

# Geometric algorithms for classification and retrieval in high dimension

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# Retrieval and classification

$\mathcal{X}$  = space of data items

- images
- documents
- speech recordings
- medical records
- ...



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- **Statistical question: how much data is needed to find a good rule?**

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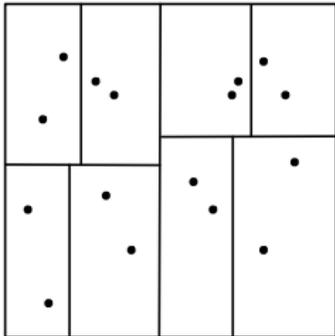
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One way to conceptualize and manage this:

- Actual **degrees of freedom** are often much smaller than the apparent dimension  $d$
- Formalize a notion of **intrinsic dimension**
- Develop methods for retrieval and classification whose complexity scales with the intrinsic dimension, not with  $d$

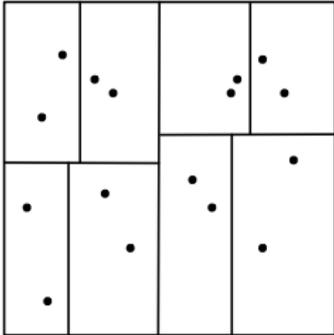
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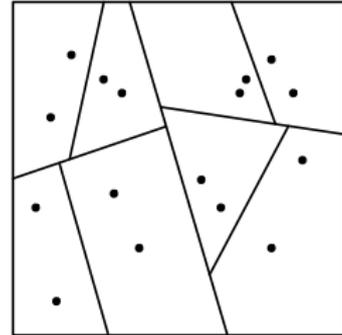


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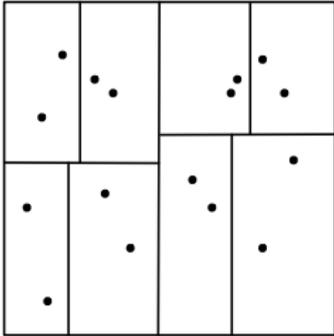


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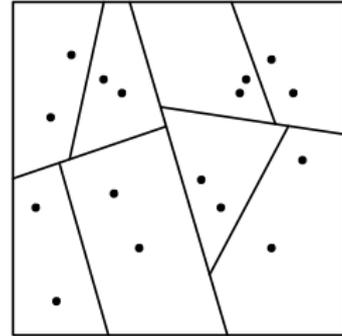


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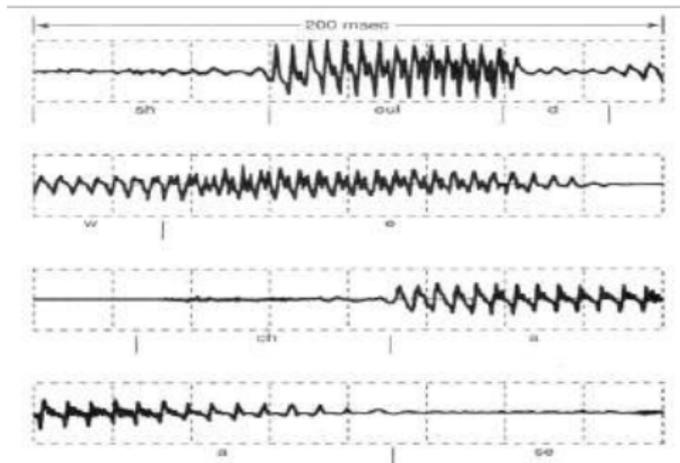
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The same method yields state-of-the-art nearest neighbor search.

# Outline

- ① Intrinsic dimension
- ② Classification
- ③ Retrieval

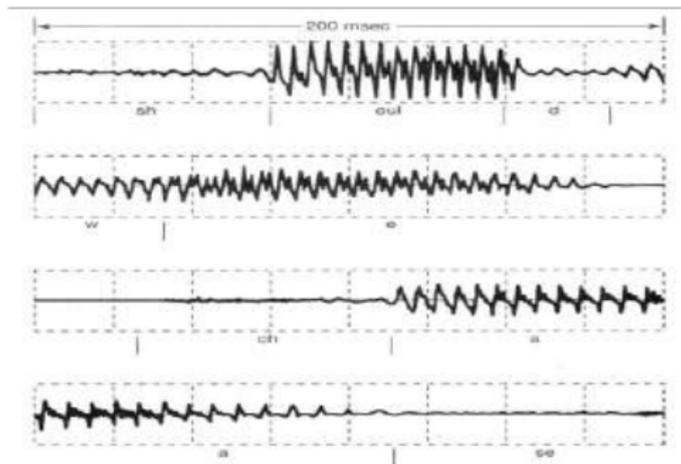
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But the speech has been produced by a physical system (vocal tract) with a fixed number of degrees of freedom.

