Approximate Nearest Neighbor Search based on Product Quantization

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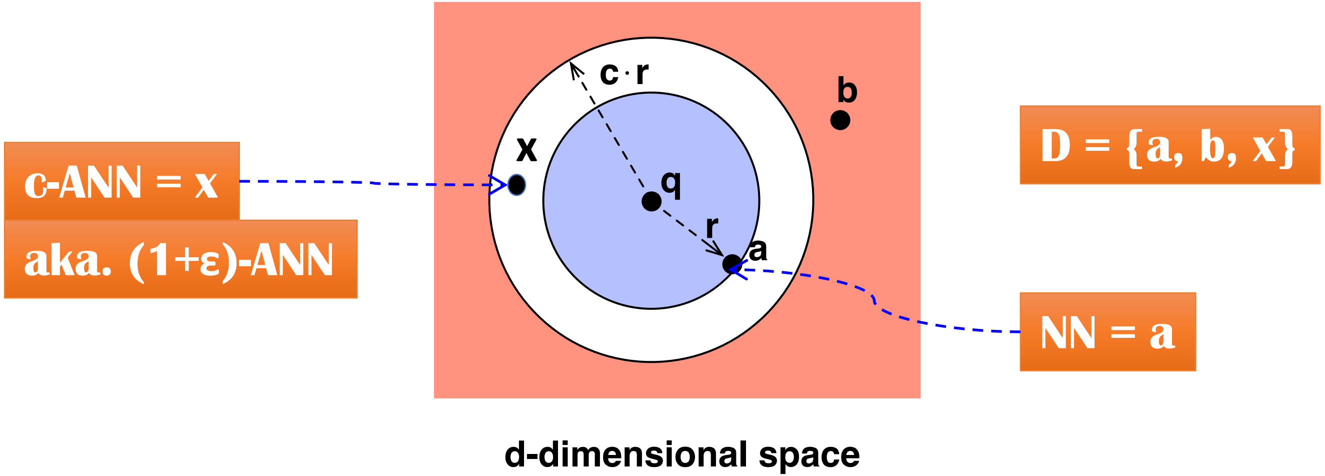
Nearest Neighbor (NN) and its Variants



- Given: n points in d-dimensional Euclidean space
- NN query: find the closest point, o*, in D, wrt a query point q
- Approximate NN query: find a near point
- All extendible to kNN versions for k > 1

Motivations

- Theoretical interest
  - Fundamental geometric problem: “post-office problem”
  - Known to be hard due to high-dimensionality
- Many applications
  - Feature vectors: Data Mining, Multimedia DB
  - Applications based on similarity queries, e.g.,
    - Quantization in coding/compression
    - Recommendation systems
    - Bioinformatics/Chemoinformatics
  - Machine Learning
    - Representation learning (e.g., embedding)
    - Dimensionality reduction; collaborative filtering; kNN classifier; Kernel?

