AIMS-CDT Michaelmas 2019

# Discriminative Learning and Big Data

## Approximate Nearest Neighbours

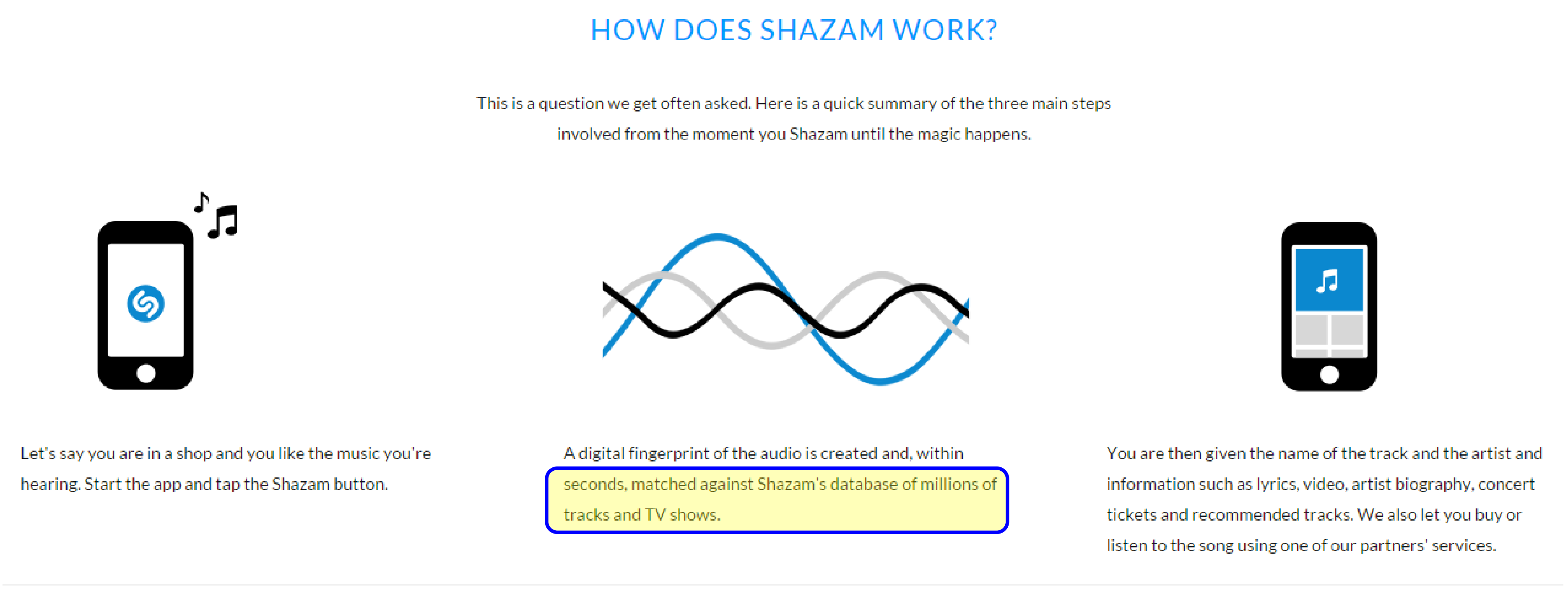
Relja Arandjelović

DeepMind
www.relja.info

# NN Applications: What is this?

Search for the query descriptor in a large database

Copy the meta-data of the nearest neighbour



HOW DOES SHAZAM WORK?

This is a question we get often asked. Here is a quick summary of the three main steps involved from the moment you Shazam until the magic happens.

Let's say you are in a shop and you like the music you're hearing. Start the app and tap the Shazam button.

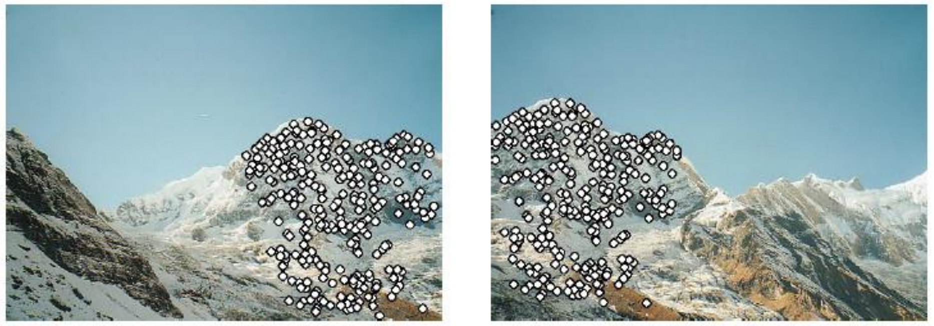
A digital fingerprint of the audio is created and, within seconds, matched against Shazam's database of millions of tracks and TV shows.

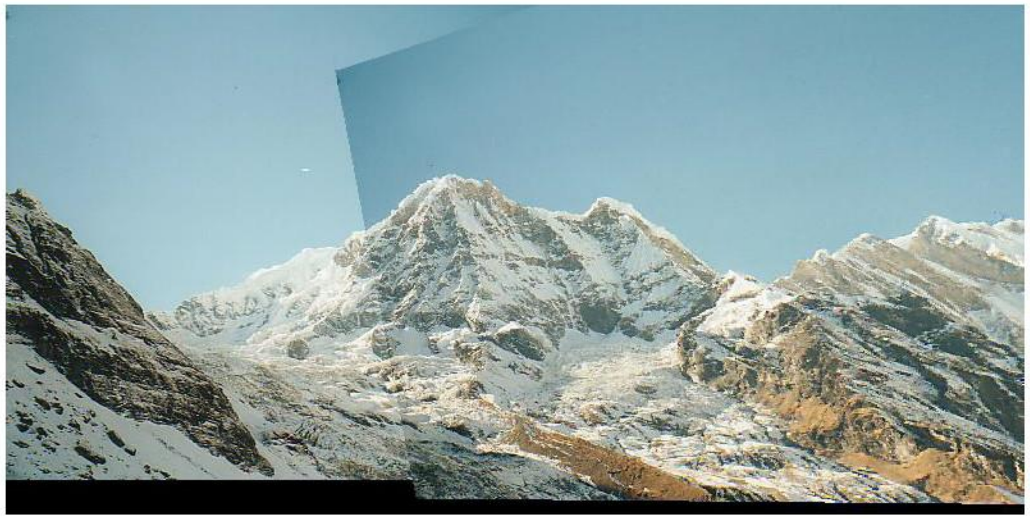
You are then given the name of the track and the artist and information such as lyrics, video, artist biography, concert tickets and recommended tracks. We also let you buy or listen to the song using one of our partners' services.

From www.shazam.com

## NN Applications: Automatic panorama creation

Match local patches, estimate the geometric transformation


(c) SIFT matches 1 (d) SIFT matches 2

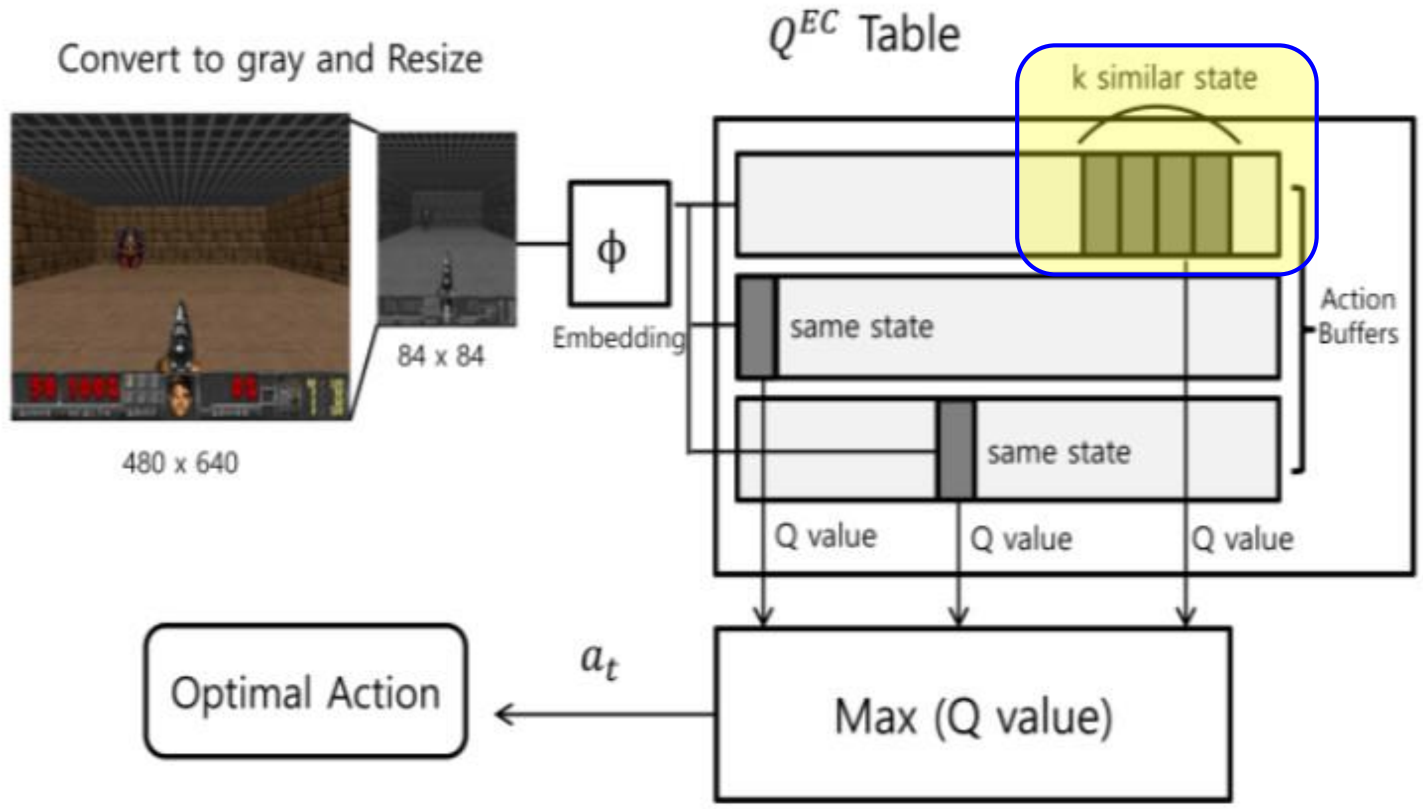

(e) Images aligned according to a homography

From Brown & Lowe “Automatic Panoramic Image Stitching using Invariant Features”