# Low dimensional manifolds

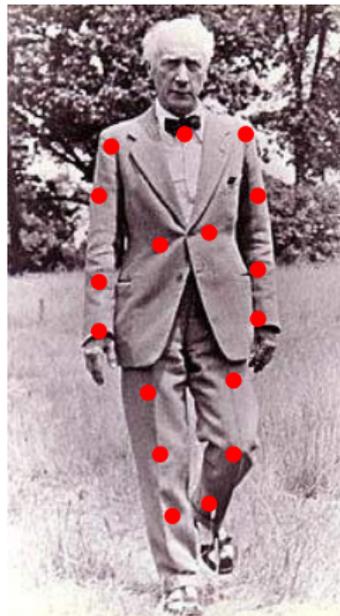
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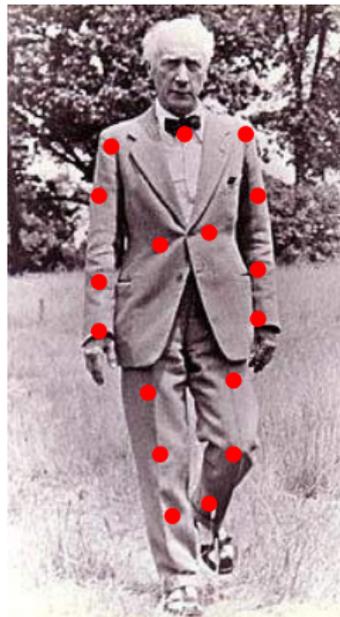


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Typical approach: approximately identify the manifold and use this to reduce dimension



# Another example of low intrinsic dimension

## Bag-of-words document model

It was the best of times, it was the worst of times, it was the age of wisdom, it was the age of foolishness, it was the epoch of belief, it was the epoch of incredulity, it was the season of Light, it was the season of Darkness, it was the spring of hope, it was the winter of despair, we had everything before us, we had nothing before us, we were all going direct to Heaven, we were all going direct the other way – in short, the period was so far like the present period, that some of its noisiest authorities insisted on its being received, for good or for evil, in the superlative degree of comparison only.



1	despair
2	evil
0	happiness
1	foolishness

- Fix a vocabulary of size  $d$
- A document is represented by a  $d$ -dimensional vector indicating, for each word, whether it appears (or how often)

Average number of nonzero entries in these vectors is  $d_o \ll d$ .

# Unifying notion of intrinsic dimension?

There are several widely-occurring types of low intrinsic dimension.

Can we:

- Find a broad notion of dimensionality that captures at least a few of these?
- Develop methods for classification and retrieval whose complexity depends only on this refined notion rather than on the superficial apparent dimension?

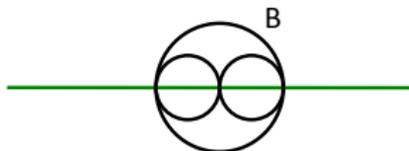
# Doubling dimension

Set  $S \subset \mathbb{R}^d$  has *doubling dimension*  $d_0$  if for any (Euclidean) ball  $B$ , the subset  $S \cap B$  can be covered by  $2^{d_0}$  balls of half the radius [Assouad, Gupta-Krauthgamer-Lee].

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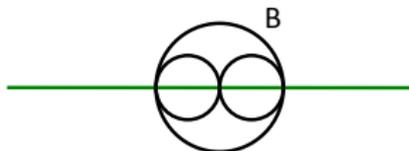
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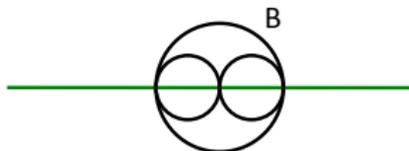


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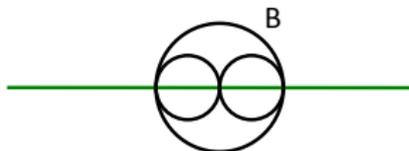


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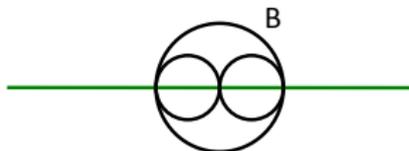


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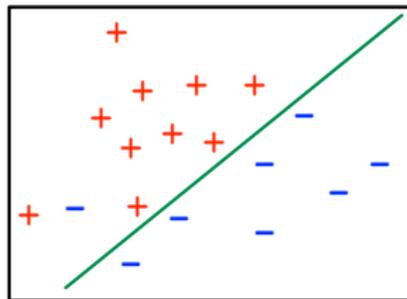
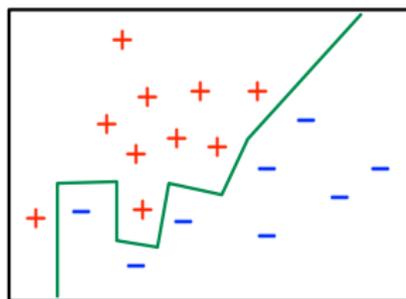
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- 5 If  $S$  has doubling dimension  $d_o$ , then so does any subset of  $S$ .

