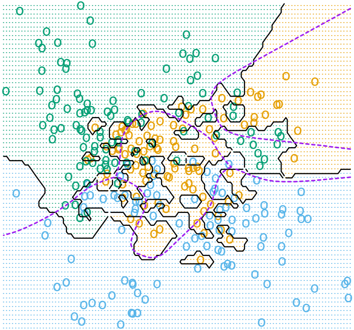
Example: OCR with k-NN classifier

k	1	3	5	7	9
$\mathrm{err}(\hat{f}_k, T)$	0.0309	0.0295	0.0312	0.0306	0.0341

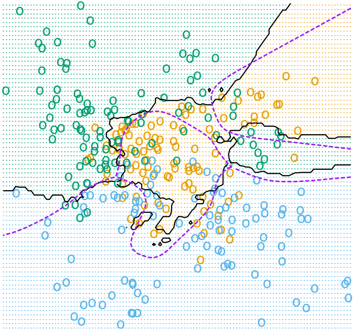
Effect of k

In general:

- Smaller $k \Rightarrow$ smaller training error. ($k = 1 \Rightarrow$ has zero training error.)
- Larger $k \Rightarrow$ predictions are more "stable" due to voting.



1-NN



15-NN

Purple dotted lines: Bayes classifier's decision boundaries.
Black solid lines: k-NN's decision boundaries.

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the difference is at k's value!!!

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hold one point out for test

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More on this later in the course.

Consistency of k-NN

Say a learning algorithm is **consistent** if

$$\lim_{n \to \infty} \mathbb{E}\Big[\text{error of learned classifier with training sample size } n\Big] \;=\; \mathrm{err}(f^{\star}).$$

Consistency of k-NN

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the best classifier!

$$\lim_{n\to\infty} \mathbb{E}\Big[\text{error of learned classifier with } \boxed{\text{training sample size } n}\Big] = \boxed{\operatorname{err}(f^\star).}$$

k-**NN is consistent** provided that $k := k_n$ is chosen as an increasing but sublinear function of n:

$$\lim_{n\to\infty} k_n = \infty, \quad \lim_{n\to\infty} \frac{k_n}{n} = 0$$

(some other mild conditions might also have to hold).

as the size of training sample grows up. the error of the learned classifier getting closer to err(f).

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1-**NN is not consistent unless** $\boxed{\mathrm{err}(f^\star) = 0,}$ although

$$\lim_{n\to\infty} \mathbb{E}\Big[\mathrm{err}(\hat{f}_1)\Big] \;\le\; 2\,\mathrm{err}(f^\star)\cdot\left(1 - \frac{K}{2(K-1)}\,\mathrm{err}(f^\star)\right).$$

Nearest neighbor search

- Naïve implementation of NN classifiers uses n distance computations to compute $\hat{f}_k(\boldsymbol{x})$ for any test point $\boldsymbol{x} \in \mathcal{X}$.

NEAREST NEIGHBOR SEARCH

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- **Alternatives**:
  1. Settle for an approximate nearest neighbor using *locality sensitive hash functions*.
  2. Store the n training data in a geometric data structure that permits fast NN queries.

Locality sensitive hash functions

(Informally:) A family $\mathcal{H}$ of hash functions from $\mathbb{R}^d$ to $\mathbb{Z}$ is a **locality-sensitive hash family** if

- For any points $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in \mathcal{X}$ with $\|\boldsymbol{a} - \boldsymbol{b}\|_2 \ll \|\boldsymbol{a} - \boldsymbol{c}\|_2$,

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It turns out there are such hash families!