# NN Applications: Reinforcement Learning

Act in the environment by consulting past memories

Search memories using the current state

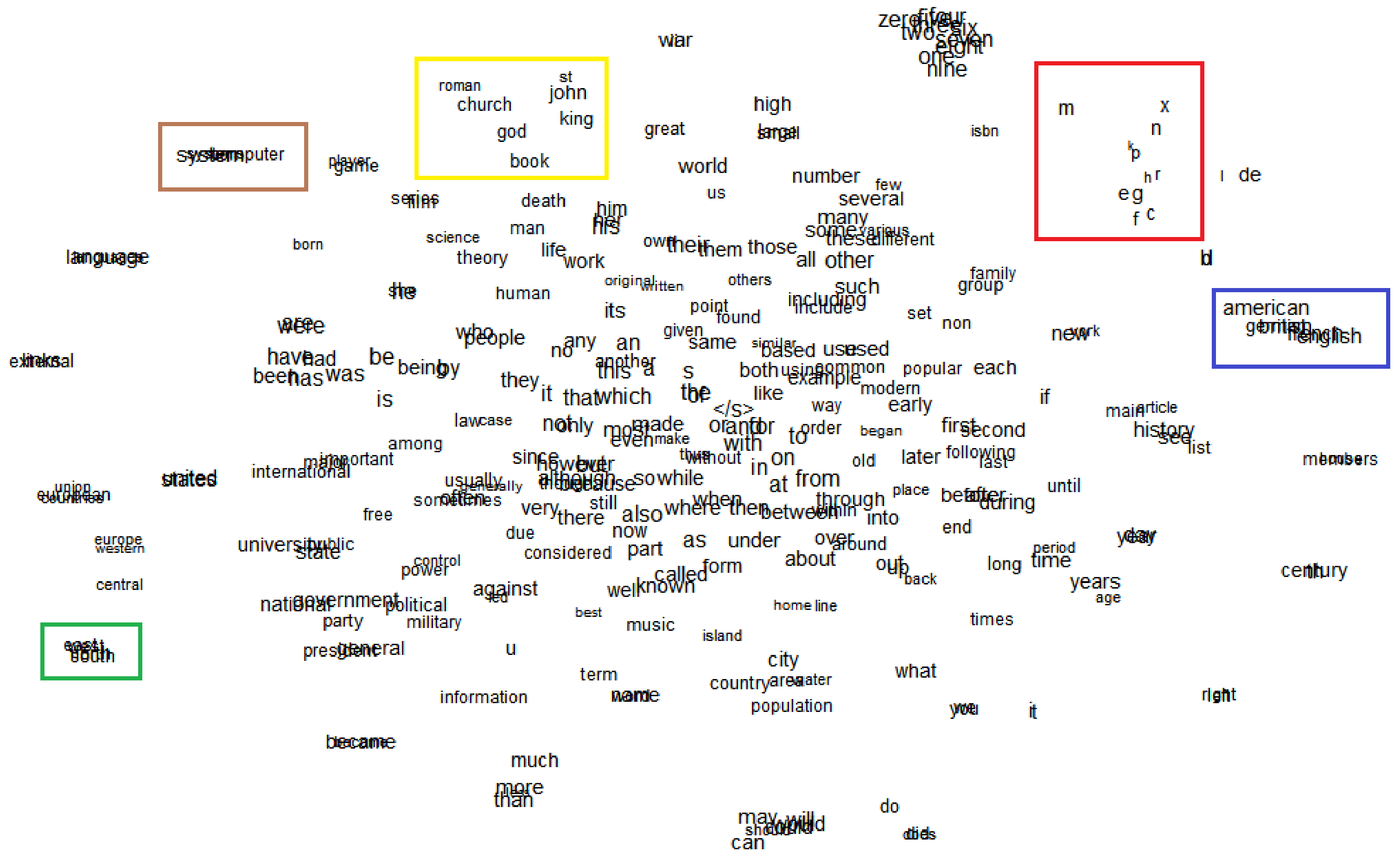


From Min & Kim “Learning to Play Visual Doom using Model-Free Episodic Control”

# NN Applications: Data Visualization (t-SNE)

Compute nearest neighbours for all points

Flatten the high dimensional data preserving the neighbourhood structure



Taken from https://theconceptcenter.com/simple-research-study-similarity-between-two-words/

## NN Applications: Other

- k-NN classification and regression
- Clustering
- Hard negative mining
- Semi-supervised learning

…

## Efficient implementations

Cost O(nd) but many optimization tricks

- Scalar product instead of distance if possible
- Special CPU instructions (SIMD in SSE)
- Pipelining / loop expansion
- Multiple queries: clever use of cache

For best performance use standard libraries

- Lower-level: BLAS
- Higher-level: Vectorized MATLAB, numpy, ..
- Good free libraries:
    - yael_nn ( http://yael.gforge.inria.fr/ )
    - FAISS (https://github.com/facebookresearch/faiss )

## The cost of (efficient) exact matching

But what about the actual timings ? With an efficient implementation!

Finding the 10-NN of 1000 distinct queries in 1 million vectors

- Assuming 128-D Euclidean descriptors
- i.e., 1 billion distances, computed on a 8-core machine

**How much time?**

Slide: Hervé Jégou

## How to speed up?

Dimensionality reduction?

- Reasonable first step, but typically insufficient

Use GPU?

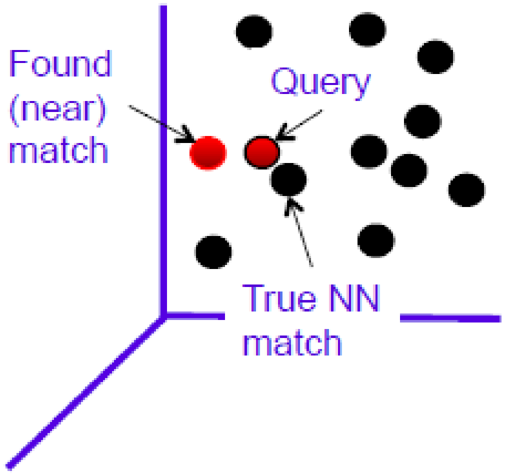
- Adds lots of complexity
- Insufficient memory
- Overhead for memory copying between CPU & GPU

Buy more machines?

- Costs money to buy, maintain, ..
- Adds lots of complexity
- For real-time systems: communication overhead
- Still often insufficient, e.g. if all pairwise distances are needed (e.g. building a neighbourhood graph, clustering, ..)

# Finding *approximate* nearest neighbour vectors

- Approximate method is not guaranteed to find the nearest neighbour.
- Can be much faster, but at the cost of missing some nearest matches



128D descriptor space

## Approximate Nearest Neighbours (ANN)

Is finding only approximate nearest neighbours acceptable?

- Often there is no choice
  - Use ANN or not = have Google or not
- Often it is good enough
  - What is this?

?

Big Ben

## Approximate Nearest Neighbours (ANN)

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Big Ben

## Approximate Nearest Neighbours (ANN)

Is finding only approximate nearest neighbours acceptable?

- Often there is no choice
  - Use ANN or not = have Google or not
- Often it is good enough
  - What is this?
  - Geometric matching: Only need sufficient number of matches
  - Data visualization: Rough nearest neighbours are fine

## Approximate Nearest Neighbours (ANN)

Three (contradictory) performance criteria for ANN schemes

- Search quality
  - Retrieved vectors are actual nearest neighbors
- Speed
- Memory footprint
  - Representation must fit into memory, disk is too slow

## Approximate Nearest Neighbours (ANN): Methods

Broad division

1. Approximate the vectors => do faster distance computations
   - Brute-force search, visit all points: O(n)

2. Approximate the search => do fewer distance computations
   - Do not visit all points

Can (and should) mix and match: approximate both, rerank (1.) with original vectors, etc

## Approximate Nearest Neighbours (ANN): Methods

Broad division

1. **Approximate the vectors => do faster distance computations**
   - Brute-force search, visit all points: O(n)

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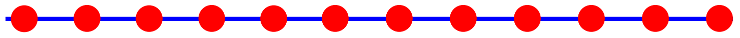
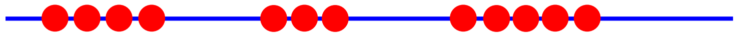
   - Do not visit all points

## ANN via approximating vectors

- Objectives
  - Approximate vectors as well as possible
  - Make the distance computation fast
  - Effectively: quantization, compression

- Do we need all 32 bits in a float?
  - Sometimes yes: 
  - Sometimes no: 
  - The limit is entropy (amount of information)
  - Betting on exploiting underlying structure
    - Otherwise there is no hope
    - zip, jpeg, mpeg, .. do not always compress!

## ANN via approximating vectors: Methods

- Hashing
  - LSH

- Vector Quantization
  - Product Quantization

## Hashing (for approximating vectors)

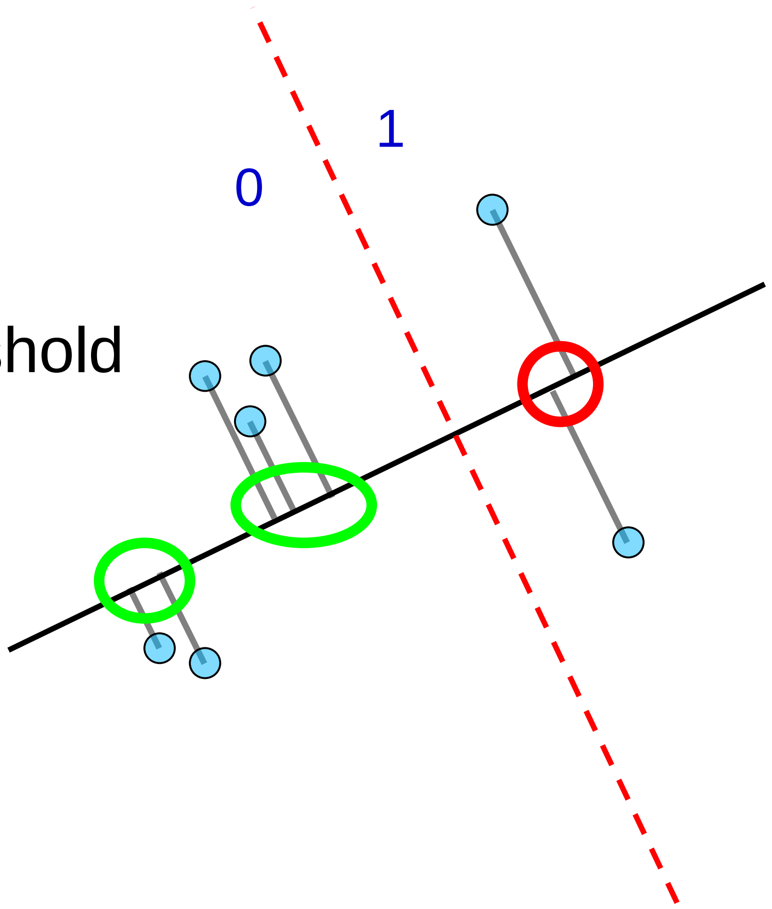
- Key idea
  - Convert the input real-valued vector into a binary vector
  - Compare binary vectors using Hamming distance

```
x: 00100101
y: 10100011
   --------------
   10000110 => Hamming distance = sum(1's) = 3
```