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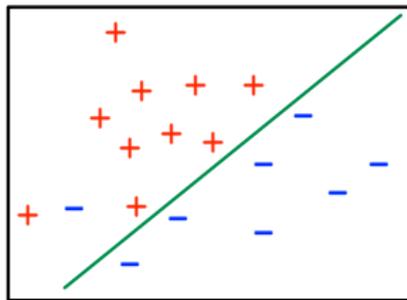
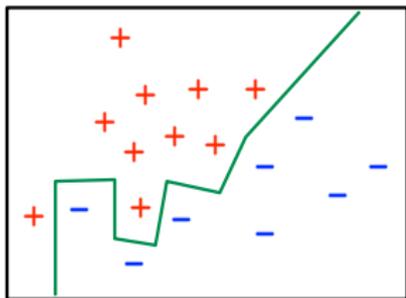
# Nonparametric classification

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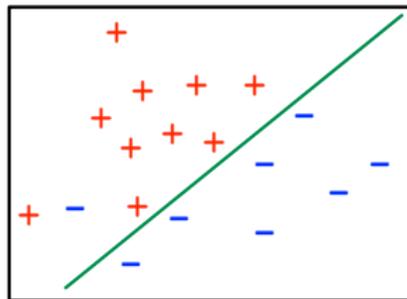
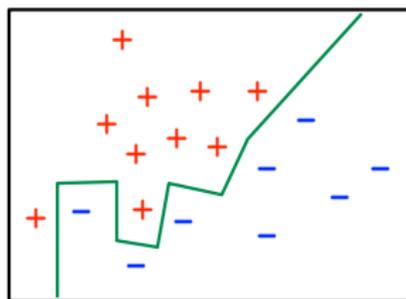
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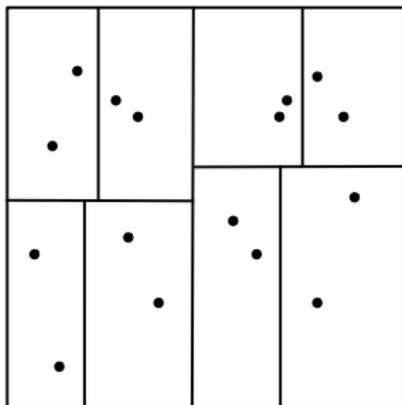
But they suffer a severe curse of dimension.

Consider random pair  $(X, Y)$ , where  $X \in \mathbb{R}^d$  and  $Y \in \{0, 1\}$  is a label.

- Want to infer  $f(x) = \mathbb{E}[Y|X = x]$ .
- Let  $f_n$  be an estimator based on  $n$  data points. It is common to judge it by its squared loss  $\mathbb{E}(f_n(X) - f(X))^2$ .
- Stone 1982: Loss  $\geq n^{-2p/(2p+d)}$ , where  $p$  captures smoothness of  $f$ .

# Spatial partitioning for nonparametric estimation

e.g. the  $k$ -d tree:



To split a cell with points  $S$ :

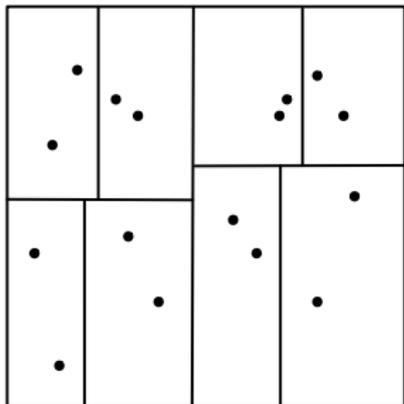
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These estimators are consistent if, as  $n \rightarrow \infty$ ,

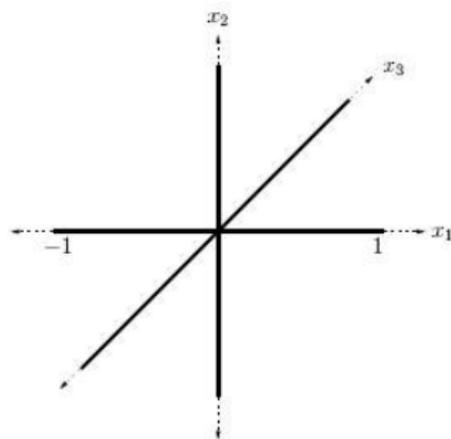
- ① the diameter of the leaf cells goes to zero, and
- ② the number of samples in each leaf goes to infinity.

Rate of convergence depends on relative speed of these two effects.

## $k$ -d trees are not adaptive to intrinsic dimension

As one moves down a  $k$ -d tree, how rapidly does the cell diameter shrink?

Consider the data set  $S = \cup_{i=1}^d \{te_i : -1 \leq t \leq 1\}$ .

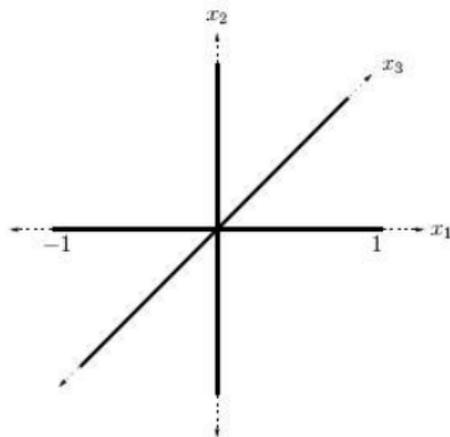


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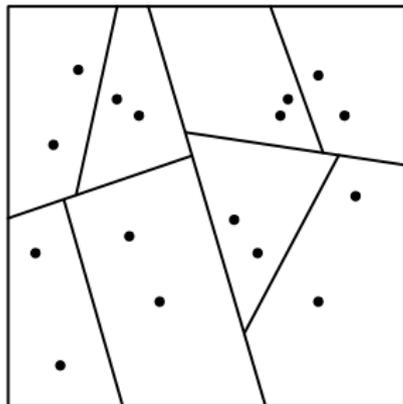


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Yet  $S$  has doubling dimension just  $d_o = 1 + \log d$ .