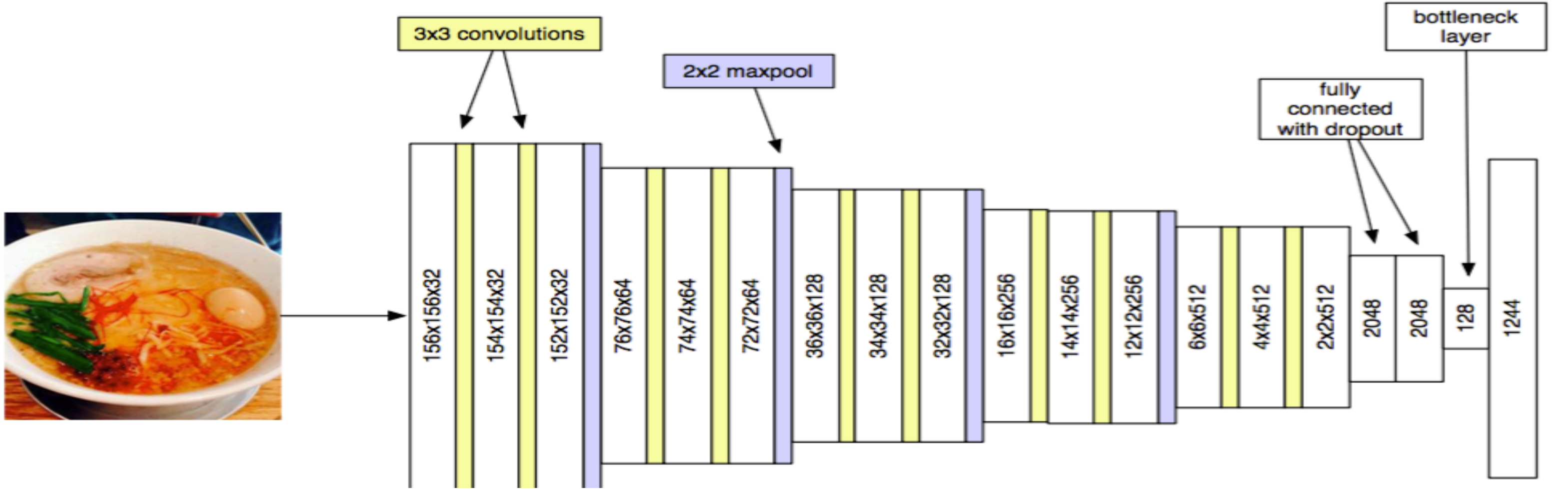
Dimensionality reduction for ML

- Start with high-dimensional data
- Run dimensionality reduction
- Do stuff in a small dimensional space

Erik Bernhardsson, “Approximate nearest neighbor methods and vector models”, 2015

Deep Learning for food

- Deep model trained on a GPU on 6M random pics downloaded from Yelp



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Distance in Smaller Space

1. Run image through the network
2. Use the 128-dimensional bottleneck layer as an item vector
3. Use cosine distance in the reduced space

$f($  $) = \mathbf{v} \qquad (\mathbf{v} \in \mathbb{R}^{128})$

$$d(\mathbf{u}, \mathbf{v}) = \left(\frac{\mathbf{u}}{|\mathbf{u}|} - \frac{\mathbf{v}}{|\mathbf{v}|} \right)^2$$

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Nearest Neighbor Food Pics

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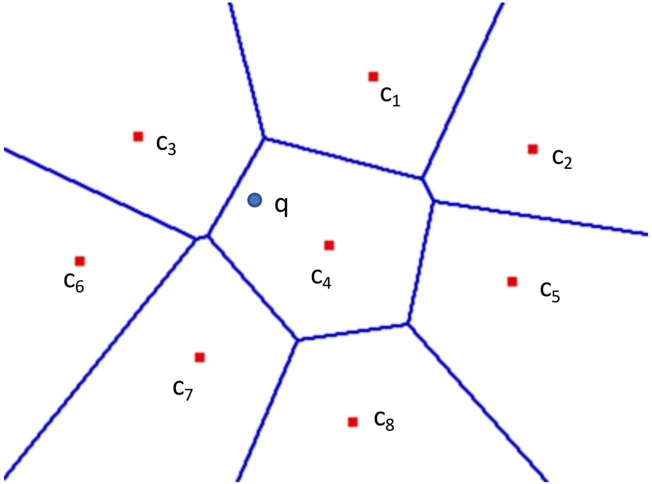
Preliminary: Vector Quantization (with K-means)

- Idea: compressed representation of vectors
  - Each D-dim vector x is represented by QZ(x), where QZ() is a quantizer
  - dist(x, o) ≈ dist(x, QZ(o))
- Encode the vectors:
  - Learn a codebook $W = \{c_1, c_2, \ldots, c_K\}$ via K-means
  - Assign o to its **nearest** codeword in W
    - E.g., $QZ(o) = c_i$ ($i \in 1 \ldots K$), such that $dist(x, c_i) \leq dist(x, c_j)$ for $\forall j$
  - Represent each vector o by its assigned codeword
- Assume D = 256, $K = 2^{16}$
  - Before: 4 bytes * 256 = 1024 bytes for each vector
  - Now:
    - data: 16 bits = 2 bytes
    - codebook: $4 * 256 * 2^{16}$