- Pros
  - Memory savings: d*32 bits -> b bits
  - Extremely fast distance computation: *popcnt(xor(x,y))*
- Cons
  - Can be hard to design a good hashing function

# Locality Sensitive Hashing (LSH)

- Choose a random projection
- Project points, pick a random threshold
- Points close in the original space remain close under the projection
- Unfortunately, converse not true



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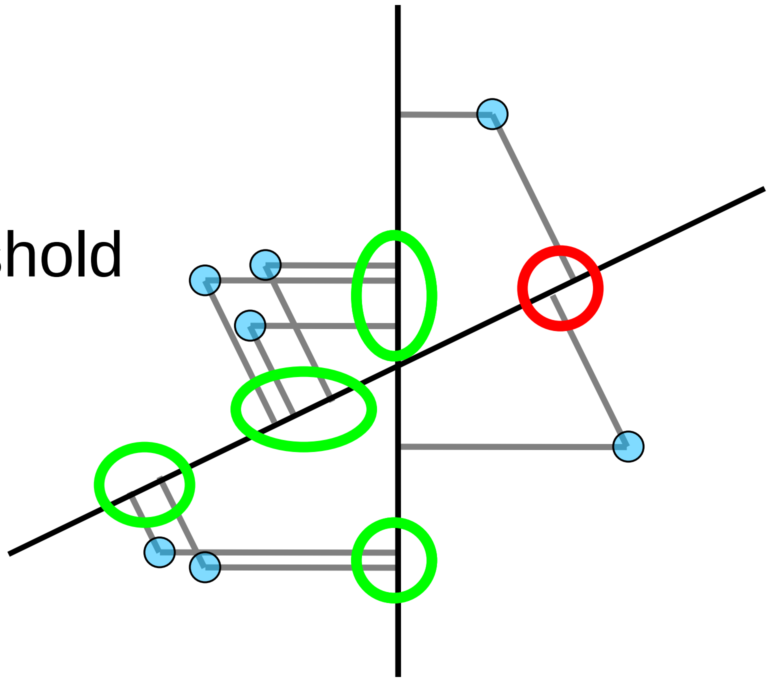
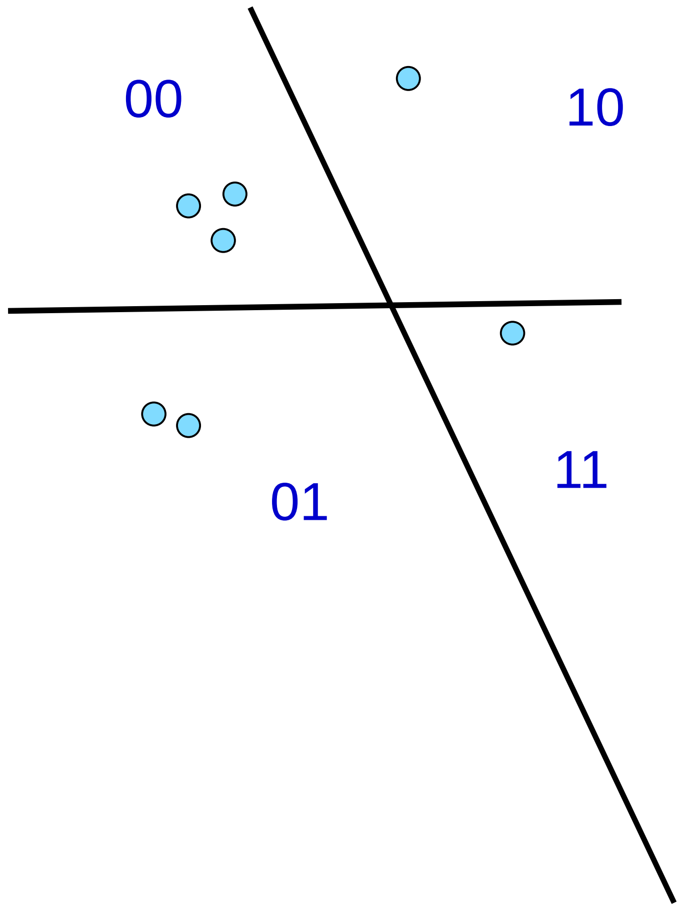


- Solution: use multiple quantized projections which define a high-dimensional “grid”

# Locality Sensitive Hashing (LSH): Discussion

- Pros
  - Very simple to implement
  - Very fast
  - Good for embedded systems



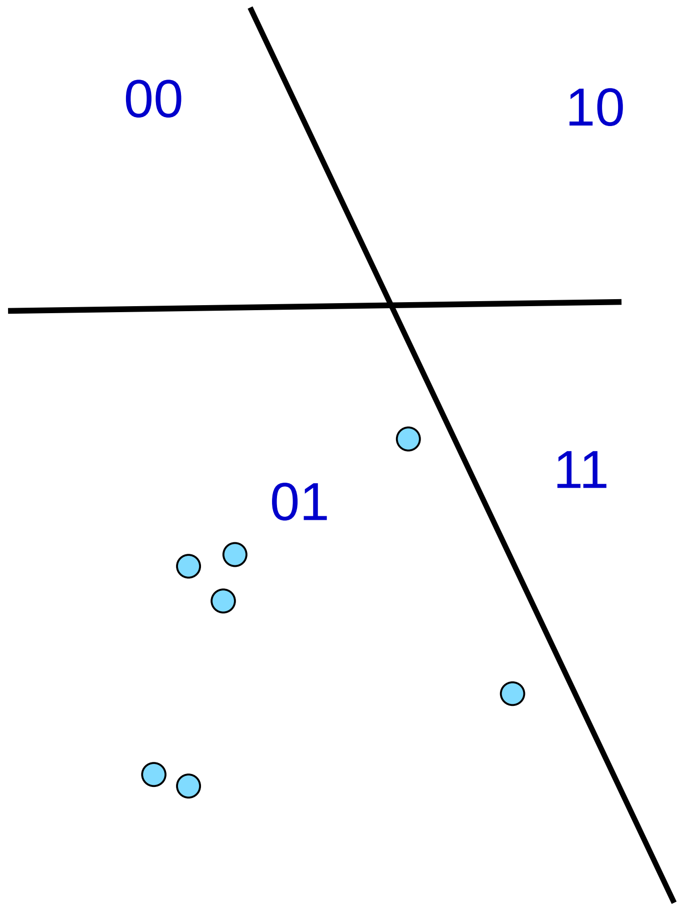
## Locality Sensitive Hashing (LSH): Discussion

- Pros
  - Very simple to implement
  - Very fast
  - Good for embedded systems

*“Choose a random projection”* ??

*“Betting on exploiting underlying structure”*

- Cons
  - Data-agnostic = blind
  - Need a large number of projections (=bits=a lot of memory) for decent performance compared to alternatives
- The way to go: data-dependent hashing
  - Iterative Quantization [Gong & Lazebnik 2011], Spectral Hashing [Weiss et al. 2009], …



## ANN via approximating vectors: Methods

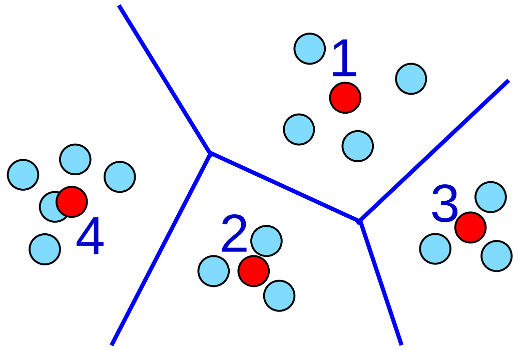
- Hashing
  - LSH
- **Vector Quantization**
  - Product Quantization

## Vector Quantization

Hard to design the conversion real vector -> binary vector, such that distances in binarized space are meaningful

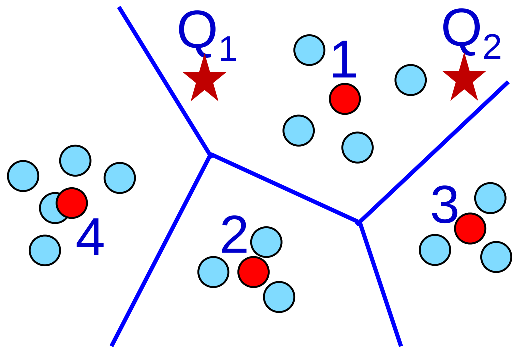
Idea

- Scrap using Hamming distance to compare codes
- Codebook (vocabulary) of *k* vectors (codewords)
- Code for vector = ID of the nearest codeword ($\log_2 k$-bits)
- Learn codebook to optimize for quantization quality



## Vector Quantization: Pros

- Great data dependence
- Easy to learn good codebook: k-means
- Fast search
  - Offline: Pre-compute all distances between codewords
  - Online: $d(x, y) \approx d(q(x), q(y))$ ; lookup table
- Asymmetric distance
  - No need to quantize the query!
  - Online:
    - Compute all d(x, codeword)
    - $d(x, y) \approx d(x, q(y))$ ; lookup table



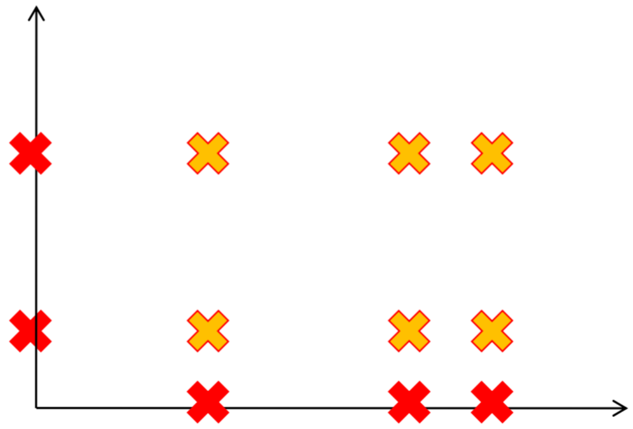
## Vector Quantization: Cons

- Not scalable at all
  - E.g. for a standard 64-bit size code
    - Codebook size $k=2^{64}=1.8 \times 10^{19}$
    - Not possible to learn
      - Slow
      - Insufficient training data
    - Huge memory requirements for codebook and lookup tables
    - Huge cost of distance pre-computation