# Random projection trees

A randomized variant of the  $k$ -d tree

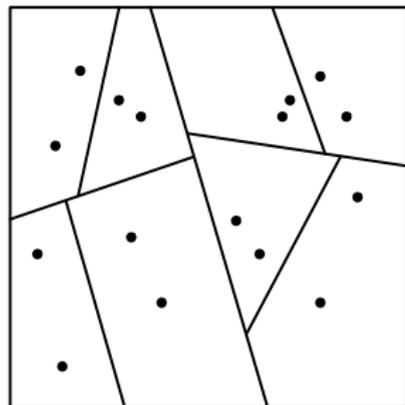


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**Theorem:** Pick any cell  $C$  in the tree. With probability at least  $1/2$ , every descendant cell  $C'$  which is more than  $d_0 \log d_0$  levels below  $C$  has  $\text{diam}(C') \leq \text{diam}(C)/2$ .

Here,  $\text{diam}(C)$  is the maximum interpoint distance of data in cell  $C$ .

# Properties of random projection

Pick a random vector  $U$  from the unit sphere in  $\mathbb{R}^d$ . Mapping:

$$\Pi(x) = U \cdot x$$

Almost the same: pick  $U \sim N(0, (1/d)I_d)$ .

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Pick any  $x$ . As  $U$  varies, projection  $\Pi(x)$  has a Gaussian distribution with mean zero and variance  $\|x\|^2/d$ .

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## 2 To extend to sets of points, generally need to take a union bound.

## 3 Median of projected points.

If  $S \subset B(x_o, \Delta)$ , then

$$|\text{median}(\Pi(S)) - \Pi(x_o)| \leq O\left(\frac{\Delta}{\sqrt{d}}\right).$$

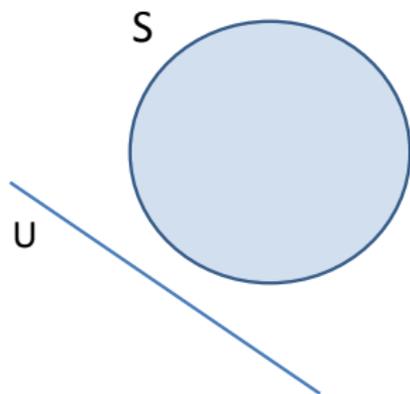
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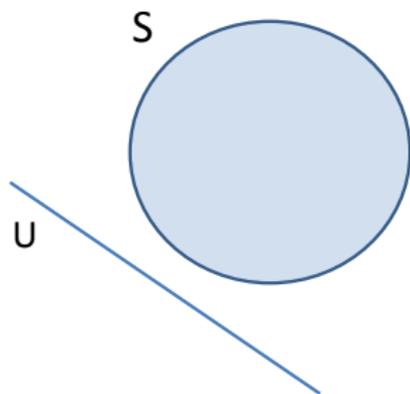
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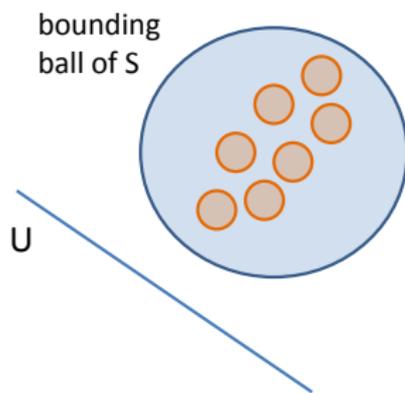
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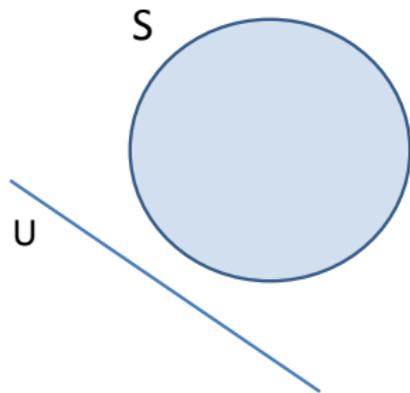
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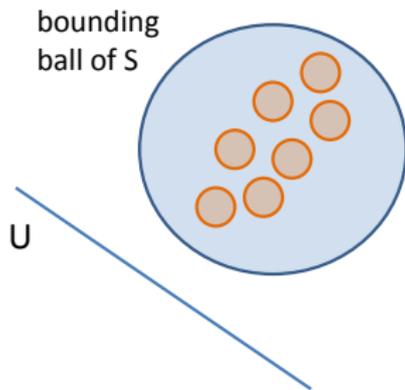
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In the latter case,  $\text{diam}(\Pi(S))$  is at most about  $\text{diam}(S) \cdot \sqrt{d_o/d}$ .

# Random projection and diameter

**Theorem:** If  $S \subset \mathbb{R}^d$  has doubling dimension  $d_o$ , then with probability at least  $1 - \delta$ , the diameter of  $\Pi(S)$  is at most

$$4 \cdot \frac{\text{diam}(S)}{\sqrt{d}} \cdot \sqrt{2 \left( d_o + \ln \frac{2}{\delta} \right)}.$$

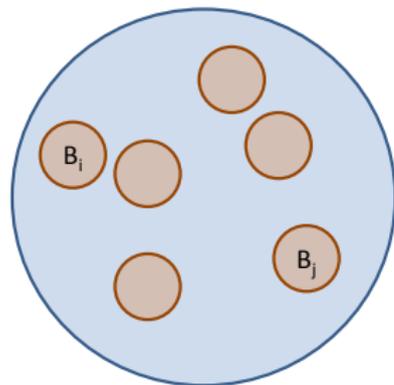
Proof: We'll prove a weaker version with factor  $\sqrt{(d_o \log d)/d}$ .

