POLITECNICO DI TORINO
Telecommunications Engineering
Information Theory and Signal Processing Applications

Master Degree Dissertation

Nearest Neighbour Search using binary clustered Neural Networks

Applied to object retrieval and classification

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PRESENTATION OVERVIEW

PROBLEM STATEMENT

NEAREST NEIGHBOUR SEARCH

The problem of searching for the Nearest Neighbour is formulated as:

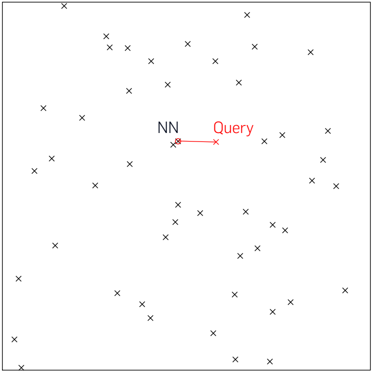
> "**Given a collection of data points and a query point in a hyper-dimensional metric space, find the data point that is closest to the query one.**" [Kevin Beyer, 1998]

The closeness metric is generally considered as **Euclidean Distance**.

Motivations can be found in its wide set of applications, mainly related to the domains of Data Processing and Machine Learning:

- → **Object Retrieval**
- → **Classification**
- Computational Statistics
- Pattern Recognition
- Computer Vision
- Data Mining.

PROBLEM STATEMENT



Example of Nearest Neighbour search query over a two-dimensional set of uniform distributed points.

Running an **Exhaustive Search**:

→ Computing Euclidean Distances,

→ Retrieving the minimum one.

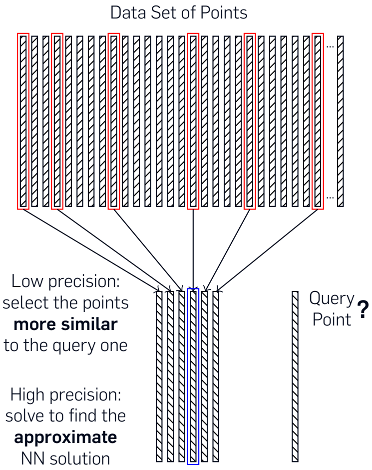
The **Computational Complexity** is:

→ Linear with the number of data points, considered to be N,

→ Linear with the dimensionality of the search space d.

It may hence be denoted as $\mathcal{O}(N \cdot d)$.

PROPOSED SOLUTION

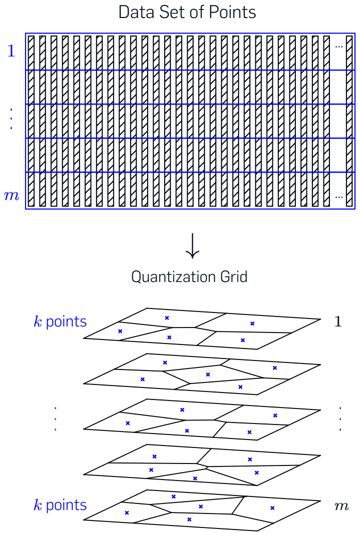


The proposed solution is structured as:

- **Training Stage**
  - → Coarse Vector Quantization acts on the data dimensionality,
  - → Neural Networks Learning allows a quick data access.
- **Query Stage**
  - → Neural Networks Polling acts on the data cardinality.
  - → Fine Vector Quantization Despite a higher compression rate, it works at low dispersion.

VECTOR QUANTIZATION

VECTOR QUANTIZATION

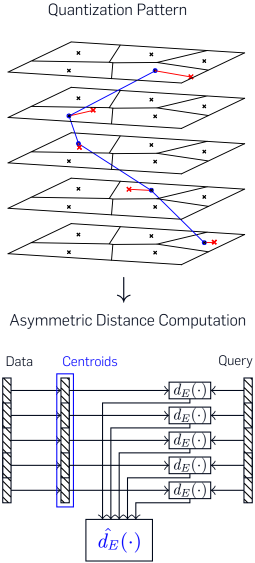


The quantization grid is computed empirically over the data set of points.