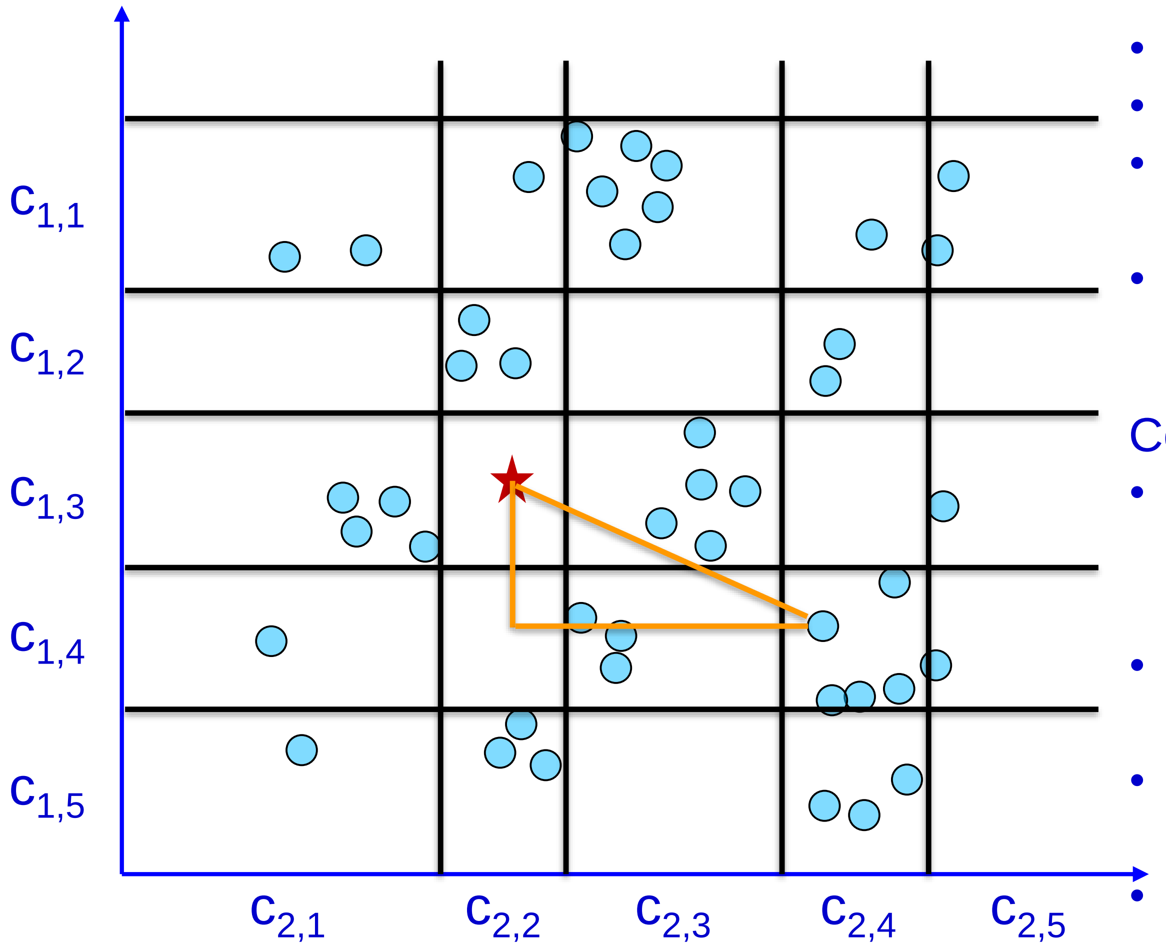
# Product Quantization (PQ)

Key idea

- Divide vectors into *m* subvectors (blocks)
- Vector Quantize each subvector independently
- E.g. for a standard 64-bit size code
  - 8 blocks quantized with 8 bits each
  - Sub-codebook size: $2^8$=256
  - Equivalent to vector quantizing with a $2^{64}$=1.8 x $10^{19}$ codebook
  - Effective codebook: codewords are the Cartesian product of block-wise codewords



# Product Quantization: Distance computation



Toy example

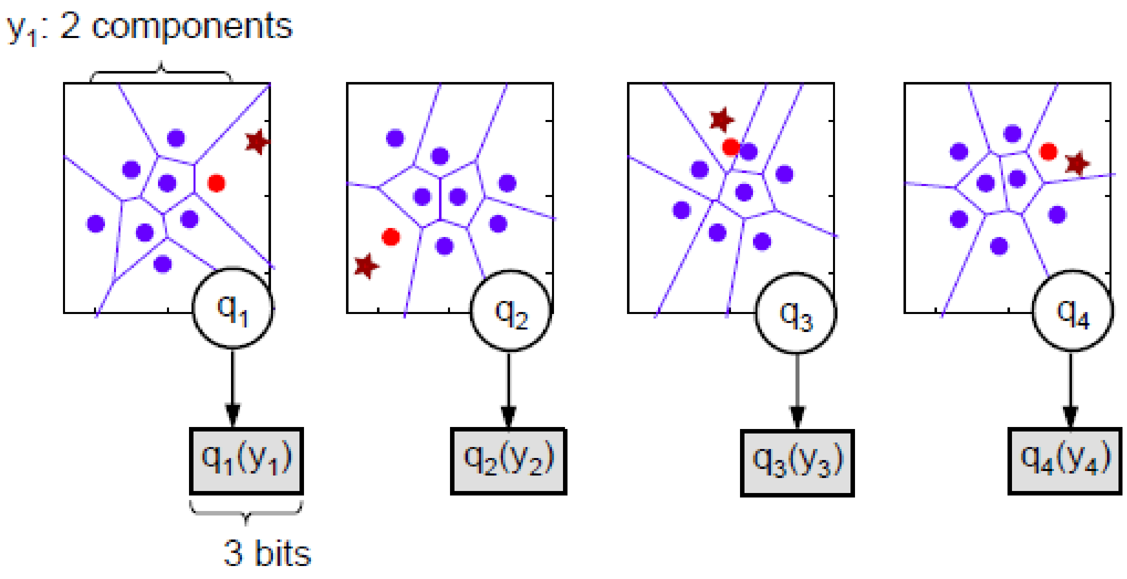
- 2-D vectors
- Split into m=2 1-D subspaces
- Sub-codebooks of size 5
- Equivalent "product" codebook size = 25
- Assumes subspace independence

Computing distances

- Pythagoras: sum squared distances from orthogonal subspaces
- Compute squared distances in each subspace independently
- Precompute squared distances to all sub-codebook centroids
- Product quantization: 5+5 distance computations
- Vector quantization: 25 distance computations

# Searching using Product Quantization

- Vector split into m subvectors: $y \rightarrow [y_1 \dots y_m]$
- Subvectors are quantized separately
- Toy example: y = 8-dim vector split into 4 subvectors of dimension 2



$8^4$=4,096 centroids induced

for a quantization cost equal to that of 8 centroids

- In practice: 8 bits/subquantizer (256 centroids)

Jegou *et al,* PAMI 2011

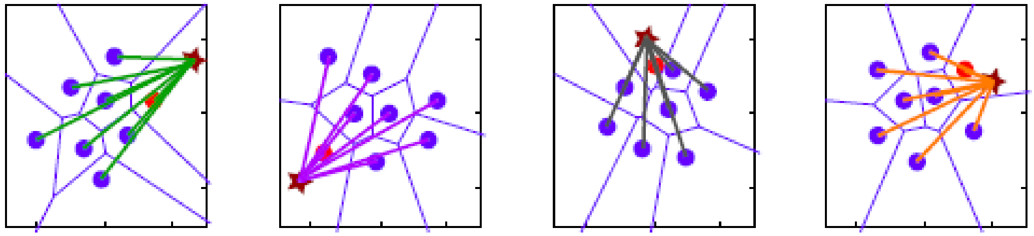
# Searching using Product Quantization

- Estimate distances **in the compressed domain**

$$d(x,y)^2 = \sum_{i=1}^{m} d(x_i, y_i)^2 \approx \sum_{i=1}^{m} d(x_i, q_i(y_i))^2$$

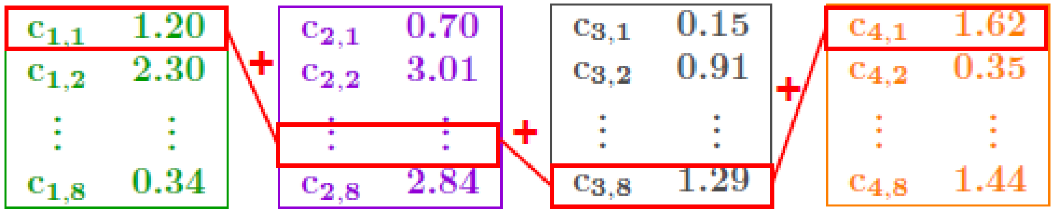
- To compute distances between query $x$ and **many** codes:

I-



$\rightarrow$ Precompute all distances between query subvectors and centroids:

$$d\left(x_i, c_{i,j}\right)^2$$



|  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|
| $c_{1,1}$ | 1.20 | $c_{2,1}$ | 0.70 | $c_{3,1}$ | 0.15 | $c_{4,1}$ | 1.62 |
| $c_{1,2}$ | 2.30 | $c_{2,2}$ | 3.01 | $c_{3,2}$ | 0.91 | $c_{4,2}$ | 0.35 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $c_{1,8}$ | 0.34 | $c_{2,8}$ | 2.84 | $c_{3,8}$ | 1.29 | $c_{4,8}$ | 1.44 |

$\rightarrow$ Stored in look-up tables computed per query descriptor

II- For each database vector: sum the elementary square distances

- **m-1 additions per distance**

Jegou *et al*, PAMI 2011

## Example stats

3 Million key frames

Use PQ with 4 dim sub-vectors, and 1 byte per sub-vector (256 centres)

Original descriptors 8k dimension

- Memory footprint: 8k x 4 x 3M = 96 GB

Product Quantization: 8k x 4 -> 2k

- Memory footprint: 2k x 3M = 6 GB

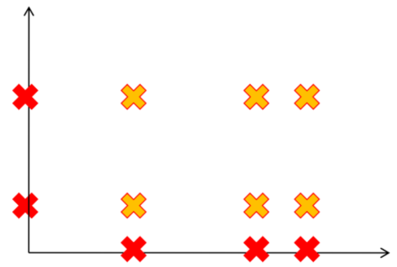
Product Quantization for vector compression,
Jegou *et al.*, PAMI 2011

# Product Quantization (PQ)

Pros

- Large reduction in memory footprint
- Large speedup in NN search (c.f. exhaustive search)
- Good performance in practice