- 1 WLOG  $S$  has diameter 1 and  $S \subset B(0, 1)$ .
- 2 Cover  $S$  by balls of radius  $\sqrt{d_o/d}$ . At most  $(d/d_o)^{d_o/2}$  balls are needed.
- 3 Pick any of these balls. With probability  $1 - (1/d)^{d_o}$ , its center is projected to a point within distance  $\sqrt{(d_o \log d)/d}$  of the origin; and thus the entire projected ball lies in an interval within distance  $\sqrt{(d_o \log d)/d} + \sqrt{d_o/d}$  of the origin.
- 4 Take a union bound over all the balls.

# Proof outline for RP trees

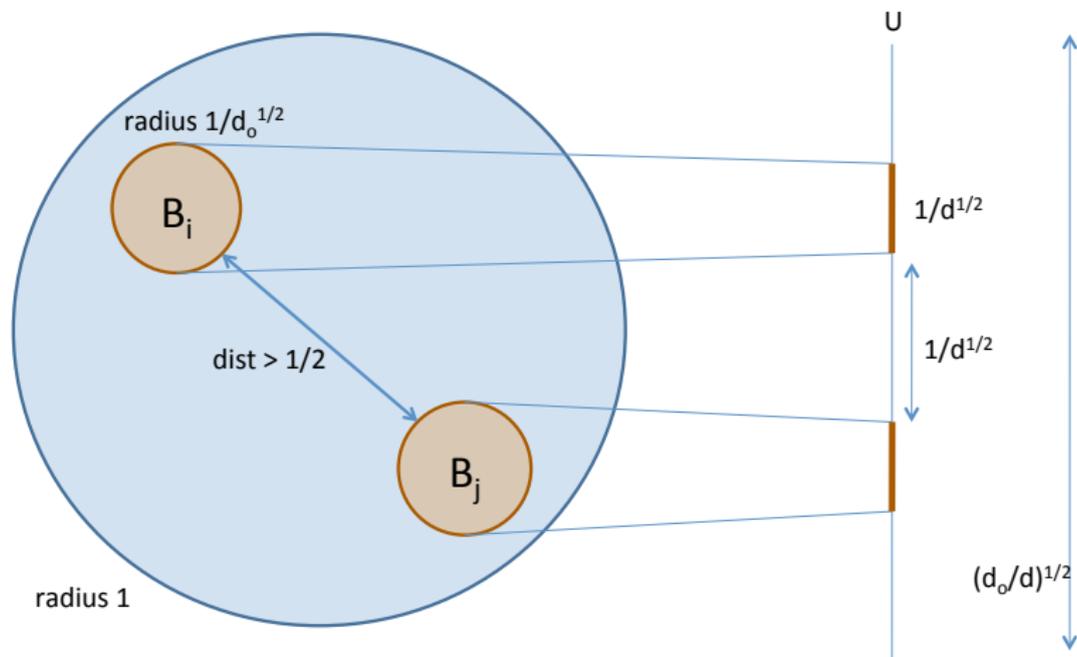
Suppose  $S \subset \mathbb{R}^d$  has doubling dimension  $d_o$  and lies in a ball of radius 1. We need to show that if an RP tree is built on  $S$ , then with constant probability, every cell  $O(d_o \log d_o)$  levels below is contained in ball of radius  $1/2$ .

Current cell (radius  $\leq 1$ ):



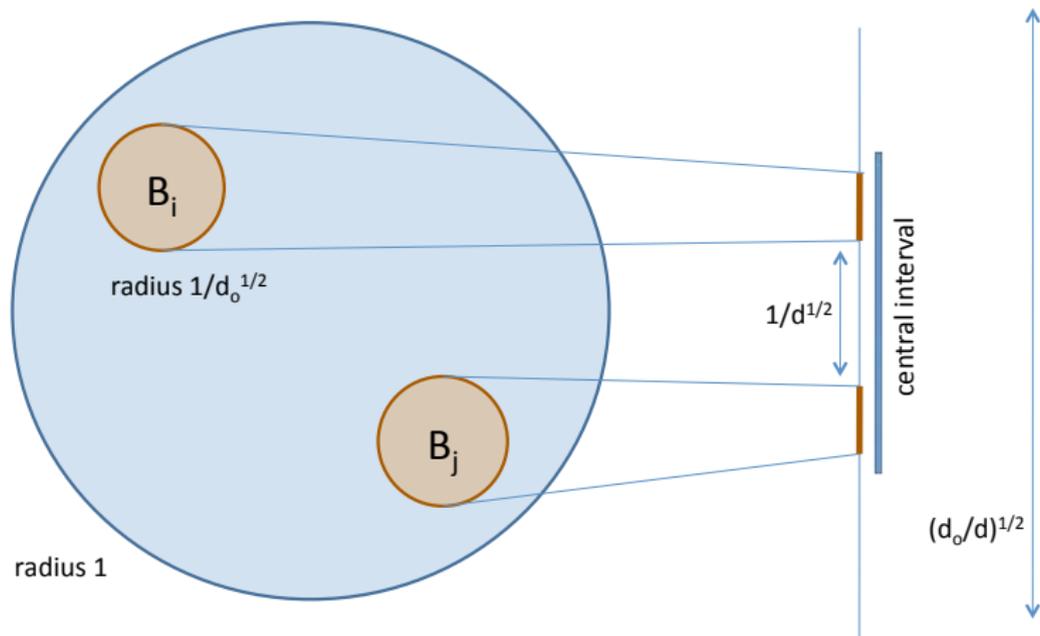
- 1 Cover  $S$  by  $d_o^{d_o/2}$  balls  $B_i$  of radius  $1/\sqrt{d_o}$ .
- 2 Consider any pair of balls  $B_i, B_j$  that are distance  $> 1/2 - 1/\sqrt{d_o}$  apart. We'll see that a single random split has constant probability of cleanly separating them.
- 3 There are at most  $d_o^{d_o}$  such pairs, so after  $O(d_o \log d_o)$  splits, with constant probability every faraway pair of balls will be separated. Thus all cells at that level will have radius  $\leq 1/2$ .