- **Splitting over m layers**
  - → The search space is split in contiguous orthogonal sections.
- **Clustering the layers to k points**
  - → Each data points section is processed to determine the best set of **cluster centroids**.

The optimality criteria considered is the minimum average dispersion one,
Its achievement is sought in the use of a specific procedure known as **k-means**.

PRODUCT QUANTIZATION



Product Quantization (PQ) is a state-of-the-art technique to solve Approximate NN (ANN) search:

- **Data Points Approximation**
  → Associate them centroids sets called **Quantization Patterns**.
- **Distance Metric Approximation**
  → The Euclidean Distance is computed as **Sum of Distances** over lower-dimensional layers.

The scan search can be accelerated by using a Look Up Table approach.

NEURAL NETWORKS

ARTIFICIAL NEURAL NETWORKS

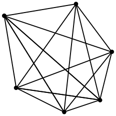
Artificial Neural Networks are a family of computational models able to accelerate the **data access** with a neuro-inspired approach.

Based on the biological model of **synaptic interaction**, it concerns a system of interconnected neural cells exchanging information messages.

The connections have numeric weights that can be tuned based on experience, making them capable of **learning** and **retrieving** messages.

They may be represented in two equivalent ways:

Weighted, Undirected Graphs



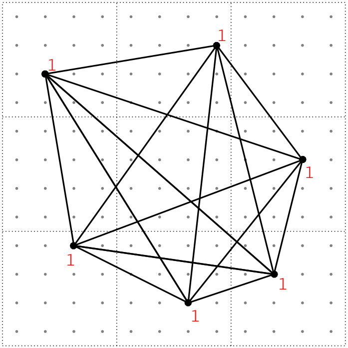
Nodes represent neurons, whereas edges are their interconnections.
They always generate fully connected polyhedra.

Connections Matrices

$$\begin{matrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{matrix}$$

Each of the elements expresses the activation of a cell, hence the weight of the connections between couple of nodes.

ADOPTED MODEL



Peculiar properties of the adopted model, can be expressed by:

→ **Binary Connections Weights**
Ones in the matrix establish active nodes, i.e. they identify only the existence of edges among nodes.

→ **Clustered neural activations**
The connections matrix is partitioned in such a way that only unique activations occur within each cluster.

The activation co-occurrences within clusters identify a fully connected sub-graph, or **Connections Pattern**.

FUNCTIONALITIES

Learning Rule

Considering $\mathbf{z}$ to be one of the **binary messages** in the **learning set** $\mathcal{Z}$ with a clustered structure, the **adjacency connections matrix** $W(\mathcal{Z})$ is generated as:

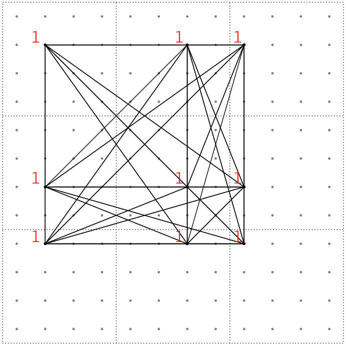
$$W(\mathcal{Z}) = g\left[\sum_{\mathbf{z}\in\mathcal{Z}} \left(\mathbf{z}\cdot\mathbf{z}^T\right)\right], \quad g(\xi) = \begin{cases} 1 & \text{if } \xi > 0 \\ 0 & \text{otherwise} \end{cases}, \; \xi \in \mathbb{Z}^*$$

Polling Rule

Being $\mathbf{z}_0$ a **binary query message**, still matching the clustering structure, the polling rule for the neural network trained by the set $\mathcal{Z}$ is expressed by the **score**:

$$s(\mathbf{z}_0, \mathcal{Z}) = \frac{\mathbf{z}_0^T \cdot W(\mathcal{Z}) \cdot \mathbf{z}_0}{(\mathbf{z}_0^T \cdot \mathbf{z}_0)^2}, \in [0,1] \subset \mathbb{R}$$

MOTIVATIONS OF USE



The choice of a binary, clustered model is motivated by many reasons:

→ Binary connection weights
Reduced **computational complexity** and preserve **memory occupancy**.

