Self-Taught Hashing for Fast Similarity Search

Dell Zhang, Jun Wang, Deng Cai, Jinsong Lu

Birkbeck, University of London
dell.z@ieee.org

The 33rd Annual ACM SIGIR Conference
19-23 July 2010, Geneva, Switzerland
Outline

1. Problem
2. Related Work
3. Our Approach
4. Experiments
5. Conclusion
Problem

Similarity Search (aka Nearest Neighbour Search)

— Given a query document, find its most similar documents from a large document collection

- Information Retrieval tasks
  - near-duplicate detection, plagiarism analysis, collaborative filtering, caching, content-based multimedia retrieval, etc.
- k-Nearest-Neighbours (kNN) algorithm
  - text categorisation, scene completion/recognition, etc.

“The unreasonable effectiveness of data”
If a map could include every possible detail of the land, how big would it be?
A promising way to accelerate similarity search is **Semantic Hashing**

- Design compact *binary* codes for a large number of documents so that semantically similar documents are mapped to similar codes (within a short Hamming distance)
  - Each code can be regarded as a *cluster*
  - Clustering similar documents into nearby codes (buckets) in the hash table
- Then similarity search can done extremely fast by just checking a few nearby codes (memory addresses)
  - For example, 0000 $\rightarrow$ 0000, 1000, 0100, 0010, 0001.
Problem
Problem
Related Work

Fast (Exact) Similarity Search in a *Low*-Dimensional Space

- Space-Partitioning Index
  - KD-tree, etc.
- Data Partitioning Index
  - R-tree, etc.
Related Work

Figure: An example of KD-tree (by Andrew Moore).
Related Work

Fast (Approximate) Similarity Search in a \textit{High}-Dimensional Space

- Data-Oblivious Hashing
  - Locality-Sensitive Hashing (LSH)
- Data-Aware Hashing
  - binarised Latent Semantic Indexing (LSI), Laplacian Co-Hashing (LCH)
  - stacked Restricted Boltzmann Machine (RBM)
  - boosting based Similarity Sensitive Coding (SSC) and Forgiving Hashing (FgH)
  - \textbf{Spectral Hashing (SpH)} — \textit{the state of the art}
    - Restrictive assumption: the data are uniformly distributed in a hyper-rectangle
## Related Work

**Table:** Typical techniques for accelerating similarity search.

<table>
<thead>
<tr>
<th>low-dimensional space</th>
<th>exact similarity search</th>
<th>data-aware</th>
<th>KD-tree, R-tree</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>data-oblivious</td>
<td>LSH</td>
</tr>
<tr>
<td>high-dimensional space</td>
<td>approximate similarity search</td>
<td>data-aware</td>
<td>LSI, LCH, RBM, SSC, FgH, SpH, STH</td>
</tr>
</tbody>
</table>

D. Zhang (Birkbeck) Self-Taught Hashing SIGIR 2010 11 / 40
Outline

1. Problem
2. Related Work
3. Our Approach
4. Experiments
5. Conclusion
Our Approach

Input:
- \( X = \{x_i\}_{i=1}^n \subset \mathbb{R}^m \)

Output:
- \( f(x) \in \{-1, +1\}^l \): hash function
  - \(-1 = \) bit off; \(+1 = \) bit on
  - \( l \ll m \)
Our Approach

Figure: The proposed STH approach to semantic hashing.
Our Approach

Stage 1: Learning of Binary Codes

- Let $y_i \in \{-1, +1\}$ represent the binary code for document vector $x_i$
  - $-1 = \text{bit off}; \ +1 = \text{bit on}$.
- Let $Y = [y_1, \ldots, y_n]^T$
Our Approach

Criterion 1a: Similarity Preserving

- We focus on the *local* structure of data
- $N_k(x)$: the set of $k$-nearest-neighbours of document $x$
- The local similarity matrix $W$
  - i.e., the adjacency matrix of the $k$-nearest-neighbours graph
  - symmetric and sparse

$W_{ij} = \begin{cases} 
\left( \frac{x_i^T}{\|x_i\|} \right) \cdot \left( \frac{x_j}{\|x_j\|} \right) & \text{if } x_i \in N_k(x_j) \text{ or } x_j \in N_k(x_i) \\
0 & \text{otherwise}
\end{cases}$