# The big picture



Recall that random projection shrinks diameter by  $\sqrt{d_o/d}$  and individual vectors by  $1/\sqrt{d}$ .

# The big picture



Most projected points (and the median) fall in a central interval of size  $1/\sqrt{d}$ .

# Outline

- ① Intrinsic dimension
- ② Classification
- ③ Retrieval

# Nearest neighbor search

Given a data set of  $n$  points in  $\mathbb{R}^d$ , build a data structure for efficiently answering subsequent nearest neighbor queries  $q$ .

- Data structure should take space  $O(n)$
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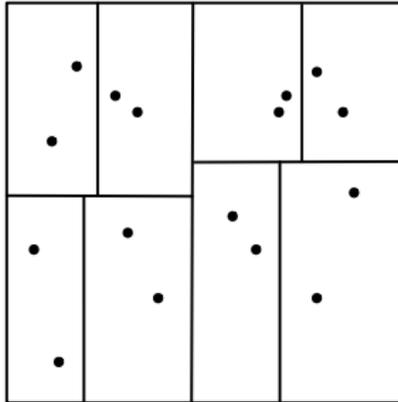
- Data structure should take space  $O(n)$
- Query time should be  $o(n)$

Unproven but common conjecture: for data structures of linear size, query time will be exponential in  $d$ .

Bad case: for any  $0 < \epsilon < 1$ ,

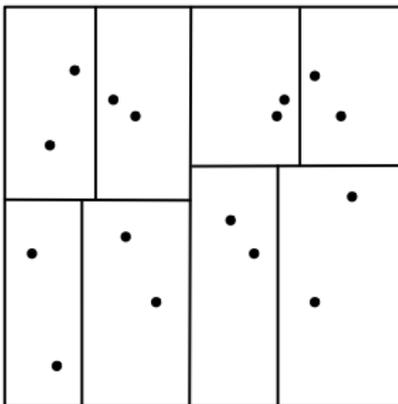
- Pick  $2^{O(\epsilon^2 d)}$  points uniformly from the unit sphere in  $\mathbb{R}^d$
- With high probability, all interpoint distances are  $(1 \pm \epsilon)\sqrt{2}$

## The $k$ -d tree, again



*Defeatist search:* return NN in query's leaf node (may not be true NN).

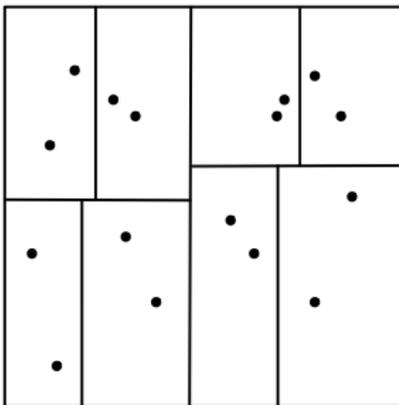
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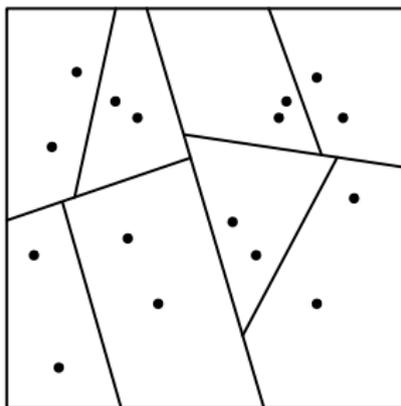
Curse of dimension: chance of returning the true NN tends to drop dramatically with dimension.

Some variants:

- Better split direction: PCA tree
- Overlapping cells (Manewongvatana and Mount; Liu et al)
- Random split directions (Liu, Moore, Gray; Muja, Lowe)

# Random projection trees

In each cell of the tree, pick split direction uniformly at random from the unit sphere in  $\mathbb{R}^d$



*Perturbed split:* after projection, pick  $\beta \in_R [1/4, 3/4]$  and split at the  $\beta$ -fractile point.

# Failure probability

Pick any data set  $x_1, \dots, x_n$  and any query  $q$ .