Cons



- Slower than hashing, but usually fast enough
- Assumes subvectors are independent
  - In practice: first decorrelate subvectors (PCA)
- Assumes subvectors contain equal amount of information
  - In practice: balance information across blocks
  - See Optimized Product Quantization [Ge et al. 2013] and Cartesian K-Means [Norouzi & Fleet 2013]

Code: FAISS (https://github.com/facebookresearch/faiss )

# ANN via approximating vectors: Comparison

Memory vs Quality

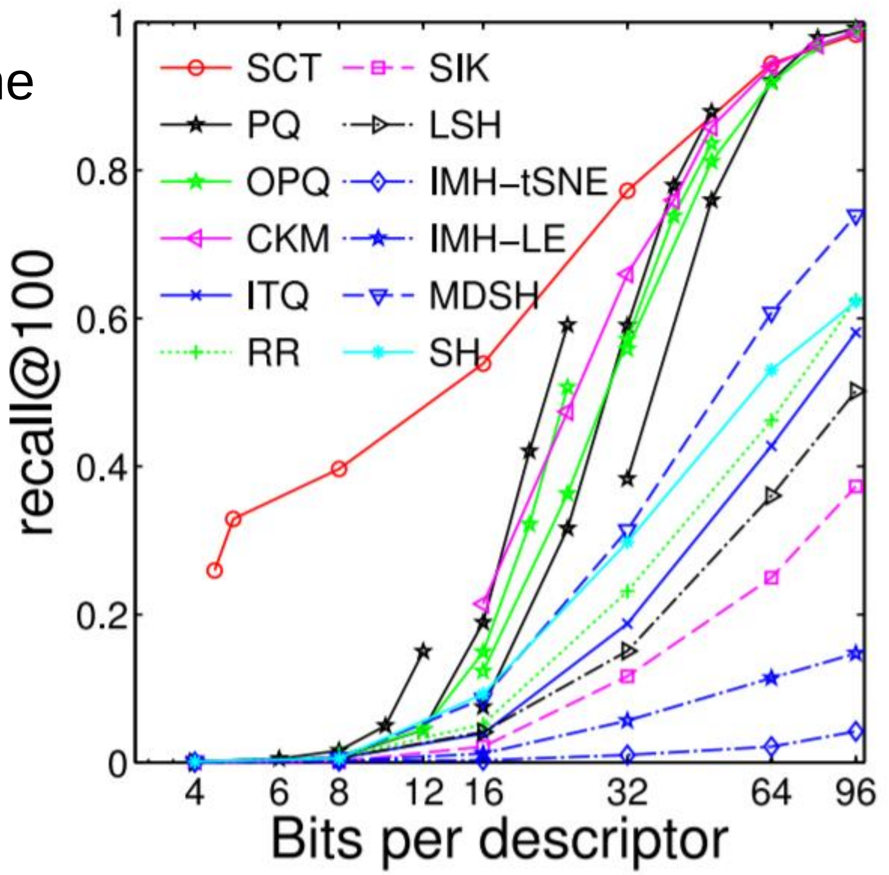
recall@100: Proportion of times the true NN is in top 100

Vector Quantization

- PQ, OPQ, CKM

Hashing

- LSH, SH, MDSH, etc



SIFT 1M 128-D

Vector Quantization beats Hashing

# ANN via approximating vectors: Comparison

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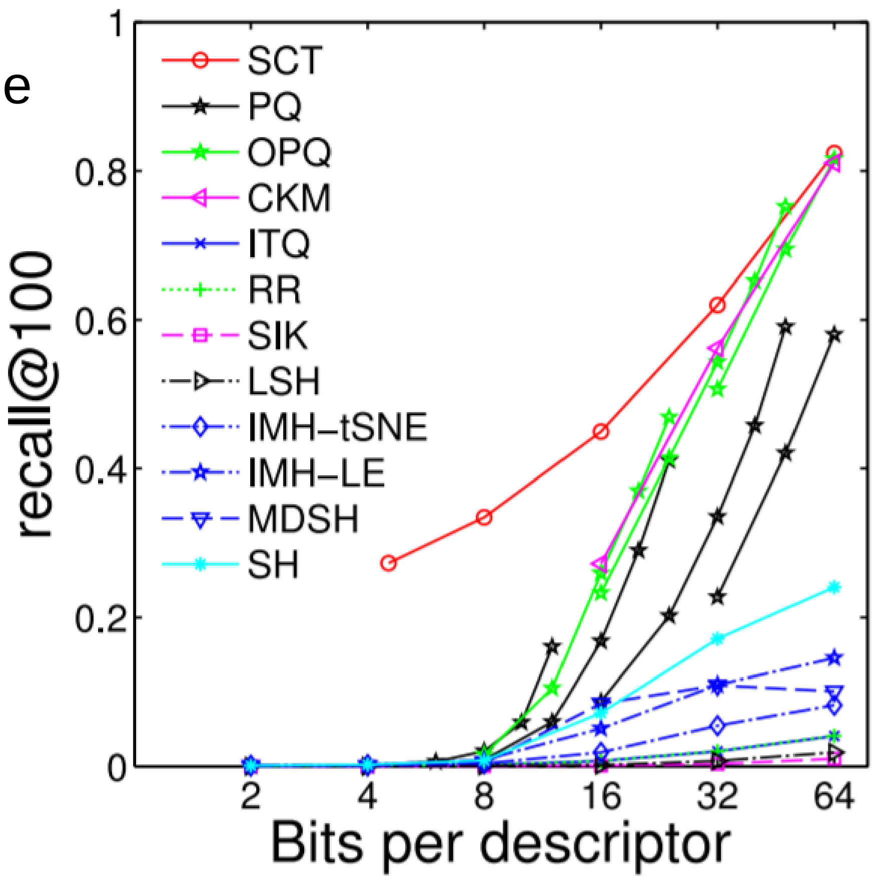

Tiny 580k 384-D

Vector Quantization beats Hashing

## Approximate Nearest Neighbours (ANN): Methods

Broad division

1. Approximate the vectors => do faster distance computations
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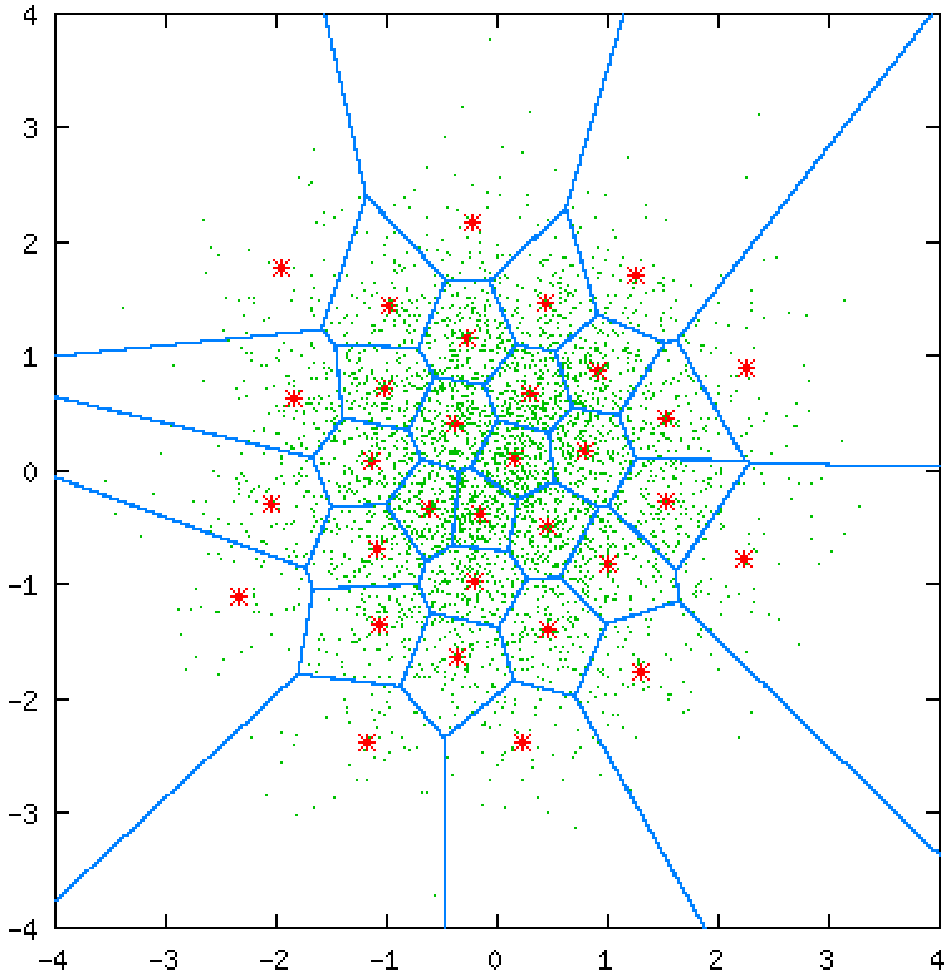
2. **Approximate the search => do fewer distance computations**
   - Do not visit all points

## ANN via approximating the search: Methods

- Space partitioning
  - Hashing
  - Vector Quantization
  - K-d trees

## Space partitioning

- Partition the vector space into C partitions
- Query
  - Search inside the nearest k partitions
- Does not decrease memory requirements
  - Can combine with quantization
- Performance
  - For C=const - still O(nd), just O(nd*k/C)
  - k/C: quality vs speed



# Curse of dimensionality

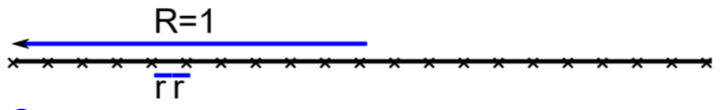
N=1 billion, r=?