$\boxed{\text{smaller when } n > 4*256*2^{16}/1022 = 65{,}664}$

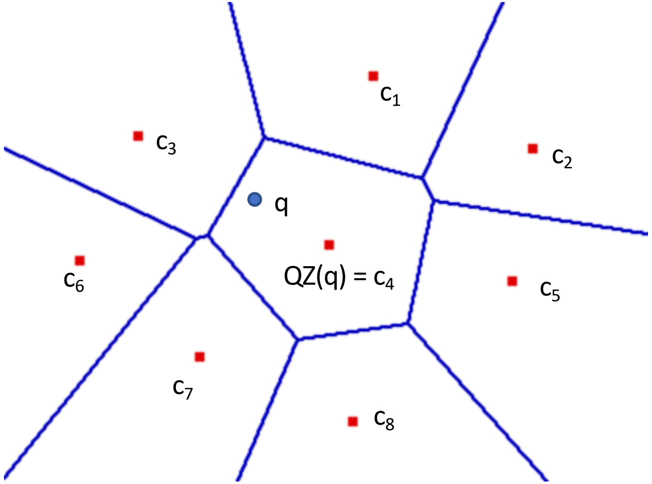
Vector Quantization – Query Processing

- Given query q, how to find a point close to q?



Vector Quantization – Query Processing

- Given query q, how to find a point close to q?
- Algorithm:
  1. Compute QZ(q)
  2. Candidate set C = all data vectors associated with QZ(q)
  3. Verification: compute distance between Q and $o_i \in C$
     - Requires loading the vectors in C



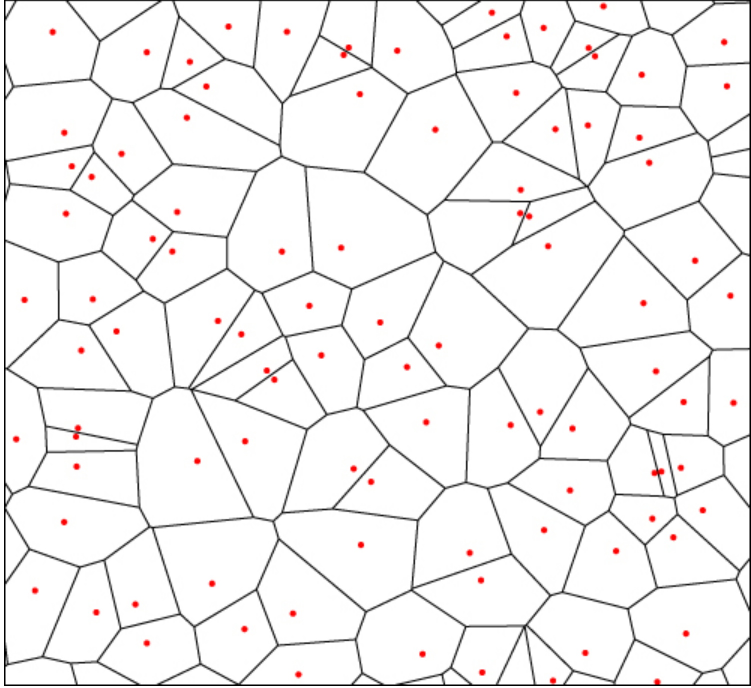
Inverted index: a hash table that maps c_j to a list of o_i that are associated with c_j

- Any problem/improvement?