- Let  $x_{(1)}, \dots, x_{(n)}$  be the ordering of data by distance from  $q$ .
- Probability of not returning the NN depends directly on

$$\Phi(q, \{x_1, \dots, x_n\}) = \frac{1}{n} \sum_{i=2}^n \frac{\|q - x_{(1)}\|}{\|q - x_{(i)}\|}$$

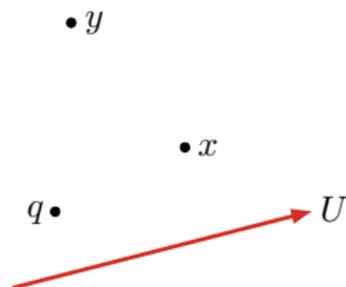
(This probability is over the randomization in tree construction.)

## Random projection of three points

Let  $q \in \mathbb{R}^d$  be the query,  $x$  its nearest neighbor and  $y$  some other point:

$$\|q - x\| < \|q - y\|.$$

Bad event: when the data is projected onto a random direction  $U$ , point  $y$  falls between  $q$  and  $x$ .

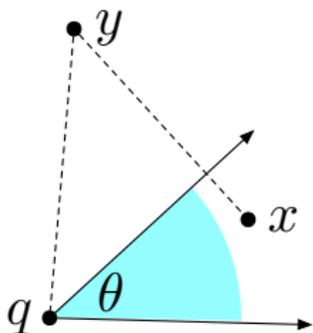


What is the probability of this?

This is a 2-d problem, in the plane defined by  $q, x, y$ .

- Only care about projection of  $U$  on this plane
- Projection of  $U$  is a random direction in this plane

## Random projection of three points



Probability that  $U$  falls in this bad region is  $\theta/2\pi$ .

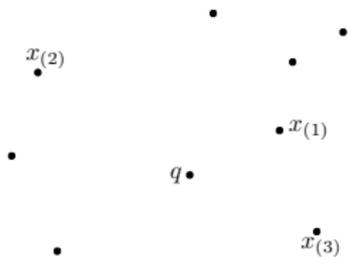
### Lemma

*Pick any three points  $q, x, y \in \mathbb{R}^d$  such that  $\|q - x\| < \|q - y\|$ . Pick  $U$  uniformly at random from the unit sphere  $S^{d-1}$  in  $\mathbb{R}^d$ . Then*

$$\Pr(y \cdot U \text{ falls between } q \cdot U \text{ and } x \cdot U) \leq \frac{1}{2} \frac{\|q - x\|}{\|q - y\|}.$$

(Tight within a constant unless the points are almost-collinear)

# Random projection of a set of points



## Lemma

Pick any  $x_1, \dots, x_n$  and any query  $q$ . Pick  $U \in_R S^{d-1}$  and project all points onto direction  $U$ . Then the expected fraction of the projected  $x_i$  that fall between  $q$  and  $x_{(1)}$  is at most

$$\frac{1}{2n} \sum_{i=2}^n \frac{\|q - x_{(1)}\|}{\|q - x_{(i)}\|} = \frac{1}{2} \Phi$$

**Proof:** Probability that  $x_{(i)}$  falls between  $q$  and  $x_{(1)}$  is at most  $\frac{1}{2} \frac{\|q - x_{(1)}\|}{\|q - x_{(i)}\|}$ . Now use linearity of expectation.

**Bad event:** this fraction is  $\Omega(1)$ . Happens with probability  $O(\Phi)$ .

# Failure probability of NN search

Fix any data points  $x_1, \dots, x_n$  and query  $q$ . For  $m \leq n$ , define

$$\Phi_m(q, \{x_1, \dots, x_n\}) = \frac{1}{m} \sum_{i=2}^m \frac{\|q - x_{(1)}\|}{\|q - x_{(i)}\|}$$

## Theorem

*Suppose an RP tree is built for data set  $x_1, \dots, x_n$  with leaf nodes of size  $n_o$ . For any query  $q$ , the probability that the NN query does not return  $x_{(1)}$  is at most*

$$\sum_{i=0}^{\ell} \Phi_{(3/4)^i n}(q, \{x_1, \dots, x_n\})$$

*where  $\ell = \log_{4/3}(n/n_o)$  is the tree's depth.*

# NN search in spaces of bounded doubling dimension

Need to bound

$$\Phi_m(q, \{x_1, \dots, x_n\}) = \frac{1}{m} \sum_{i=2}^m \frac{\|q - x_{(1)}\|}{\|q - x_{(i)}\|}$$

Suppose:

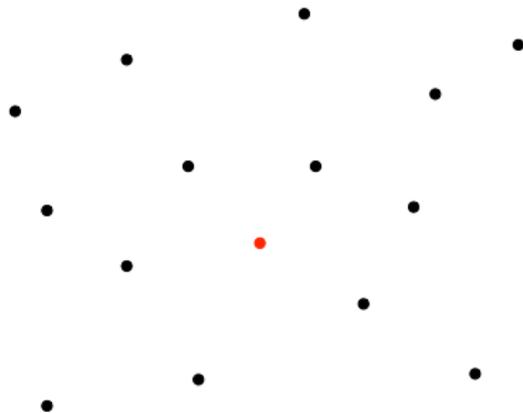
- Pick any  $n + 1$  points in  $\mathbb{R}^d$  with doubling dimension  $d_o$
- Randomly pick one of them as  $q$ ; the rest are  $x_1, \dots, x_n$

Then  $\mathbb{E}\Phi_m \leq 1/m^{1/d_o}$ .