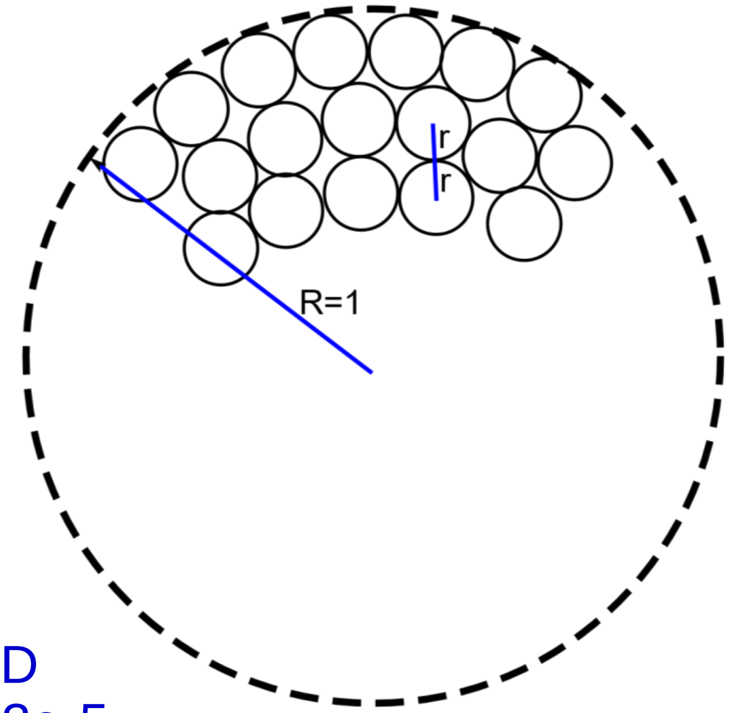
$$V_S = k_d r^d$$
$$V_L = k_d R^d = k_d$$

Packing hyper-spheres

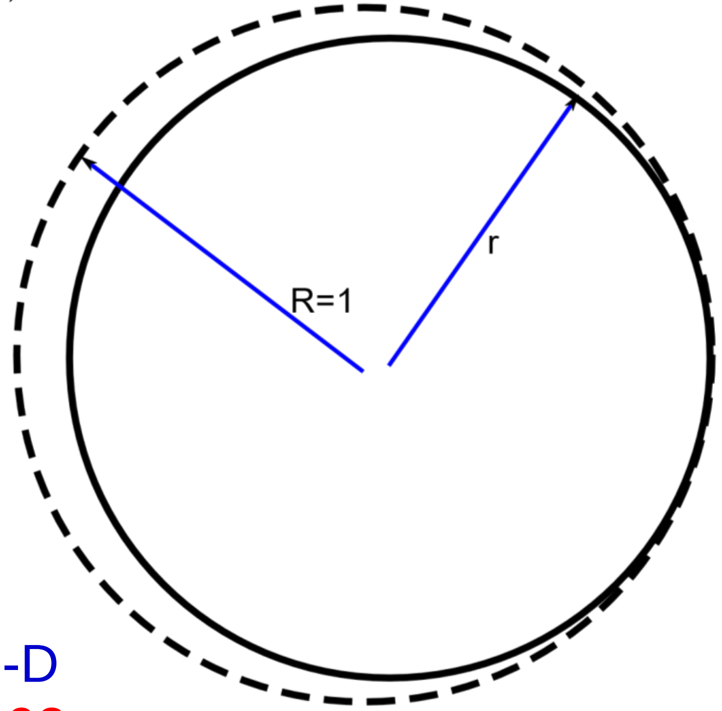
$$V_L = N V_S$$
$$k_d = N k_d r^d$$
$$r = \left(\frac{1}{N}\right)^{\frac{1}{d}}$$

1-D
r=1e-9





2-D
r=3e-5



256-D
r=0.92

## Space partitioning revisited

- Partition the vector space into C partitions
- Query
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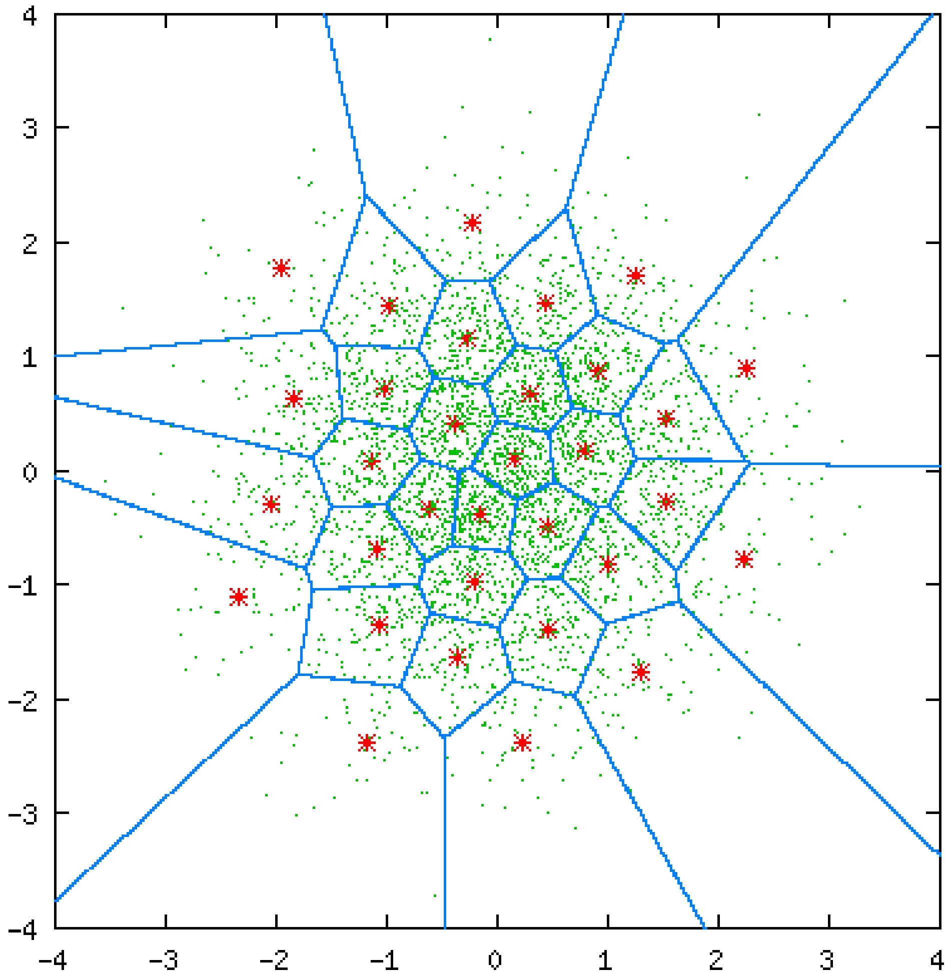

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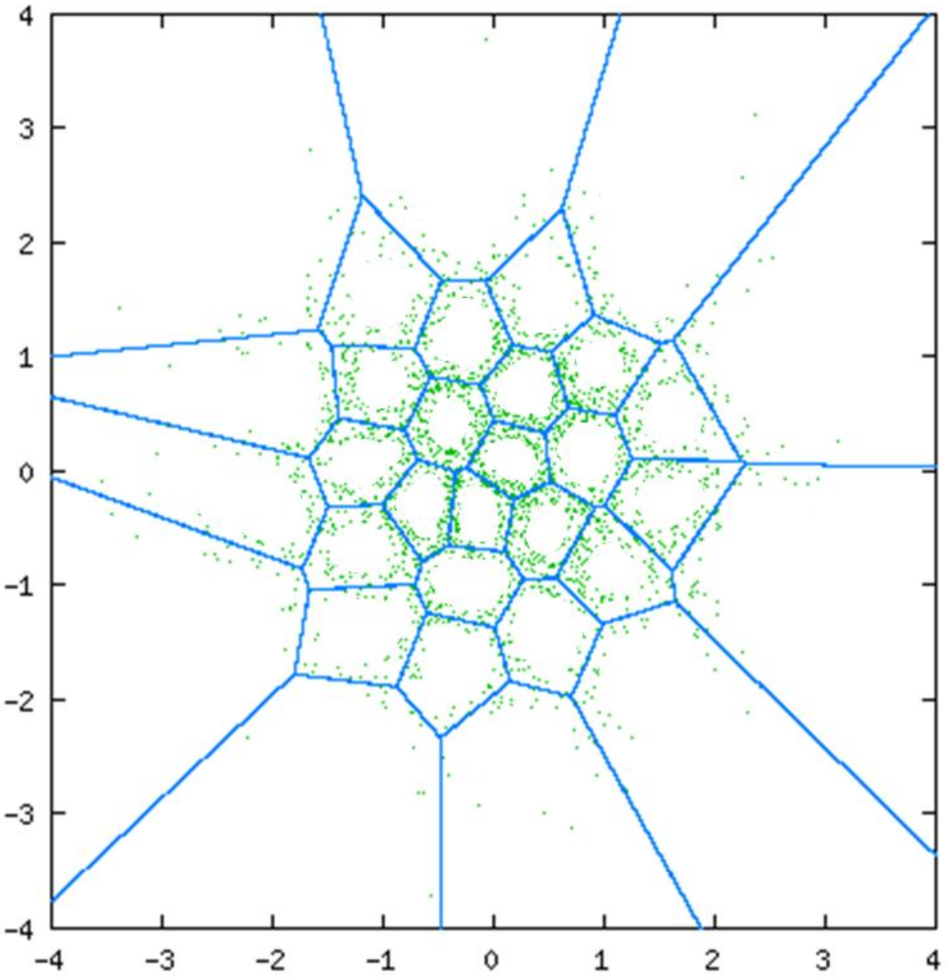
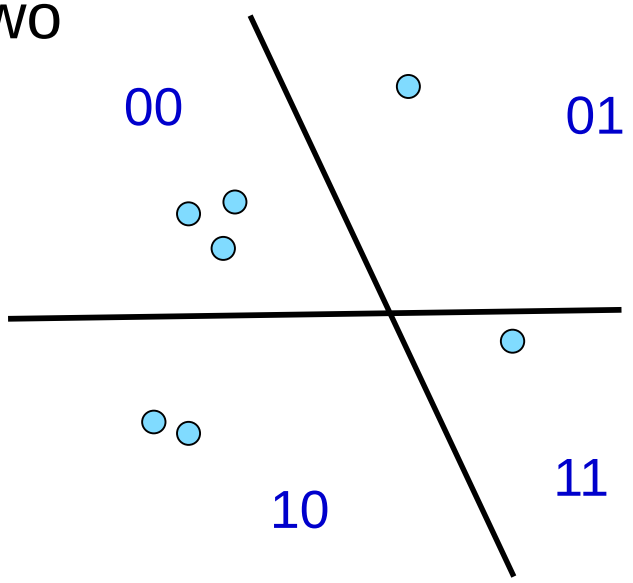


## ANN via approximating the search: Methods

- Space partitioning
  - **Hashing**
  - Vector Quantization
  - K-d trees

## Hashing (for approximate search)

Recall: Each bit partitions space into two



Query

- Visit partitions in order of increasing Hamming distance of the query hash

## Hashing (for approximate search): Discussion

How many partitions with Hamming distance r for b-bits? $\binom{b}{k}$

- For b=64, r=3: 42k
- For b=64, r=4: 635k

Necessary solution

- Multiple partitions with smaller number of bits each
- Same vector (or its ID) is stored multiple times