Limitations of VQ

- To achieve better accuracy, fine-grained quantizer with large K is needed
- Large K ➔
  - Costly to run K-means
  - Computing QZ(q) is expensive: O(K M)
  - May need to look beyond q(Q) cell

- Solutions:
  - Product Quantization, or
  - Hierarchical k-means



Product Quantization

- Idea:
  - Partition the dimension into m partitions
    - Accordingly a vector ➔ m subvectors
  - Use separate VQ with k codewords for each chunk
- Example:
  - 10-dim vector decomposed in m = 2 subvectors
    - $o^T = [o_1 : o_2]^T$
  - Each codebook has 4 codewords, denoted as $c_{i,j}$
  - Total space in bits:
    - data: m log(K)
    - codebook: m * ((D/m) * K)

7	2	-1	5	6	4	3	-5	-1	-7
-2	3	0	6	4	2	2	4	5	-8
…	…	…	…	…	…	…	…	…	…
…	…	…	…	…	…	…	…	…	…
…	…	…	…	…	…	…	…	…	…

0	1	0	0
1	0	1	1
…	…	…	…
…	…	…	…
…	…	…	…

$C_{1,1}$	5.9	2.3	-2.7	3.9	6.1
$C_{1,2}$	-1.3	1.8	7.4	5.5	0.9
$C_{1,3}$	…	…	…	…	…
$C_{1,4}$	…	…	…	…	…

$C_{2,1}$	-0.1	3.5	1.4	9.6	5.5
$C_{2,2}$	…	…	…	…	…
$C_{2,3}$	…	…	…	…	…
$C_{2,4}$	…	…	…	…	…

Distance Estimation

- Euclidean distance between a query point **q** and a data point encoded as **t**
  - Restore the virtual joint center by looking up each partition of **t** in the corresponding codebooks ➔**p**

$$d^2(\mathbf{q}, \mathbf{t}) = \sum_{i=1}^{D} (\mathbf{q}_i - \mathbf{p}_i)^2$$

  - This is the Asymmetric Distance (AD)

$$d^2(\mathbf{q}, \mathbf{t}) = \sum_{i=1}^{m} (\mathbf{q}_{(i)} - \mathbf{c}_{i,\mathbf{t}_{(i)}})^2$$

q

7	2	-1	5	6	4	3	-5	-1	-7

t

0	1	0	0

$C_{1,1}$	5.9	2.3	-2.7	3.9	6.1
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$C_{1,3}$	…	…	…	…	…
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$C_{2,3}$	…	…	…	…	…
$C_{2,4}$	…	…	…	…	…

p

-1.3	1.8	7.4	5.5	0.9	-0.1	3.5	1.4	9.6	5.5

PQ – Query Processing

q

7	2	-1	5	6	4	3	-5	-1	-7

t	0	1	0	0
t'	1	0	1	1
	1	0	1	0
	0	0	1	0
	1	1	1	1

- Naïve:
  - Perform ADC for every **t** in the database
  - Candidate = those with the k smallest AD
  - [Optional] Reranking (if k > 1):
    - Load the data vectors and compute the actual Euclidean distance
    - Return the one with the smallest distance
- Pruning:
  - AD is monotonic in each component

$$d^2(\mathbf{q}, \mathbf{t}) = \sum_{i=1}^{m} (\mathbf{q}_{(i)} - \mathbf{c}_{i,\mathbf{t}_{(i)}})^2$$

$$(\mathbf{q}_{(1)} - \mathbf{c}_{i,\mathbf{t}_{(1)}})^2 + (\mathbf{q}_{(2)} - \mathbf{c}_{i,\mathbf{t}_{(2)}})^2$$

$$(\mathbf{q}_{(1)} - \mathbf{c}_{i,\mathbf{t}'_{(1)}})^2 + (\mathbf{q}_{(2)} - \mathbf{c}_{i,\mathbf{t}'_{(2)}})^2$$

There is an optimal order to consider each encoded points!

Compute it efficiently and incrementally!

NOTE: Reusing figure in the paper. m = 2, each code book has 6 codewords, named $\mathbf{U_i}$ and $\mathbf{V_j}$