For constant failure probability, use tree with leaf size  $n_o = O(d_o^{d_o})$ , and query time  $O(n_o + \log n)$ .

## How does doubling dimension help?

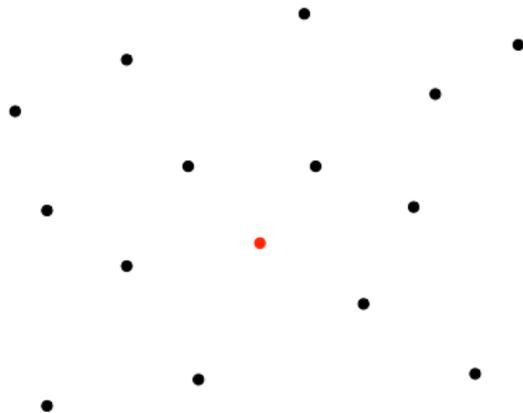
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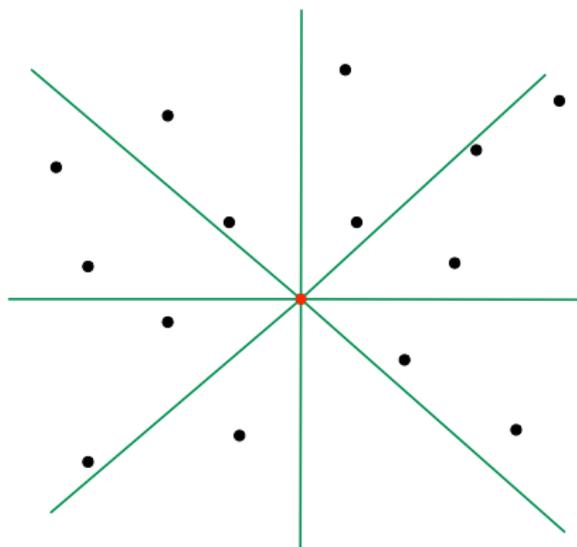
At most  $c^d$ , for some constant  $c$  [Stone].



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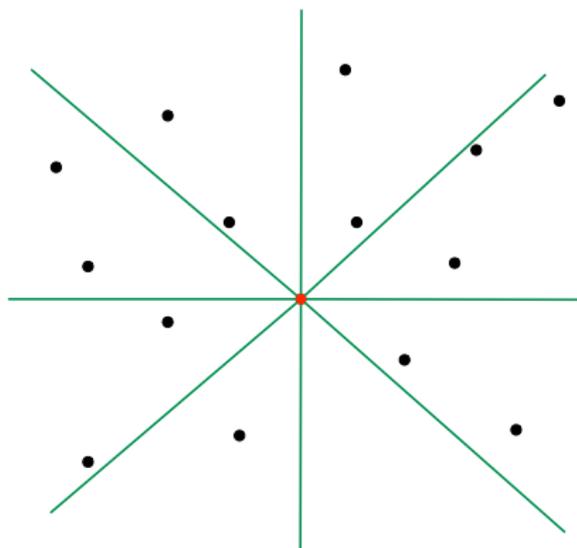
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Can (almost) replace  $d$  by the doubling dimension [Clarkson].

# Randomized forests

To exploit randomization in the data structure:

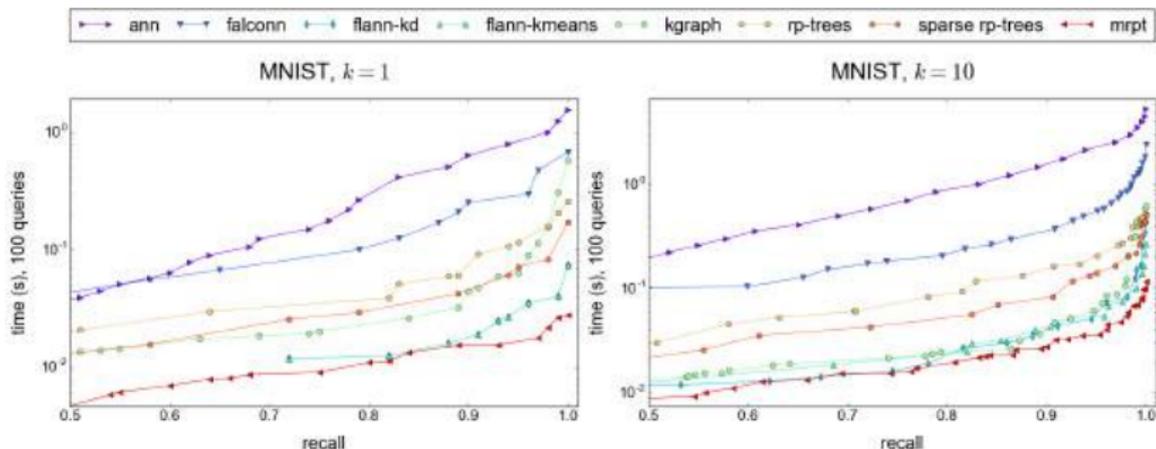
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Experiments by Roos et al:



# Open problems

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Simple randomized partition trees for metric spaces?
- ② More general notions of intrinsic dimension.  
Get closer to underlying “degrees of freedom” of input space?