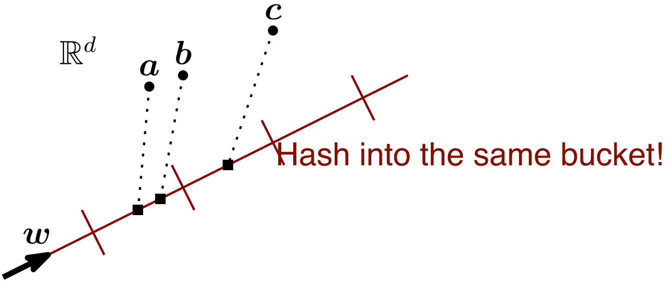
A locality sensitive hash family

A LSH family based on projections to one-dimensional subspaces

For $\boldsymbol{w} \in \mathbb{R}^d$ with $\|\boldsymbol{w}\|_2 = 1$, $r \in \{2^i : i \in \mathbb{Z}\}$, $s \in [0, r]$:

$$h_{\boldsymbol{w},r,s}(\boldsymbol{x}) := \left\lfloor \frac{\boldsymbol{w}^\top \boldsymbol{x} + s}{r} \right\rfloor .$$

- $\boldsymbol{w}$ determines the one-dimensional subspace,
- r determines a distance resolution, and
- s determines a shift of the bucket boundaries.



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Procedure:

- Select a hash function $h \in \mathcal{H}$ at random.
  (In practice, some parameters of the hash function, like r and s, may be tuned via hold-out or cross-validation.)
- Create pointer from buckets $j \in \mathbb{N}$ to points $\boldsymbol{x} \in S$ such that $h(\boldsymbol{x}) = j$.
- Given test point $\boldsymbol{x}$, search bucket $h(\boldsymbol{x})$ for nearest neighbor.
  (The bucket will generally contain far fewer than n points.)

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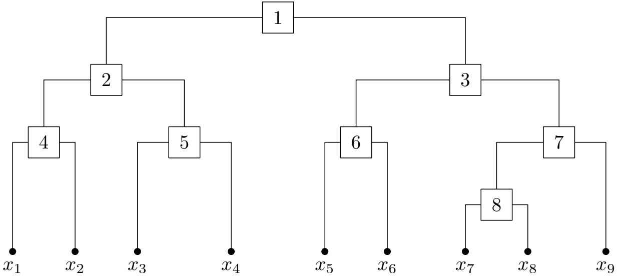
Do this with several hash functions from $\mathcal{H}$ to boost the chances that you find close neighbors.

Tree structures for one-dimensional data

A data structure for fast NN search in $\mathbb{R}^1$

Sort training data so that $x_1 \leq x_2 \leq \cdots \leq x_n$, then construct binary tree:



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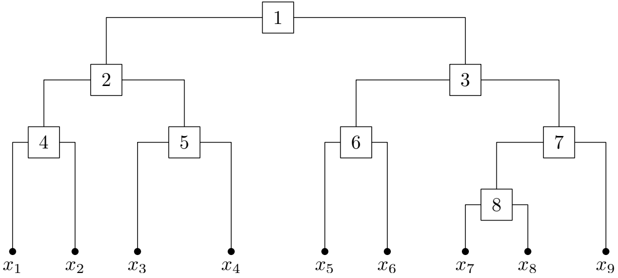

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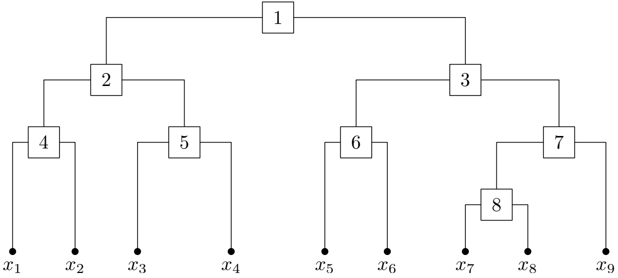

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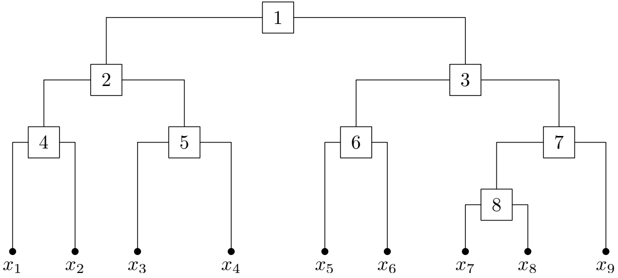

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If tree is (approximately) balanced, then $O(\log(n))$ time to find NN!