Multi-index Algorithm

1. Sort each code book in increasing order of their partial AD distance to q

2. Maintain the non-dominated combinations into a min heap H

NOTE: slightly different from the paper – Skyline algorithm

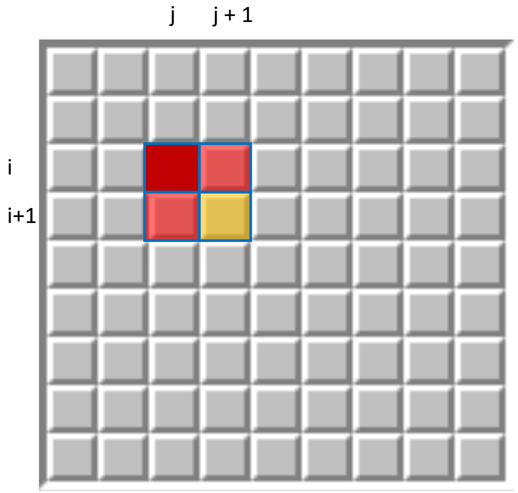
$\mathbf{q}_{(1)}$ vs. $\mathcal{U}$

i	$\mathbf{u}_{\alpha(i)}$	r
1	$\mathbf{u_3}$	0.5
2	$\mathbf{u_4}$	0.7
3	$\mathbf{u_5}$	4
4	$\mathbf{u_2}$	6
5	$\mathbf{u_1}$	8
6	$\mathbf{u_6}$	9

$\mathbf{q}_{(2)}$ vs. $\mathcal{V}$

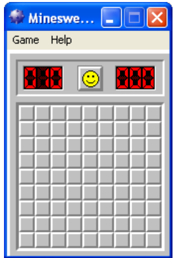
j	$\mathbf{v}_{\beta(j)}$	s
1	$\mathbf{v_4}$	0.1
2	$\mathbf{v_3}$	2
3	$\mathbf{v_5}$	3
4	$\mathbf{v_2}$	6
5	$\mathbf{v_6}$	7
6	$\mathbf{v_1}$	11

partial AD



(i,j) ➔ pushes (i+1, j) and (i, j+1) into H

Dedup: need to check if it has EVER been pushed into H or not



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5	$\mathbf{u_1}$	8
6	$\mathbf{u_6}$	9

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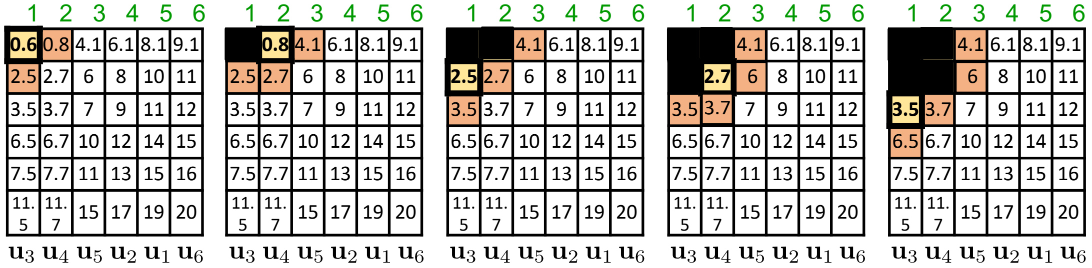
6	$\mathbf{v_1}$	11

partial AD

		1	2	3	4	5	6
$\mathbf{v}_4$	1	0.6	0.8	4.1	6.1	8.1	9.1
$\mathbf{v}_3$	2	2.5	2.7	6	8	10	11
$\mathbf{v}_5$	3	3.5	3.7	7	9	11	12
$\mathbf{v}_2$	4	6.5	6.7	10	12	14	15
$\mathbf{v}_6$	5	7.5	7.7	11	13	15	16
$\mathbf{v}_1$	6	11.5	11.7	15	17	19	20
		$\mathbf{u}_3$	$\mathbf{u}_4$	$\mathbf{u}_5$	$\mathbf{u}_2$	$\mathbf{u}_1$	$\mathbf{u}_6$



(2,2) not pushed again

(2,3) not pushed again

Exercises:

- Write out H
- How to perform dedup?
- Generalize to m-dimensional case
- [hard] perform dedup without additional data structure (and cost)

References

- Hervé Jégou, Matthijs Douze, and Cordelia Schmid. Product quantization for nearest neighbor search. TPAMI 2014.
- Artem Babenko and Victor Lempitsky. The Inverted Multi-Index. TPAMI 2014.