Pros

- If hashing is used for quantization, partitions are directly available

Cons

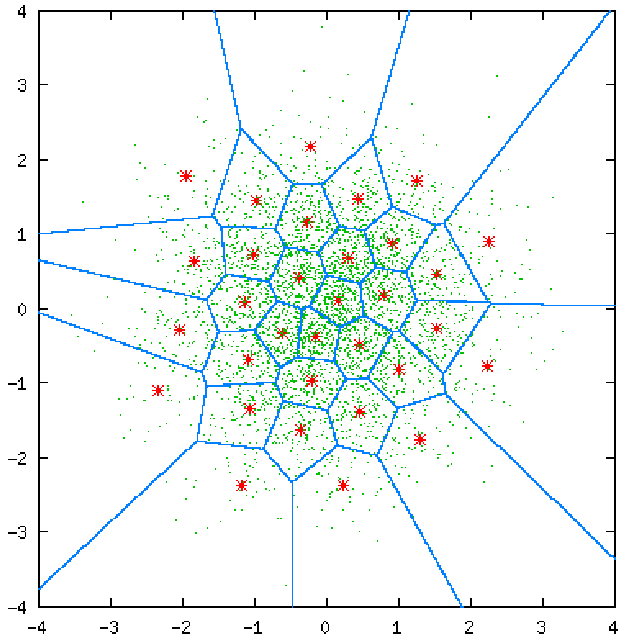
- Large memory requirements for good performance
- As before: hard to get good hashing functions

## ANN via approximating the search: Methods

- Space partitioning
  - Hashing
  - **Vector Quantization**
  - K-d trees

## Vector Quantization (for approximate search)

Partition the space using k-means



Query

- Partition visit order: k nearest partitions obtained via NN search for cluster centres

Complexity

- Ordering partitions: O(Cd)
- Searching within partitions: O(ndk/C)
- Rule of thumb: C ~ sqrt(n)

## Vector Quantization (for approximate search)

Pros

- Simple and intuitive
- As before: good data dependence
- Generally good performance

Cons

- Ordering partitions can take a significant chunk of the computation budget
    - Can do ANN for this stage as well, though usually ok

Code: FAISS (https://github.com/facebookresearch/faiss )

Further reading

- Can obtain finer partitioning through PQ, see Inverted Multi-Index [Babenko & Lempitsky 2012]

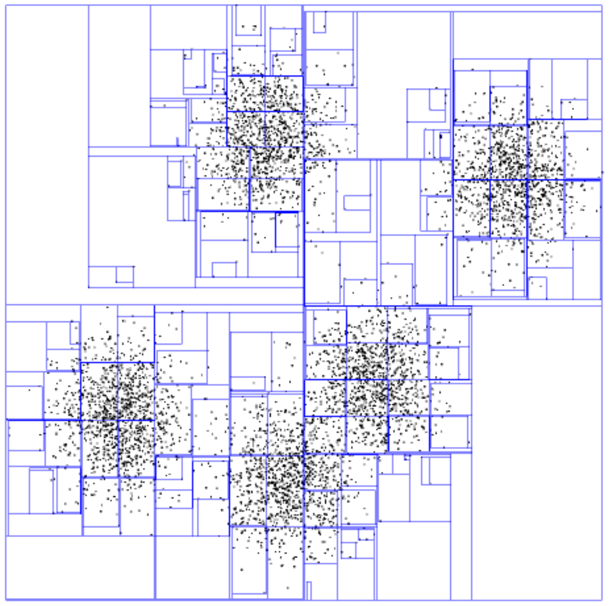
## ANN via approximating the search: Methods

- Space partitioning
  - Hashing
  - Vector Quantization
  - **K-d trees**

# K-d tree

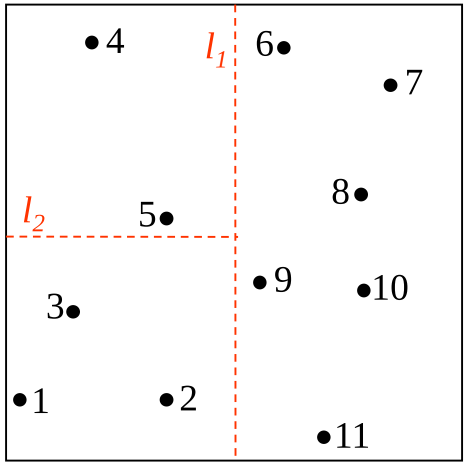
A k-d tree hierarchically decomposes the vector space

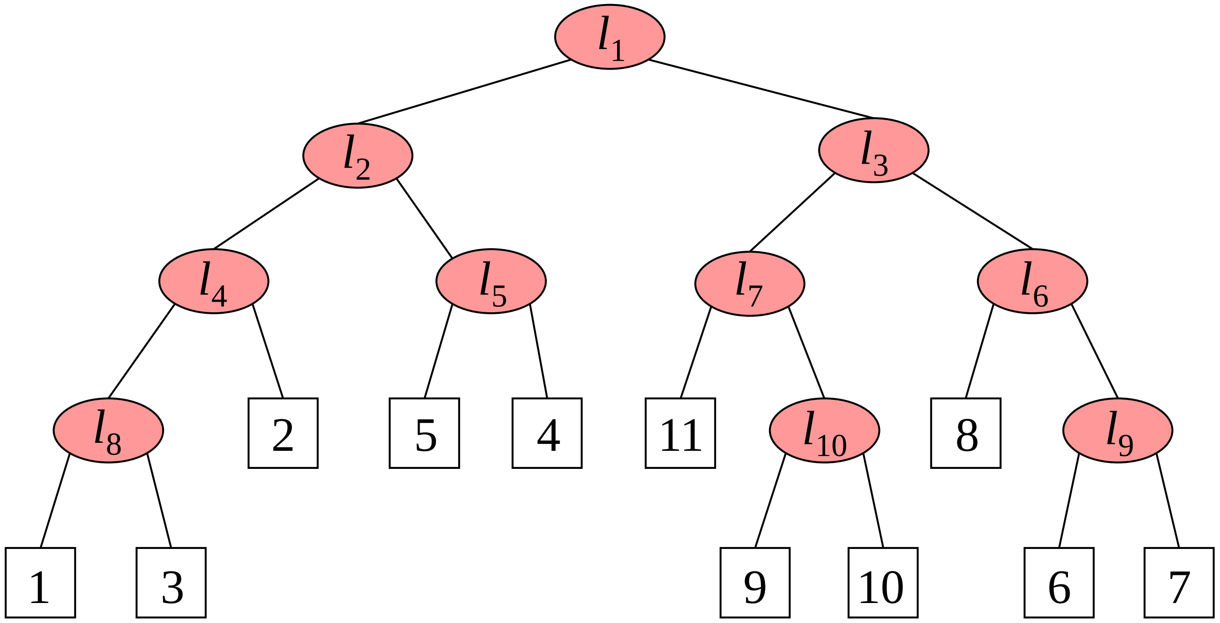
Points nearby in the space can be found (hopefully) by backtracking around the tree some small number of steps



## K-d tree

- K-d tree is a binary tree data structure for organizing a set of points in a K-dimensional space.
- Each internal node is associated with an axis aligned hyper-plane splitting its associated points into two sub-trees.
- Dimensions with high variance are chosen first.
- Position of the splitting hyper-plane is chosen as the mean/median of the projected points.