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Many options, but a popular one is the **K-D tree**.

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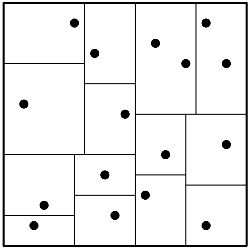
Construction procedure
Given points $S \subset \mathbb{R}^d$:

1. Pick a coordinate $j \in \{1, 2, \ldots, d\}$.
2. Let m be the median of $\{x_j : \boldsymbol{x} \in S\}$.
3. Split points into halves:

$$L := \{\boldsymbol{x} \in S : x_j < m\},$$
$$R := \{\boldsymbol{x} \in S : x_j \geq m\}.$$

4. Recurse on L and R.



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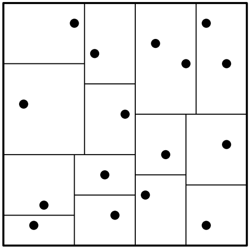

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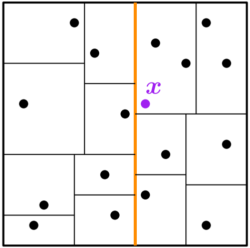

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Same $O(\log(n))$-time routing of a test point $\boldsymbol{x} \in \mathbb{R}^d$ is **overly optimistic**:
might not yield the NN!

Generic NN search procedure for binary space partition trees
Given a test point $\boldsymbol{x}$ and a tree node v (initially $v =$ root):

1. Pick most optimistic child L, recursively find NN of $\boldsymbol{x}$ in L (call it $\boldsymbol{x}_L$).
2. Let R be the other child. If

$$\|\boldsymbol{x} - \boldsymbol{x}_L\|_2 < \min_{\boldsymbol{x}' \in R} \|\boldsymbol{x} - \boldsymbol{x}'\|_2 \qquad (\star)$$

   then return $\boldsymbol{x}_L$.
3. Otherwise recursively find NN of $\boldsymbol{x}$ in R (call it $\boldsymbol{x}_R$);
   return the closer of $\boldsymbol{x}_L$ and $\boldsymbol{x}_R$.

Searching general tree structures

Generic NN search procedure for binary space partition trees
Given a test point $\boldsymbol{x}$ and a tree node v (initially $v =$ root):

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Note: can't always guarantee $O(\log(n))$ search time due to Step 3.

Question: How do you check if $(\star)$ is true?

- **Note**: it's correct (though computationally wasteful) to declare "false" in Step 2 even if $(\star)$ turns out to be true.

For K-D trees:
L and R are separated by a hyperplane $H = \left\{ \boldsymbol{z} \in \mathbb{R}^d : z_j = m \right\}$.

Using geometric properties

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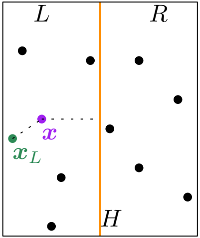

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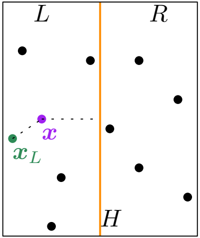

By geometry,

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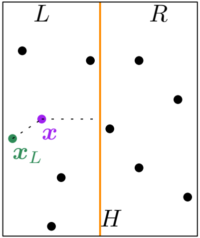

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A valid check: if $\|\boldsymbol{x} - \boldsymbol{x}_L\|_2 < |x_j - m|$, then

$$\|\boldsymbol{x} - \boldsymbol{x}_L\|_2 < \min_{\boldsymbol{x}' \in R} \|\boldsymbol{x} - \boldsymbol{x}'\|_2.$$

once there is point at left part

In this case, we can skip searching R and immediately return $\boldsymbol{x}_L$.

Efficient NN search?

For certain kinds of binary space partition trees (similar to K-D trees), enough pruning will happen so NN search typically completes in $O(2^d \log(n))$ time.

- Very fast in low dimensions.
- But can be slow in high dimensions.

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Question: Can we use trees to directly build good classifiers? (Next lecture.)