→ Clustered nodes structure
The learning process acts as **patterns overlapping**.
Clusters prevent from generating **false connections patterns**.

→ Adjacency connections matrix
For its **symmetry**, it carries a lot of **redundancy**, making it robust to **noise or memory faults**.

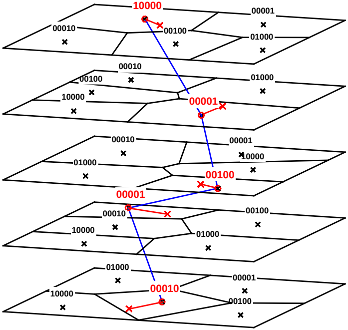
TRAINING STAGE

TRAINING STAGE OUTLINE

Set of operations executed offline, preparatory to the Query stage.

- Run a first **Coarse Vector Quantization**
  - → Build the Quantization Grids over m_c **layers**, each of them composed of k_c **centroids**, obtained by running k-means;
  - → Assign each data point to a **Quantization Pattern**.
- Go to the **Neural Networks Learning Stage**
  - → Convert the quantized data points to **binary messages**, so that they can be leant by binary neural networks.
  - → Identify L **learning sets** of binary messages to be learnt.
  - → applying the **learning rule** over all of the neural networks.

CLUSTERED BINARY LABELLING



$$\mathbf{z} = [\mathbf{10000\ 00001\ 00100\ 00001\ 00010}]$$

Quantization Patterns → Connections Patterns

Centroids Layers → Networks Clusters

It is performed a **Binary Labelling**:

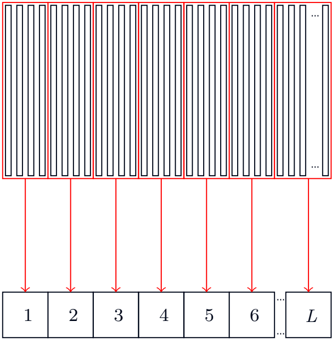
- → All of the centroids, over each layer are associated to **unitary Hamming weight**, from the canonical basis of order k.
- → For the network structure, only a **single activation** is allowed for each cluster.

Once all of the vectors are labelled, the whole search space is mapped to its binary version.

At this point, it is foreseen the use of a preprocessing step, aiming to partition the search space in a convenient way.

PREPROCESSING FOR ALLOCATION

Binary Labelled Data Set



Learning Sets

↓

Neural Networks: apply Learning Rule

$$W(\mathcal{Z}_l) = g\left[\sum_{\mathbf{z}\in\mathcal{Z}_l} (\mathbf{z}\cdot\mathbf{z}^T)\right], \quad \forall l \in [\![1, L]\!]$$

The binary labelled data set of points is partitioned in $\boldsymbol{L}$ **disjoint learning sets.**

It is used a greedy approach, aiming to:

→ **Portion of ones in the matrices**
Minimize the mutual Hamming distance within each set, hence the diversity of messages.

→ **Constant diversity**
The diversity of messages has to be uniformly distributed among the L learning sets $\mathcal{Z}_l, \forall l \in [\![1, L]\!]$.

→ **Constant cardinality**
The partition has to be fair, hence $|\mathcal{Z}_l| = n = N/L, \forall l \in [\![1, L]\!]$, in such a way that cardinality reductions do not depend on the specific query.