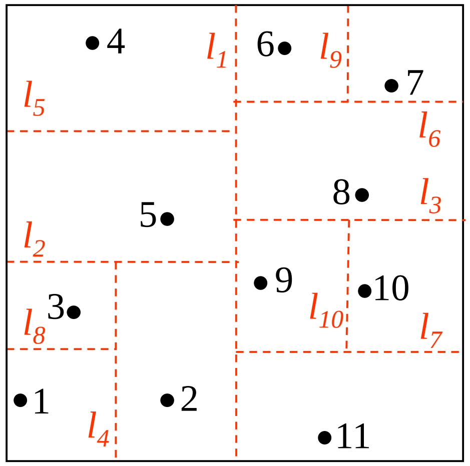


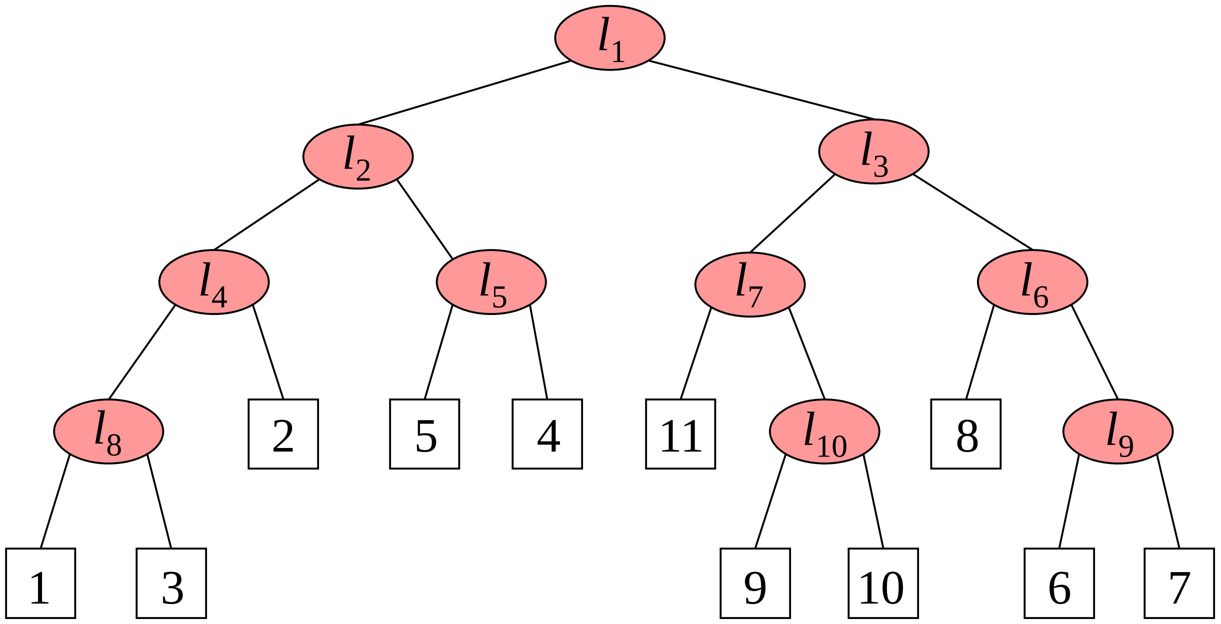


Images: Anna Atramentov

# K-d tree construction

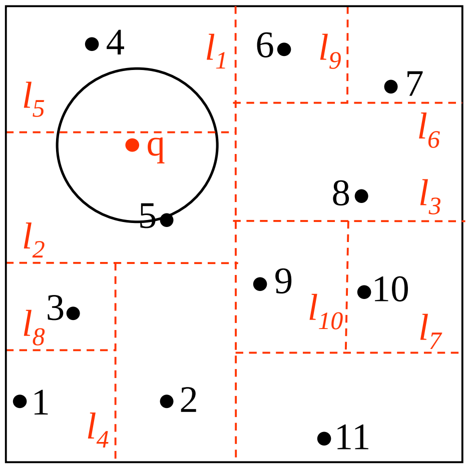
Simple 2D example

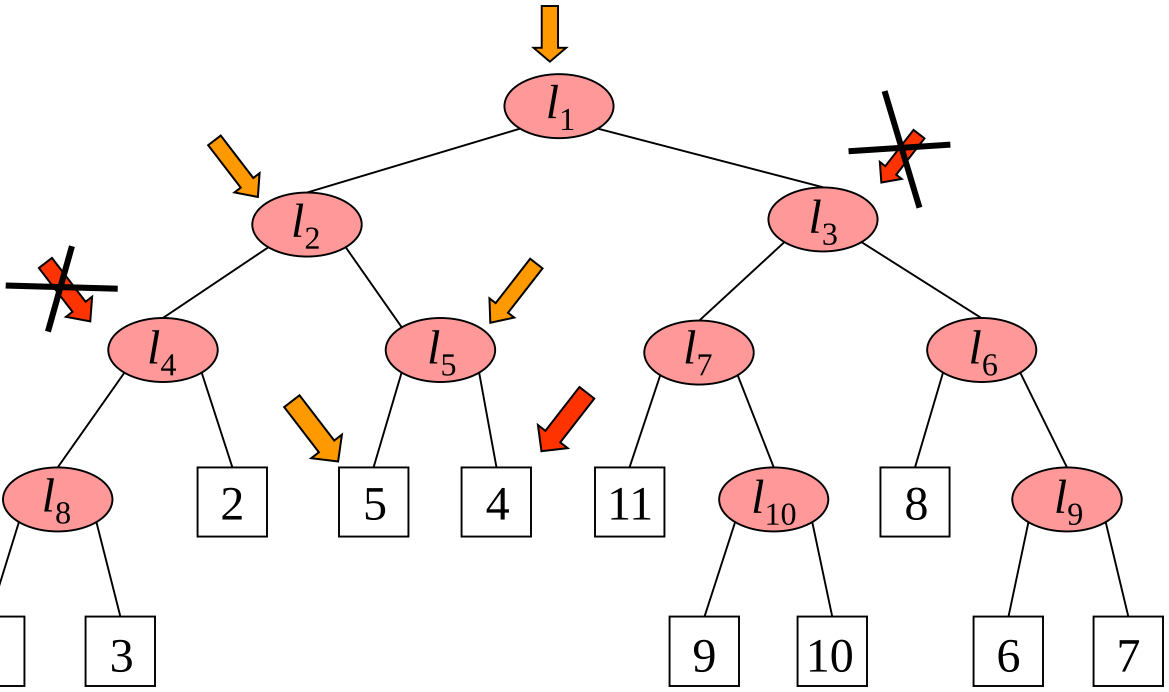




Slide credit: Anna Atramentov

# K-d tree query





Slide credit: Anna Atramentov

# K-d tree: Backtracking

Backtracking is necessary as the true nearest neighbor may not lie in the query cell.

But in some cases, almost all cells need to be inspected.

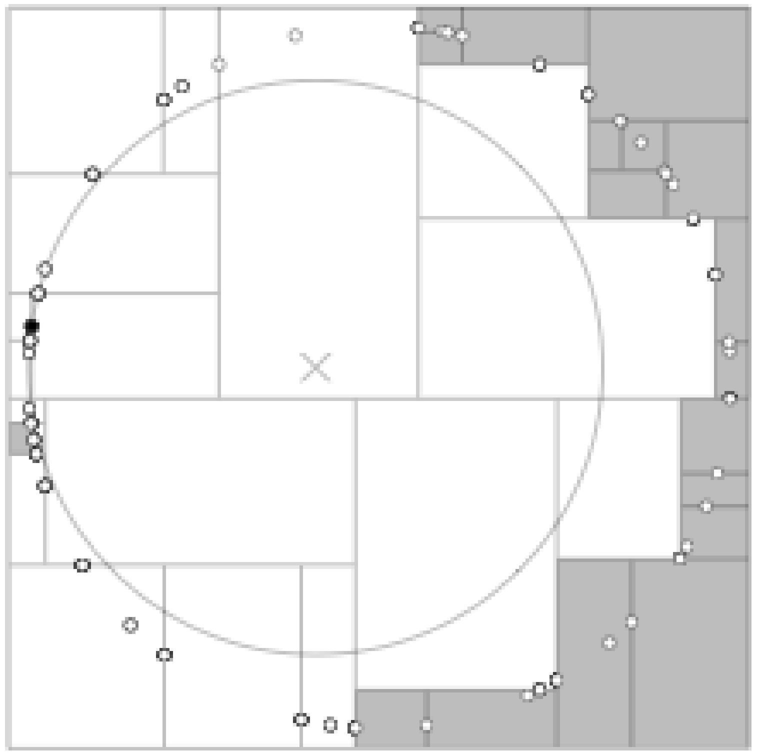


Figure 6.6

A bad distribution which forces almost all nodes to be inspected.

Figure: A. Moore

## K-d tree: Backtracking

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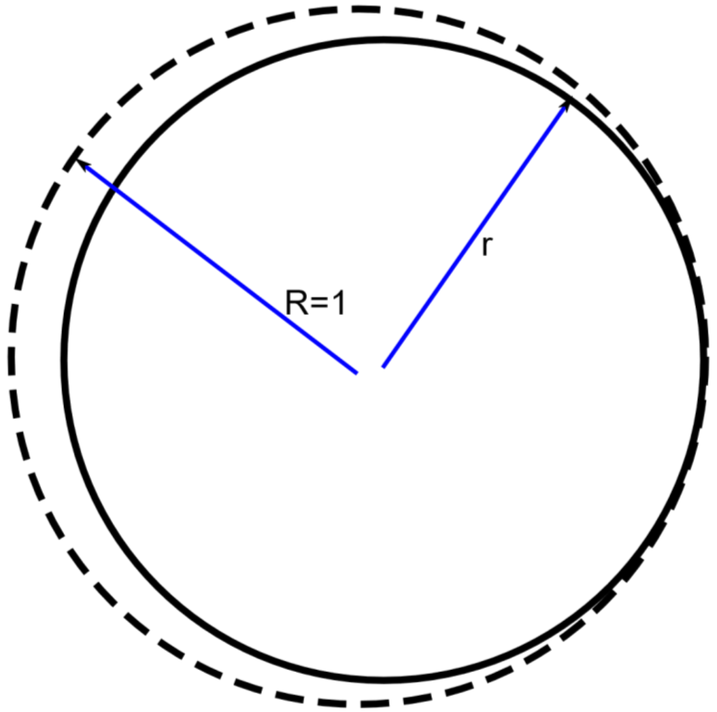
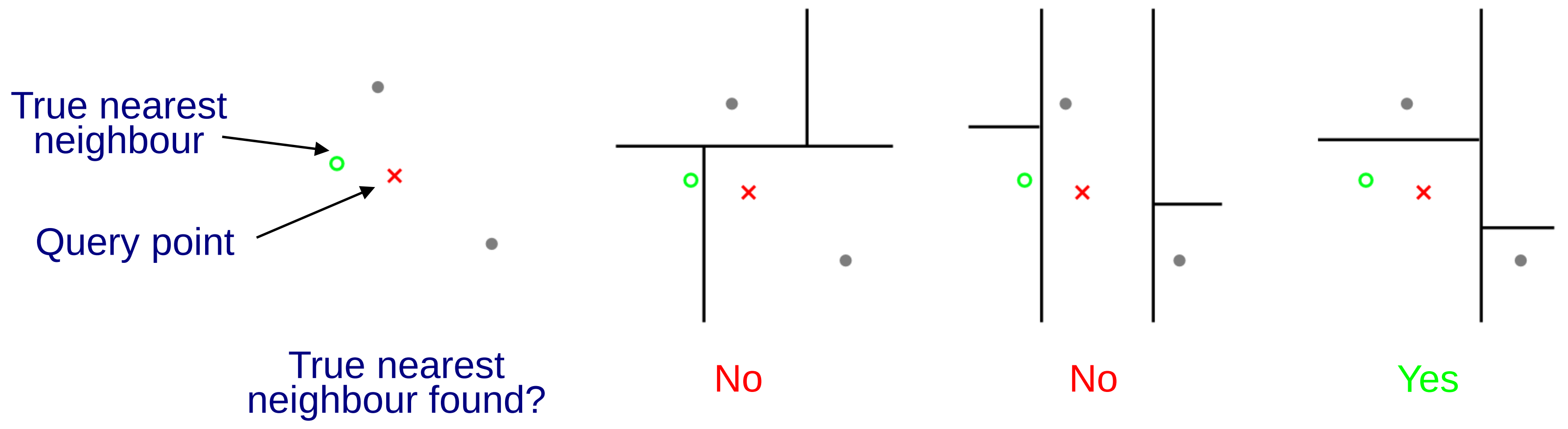


Figure: A. Moore

# Randomized K-d trees

- Multiple randomized trees increase the chances of finding nearby points (shared priority queue)



- How to choose the dimension to split and the splitting point?
  - Pick random dimension from high variance ones
  - Split at the mean/median

## Randomized K-d trees: Discussion

Pros

- Find approximate nearest neighbor in O(log n) time, where n is the number of data points
- Good ANN performance in practice for “low” dimensions (e.g. 128-D)

Cons

- Increased memory requirements: needs to store multiple (~8) trees
- Not so good in “high” dimensions

Code available online:

http://www.cs.ubc.ca/research/flann/

## Approximate Nearest Neighbour search: Overview

**Approximate the vectors**: fast distances, memory savings

- Hashing
  - LSH, see ITQ, Spectral Hashing, ..
- Vector Quantization
  - **Product Quantization**, see OPQ, Cartesian K-means, ..

**Approximate the search**

- Non-exhaustive through space partitioning
- Hashing
- **Vector Quantization**
- (Randomized) K-d trees
- Mind the dimensionality

In real life – use a **hybrid** approach

- E.g. Google Goggles/Photos 2011: Vector Quantization + OPQ

## There is more …

Inverted file indexing (Computer Vision lectures)

Beyond Euclidean distance / scalar product

- MinHash for Jaccard similarity (set overlap)
- Winner Take All hashing for rank correlation
- Other kernels: Explicit feature map

Supervised methods - current and future work

- Training representations for ANN search
  - Neural networks for hashing
    - “Supervised Hashing for Image Retrieval via Image Representation Learning” [Xia et al. 2014]
  - Neural networks for PQ
    - “SUBIC: A supervised, structured binary code for image search” [Jain et al. 2017]