$W_{ij} = \begin{cases} 
\exp \left( -\frac{\|x_i-x_j\|^2}{2\sigma^2} \right) & \text{if } x_i \in N_k(x_j) \text{ or } x_j \in N_k(x_i) \\
0 & \text{otherwise}
\end{cases}$
Figure: The local structure of data in a high-dimensional space.
Our Approach

Figure: Manifold analysis: exploiting the local structure of data.
Our Approach

Criterion 1a: Similarity Preserving

- The Hamming distance between two codes $y_i$ and $y_j$ is

  \[
  \|y_i - y_j\|^2 \\
  \frac{4}{4}
  \]

- We minimise the weighted total Hamming distance, as it incurs a heavy penalty if two similar documents are mapped far apart

  \[
  \sum_{i=1}^{n} \sum_{j=1}^{n} W_{ij} \|y_i - y_j\|^2 \\
  \frac{4}{4}
  \]

- The squared error of distance would lead to a non-convex optimisation problem
Our Approach

Spectral Methods for Manifold Analysis
— Minimising Cut-Size

For single-bit codes $f = (y_1, \ldots, y_n)^T$:

$$S = \sum_{i=1}^{n} \sum_{j=1}^{n} W_{ij} \frac{(y_i - y_j)^2}{4} = \frac{1}{4} f^T L f$$

- Laplacian matrix $L = D - W$
- $D = \text{diag}(k_1, \ldots, k_n)$ where $k_i = \sum_j W_{ij}$
Our Approach

Spectral Methods for Manifold Analysis
— Minimising Cut-Size

Figure: Spectral graph partitioning through *Normalised Cut.*
Our Approach

Spectral Methods for Manifold Analysis
— Minimising Cut-Size

- Real relaxation
  - Requiring $y_i \in \{-1, +1\}$ makes the problem NP hard
  - Substitute $\tilde{y}_i \in \mathbb{R}$ for $y_i$
- $L$ is positive semi-definite
  - Eigenvalues: $0 = \lambda_1 = \ldots = \lambda_z < \lambda_{z+1} \leq \ldots \leq \lambda_n$
  - Eigenvectors: $u_1, \ldots, u_z, u_{z+1}, \ldots, u_n$
- Optimal non-trivial division: $f = u_{z+1}$
  - The number of edges across clusters is small
Our Approach

Spectral Methods for Manifold Analysis
— Minimising Cut-Size

For $l$-bit codes $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_n]^T$:

$$S = \sum_{i=1}^{n} \sum_{j=1}^{n} W_{ij} \frac{\|\mathbf{y}_i - \mathbf{y}_j\|^2}{4} = \frac{1}{4} \text{Tr}(\mathbf{Y}^T L \mathbf{Y})$$

- Let $\tilde{\mathbf{Y}}$ be the real relaxation of $\mathbf{Y}$
Our Approach

Spectral Methods for Manifold Analysis
— Minimising Cut-Size

- Laplacian Eigenmap (LapEig)

\[
\arg\min_{\tilde{Y}} \quad \text{Tr}(\tilde{Y}^T L \tilde{Y}) \\
\text{subject to} \quad \tilde{Y}^T D \tilde{Y} = I \\
\tilde{Y}^T D 1 = 0
\]

- Generalised Eigenvalue Problem

\[
L v = \lambda D v \\
\tilde{Y} = [v_1, \ldots, v_l]
\]
Our Approach

Criterion 1b: Entropy Maximising

Best utilisation of the hash table
= Maximum entropy of the codes
= Uniform distribution of the codes (each code has equal probability)

- The $p$-th bit is on for half of the corpus and off for the other half

$$y_i^{(p)} = \begin{cases} 
+1 & \tilde{y}_i^{(p)} \geq \text{median}(v_p) \\
-1 & \text{otherwise}
\end{cases}$$

- The bits at different positions are almost mutually uncorrelated, as the eigenvectors given by LapEig are orthogonal to each other
Our Approach