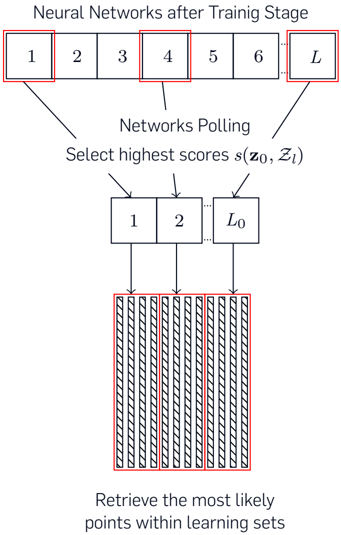
QUERY STAGE

QUERY STAGE OUTLINE

Set of operations executed on the run, when a query is performed.

- Resort to a **Neural Networks Polling**
  - → Compute the likelihood scores for all of the L networks;
  - → Select the **highest $\boldsymbol{L_0}$ scores** of likelihood;
  - → Retrieve the L_0 most likely **learning sets**.
- Apply a last **Fine Vector Quantization**
  - → Associated data points to a **fine** grid composed of $\boldsymbol{m_f}$ **layers**, with $\boldsymbol{k_f}$ **centroids** each;
  - → Approximate distance metrics with **reduced dispersion**.

NETWORKS POLLING



The selection of most likely sets is supposed to be performed as:

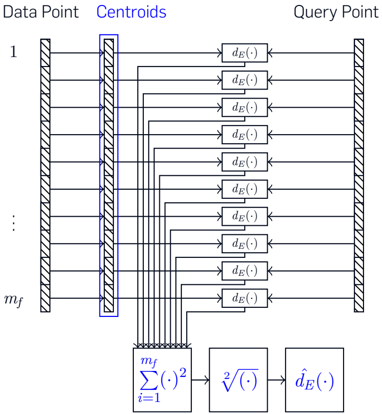
→ **Compute scores of likelihood**
For the query vector to be in the set $\mathcal{Z}_l$, learnt by the l^{th} neural network.

$$s(\mathbf{z}_0, \mathcal{Z}_l) = \frac{\mathbf{z}_0^T \cdot W(\mathcal{Z}_l) \cdot \mathbf{z}_0}{(\mathbf{z_0}^T \cdot \mathbf{z}_0)^2}, \ \forall l \in [\![1, L]\!]$$

→ **Select the highest L_0 scores**
That is, the vectors within the most likely learning sets.

Once the data points are retrieved, it is applied a better approximation to find the Nearest Neighbour with more precision.

FINE PRODUCT QUANTIZATION



Again, the quantization grid is computed empirically over the whole data set.

- → **Quantizing the data set**
  Each of the data points is associated to a fine quantization pattern.
- → **Distance Approximation**
  The distance among points is computed as the sum of distances over lower-dimensional sections.

To increase the reliability, it is foreseen the use of **multiple Recalls**.

It consists of iterative runs of the same technique, where solution obtained at each iteration is removed from the search space.

EMPIRICAL RESULTS

PERFORMANCES

→ **Metric of Evaluation**

The performances are measured in terms of success rate for **estimated solution to match the exhaustive one**, in a set of recalls of order r.

$$\eta_r = \begin{cases} 1 & \text{if } r\text{-th rank NN matches the exhaustive solution} \\ 0 & \text{otherwise} \end{cases}$$

→ **Computational Complexity**

Fine Product Quantization	Binary Clustered Networks
$\mathcal{O}(k_f d + \boxed{m_f N})$	$\mathcal{O}(k_f d + k_c d + \boxed{p_1 (m_c k_c)^2 L} + \boxed{m_f L_0 n})$
Distance Computation Fine Quantization	Coarse, Fine Quantization Scores Computation Distance Computation

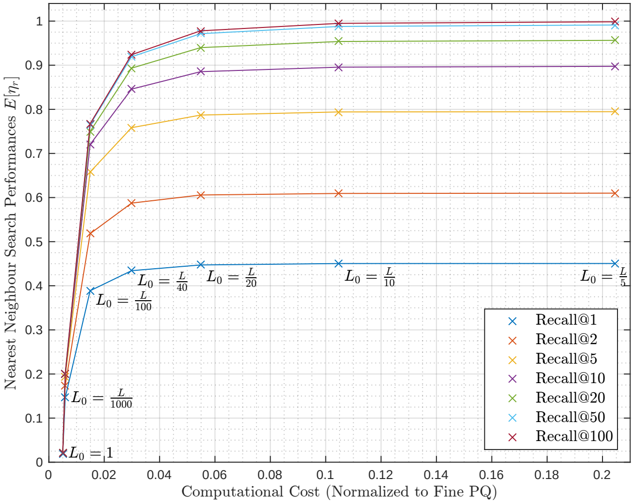
TESTED APPLICATIONS

Object Retrieval	Classification
Pictures querying within a large data collection, assuming the shape of SIFTs, i.e. extracted features local descriptors.	Identify labels associated to a large set of pictures containing handwritten digits, ranging from 0 to 9.
TEXMEX Group - INRIA, Rennes.	**MNIST Database - Yann LeCun**

In both cases, **all of the parameters of interest are trained** to work at the best settings compromise.

The achieved results are shown in the next couple of slides.

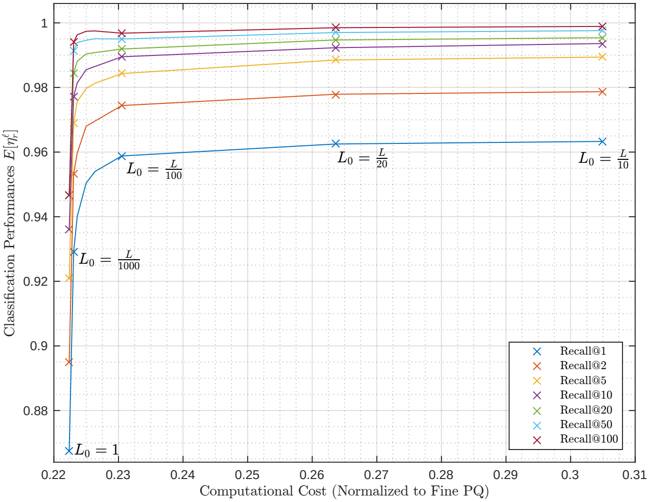
PERFORMANCES: OBJECT RETRIEVAL



Parameters list:

- Dimensionality $d = 128$
- Cardinality $N = 1000000$
- Coarse PQ $k_c = 2, m_c = 32$
- Fine PQ $k_f = 16, m_f = 256$
- Number of networks $L = 10000$

PERFORMANCES: CLASSIFICATION



Parameters list:

- Dimensionality $d = 784$
- Cardinality $N = 60000$
- Coarse PQ $k_c = 2, m_c = 32$
- Fine PQ $k_f = 16, m_f = 256$
- Number of networks $L = 2000$

CONCLUSIONS

CONCLUSIONS

This work illustrates the interest of using the introduced neural networks model to accelerate ANN search over real applications.

Future works may include different new proposals, such as:

→ Getting rid of the **Fine search** stage by implementing message retrieval strategies based with a Bayesian approach;

→ Trying to use a **Hierarchical approach**, consisting in cascading different granularity layers;

→ Proposing **refined allocation strategies** to choose which vector should be stored in which networks;

e.g. Group testing, hence the selection of non-disjoint sets

Thank you for your kind attention.