Stage 2: Learning of Hash Function

How to get the codes for new documents previously unseen? — Out-of-Sample Extension

- High computational complexity
  - Nystrom method
  - Linear approximation (e.g., LPI)
- Restrictive assumption about data distribution
  - Eigenfunction approximation (e.g., SpH)
Our Approach

Stage 2: Learning of Hash Function

- We reduce it to a supervised learning problem
  - Think of each bit $y_i^{(p)} \in \{+1, -1\}$ in the binary code for document $x_i$ as a binary class label (class-“on” or class-“off”) for that document
  - Train a binary classifier $y^{(p)} = f^{(p)}(x)$ on the given corpus that has already been “labelled” by the 1st stage
  - Then we can use the learned binary classifiers $f^{(1)}, \ldots, f^{(l)}$ to predict the $l$-bit binary code $y^{(1)}, \ldots, y^{(l)}$ for any query document $x$
Our Approach

Kernel Methods for *Pseudo*-Supervised Learning
— Support Vector Machine (SVM)
\[
y^{(p)} = f^{(p)}(x) = \text{sgn}(w^T x)
\]

\[
\begin{align*}
\text{arg min}_{w, \xi_i \geq 0} & \quad \frac{1}{2} w^T w + \frac{C}{n} \sum_{i=1}^{n} \xi_i \\
\text{subject to} & \quad \forall_{i=1}^{n} : y_i^{(p)} w^T x_i \geq 1 - \xi_i
\end{align*}
\]

- large-margin classification $\rightarrow$ good generalisation
- linear/non-linear kernels $\rightarrow$ linear/non-linear mapping
- convex optimisation $\rightarrow$ global optimum
Our Approach

Self-Taught Hashing (STH): The **Learning** Process

1. **Unsupervised Learning of Binary Codes**
   - Construct the $k$-nearest-neighbours graph for the given corpus
   - Embed the documents in an $l$-dimensional space through LapEig (1) to get an $l$-dimensional real-valued vector for each document
   - Obtain an $l$-bit binary code for each document via thresholding the above vectors at their median point, and then take each bit as a binary class label for that document

2. **Supervised Learning of Hash Function**
   - Train $l$ SVM classifiers (2) based on the given corpus that has been “labelled” as above
Our Approach

Self-Taught Hashing (STH): The **Prediction** Process

1. Classify the query document using those \( l \) learned classifiers
2. Assemble the output \( l \) binary labels into an \( l \)-bit binary code
Our Approach

The Computational Complexity of STH

- The Learning Process (offline)
  - quadratic w.r.t. the number of documents in the corpus
  - linear w.r.t. the average size of the documents in the corpus

- The Prediction Process (online)
  - linear w.r.t. the size of the query document
    - the linear projection matrix would be sparse, unlike the LSH.
Experiments

Text Datasets

- **Reuters21578**
  - Top 10 categories
  - 7285 documents
  - ModeApt split: 5228 (75%) training, 2057 (28%) testing

- **20Newsgroups**
  - All 20 categories
  - 18846 documents
  - ‘bydate’ split: 11314 (60%) training, 7532 (40%) testing

- **TDT2 (NIST Topic Detection and Tracking)**
  - Top 30 categories
  - 9394 documents
  - random split (x10): 5597 (60%) training, 3797 (40%) testing
Figure: The $F_1$ measure of STH for retrieving original nearest neighbours.
Experiments

Figure: The precision-recall curve for retrieving original nearest neighbours.

(a) Reuters21578  (b) 20Newsgroups  (c) TDT2
Figure: The $F_1$ measure of STH for retrieving same-topic documents.
Experiments

(a) Reuters21578  
(b) 20Newsgroups  
(c) TDT2

Figure: The precision-recall curve for retrieving same-topic documents.
Conclusion

- Major Contribution: Self-Taught Hashing
  - Unsupervised Learning + Supervised Learning
  - Spectral Method + Kernel Method

- Extensions (in the FGSIR Workshop on 23 Jul 2010)
  - Kernelisation
  - Supervision

- Future Work
  - Implementation using MapReduce
  - Applications in Multimedia IR
Thanks!

8-}