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Neural associative memories as accelerators for binary vector search.
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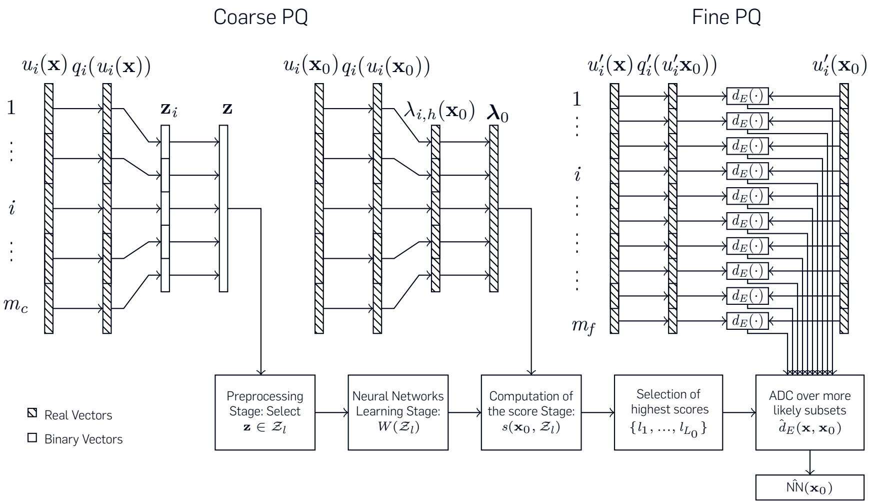
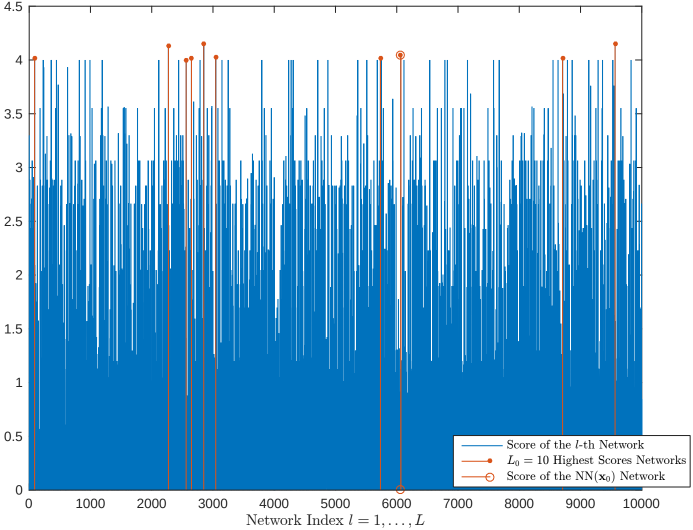
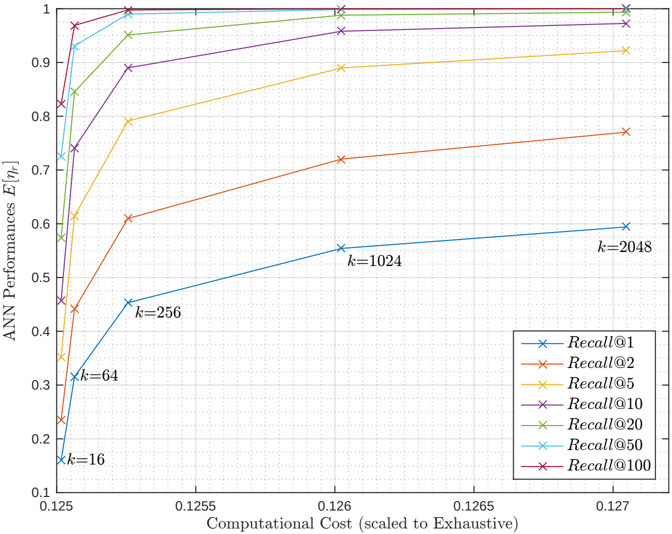
BACKUP - OVERALL TECHNIQUE SCHEME



BACKUP - RELIABILITY OF THE SCORES



BACKUP - SELECTING PARAMETERS: PQ PERFORMANCES



BACKUP - SELECTING PARAMETERS: CAOARSE GRANULARITY