Extensions to Self-Taught Hashing: Kernelisation and Supervision

Dell Zhang, Jun Wang, Deng Cai, Jinsong Lu

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

The SIGIR 2010 Workshop on
Feature Generation and Selection for Information Retrieval (FGSIR)

23 July 2010, Geneva, Switzerland

Outline

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?

Problem

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 bit can be regarded as a binary **feature**
  - Generating a few most informative binary features to represent the documents
- Then similarity search can done extremely fast by just checking a few nearby codes (memory addresses)
  - For example, 0000 $\Longrightarrow$ 0000, 1000, 0100, 0010, 0001.

Problem

Problem

Outline

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

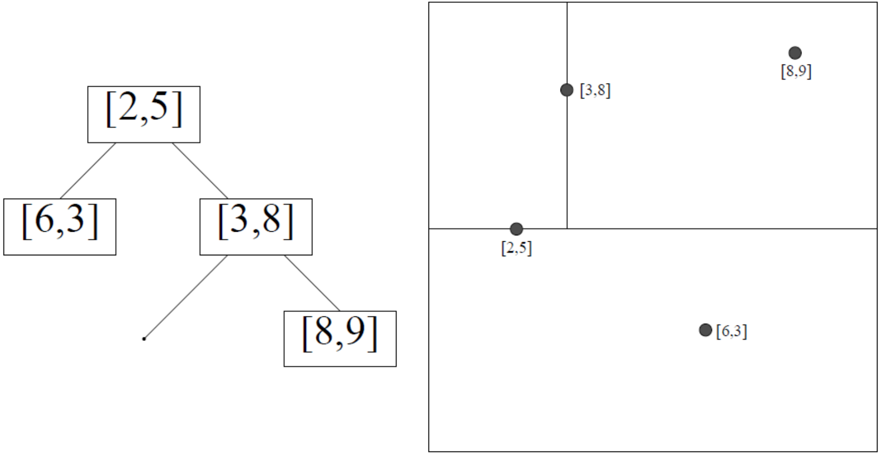


Figure: An example of KD-tree (by Andrew Moore).

Related Work

Fast (Approximate) Similarity Search in a *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)
  - **Spectral Hashing (SpH)** — *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.

low-dimensional space	exact similarity search	data-aware	KD-tree, R-tree
high-dimensional space	approximate similarity search	data-oblivious	LSH
		data-aware	LSI, LCH, RBM, SSC, FgH, SpH, STH

Outline

Review of STH

Input:

- $X = \{\mathbf{x}_i\}_{i=1}^{n} \subset \mathbb{R}^m$

Output:

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

Review of STH

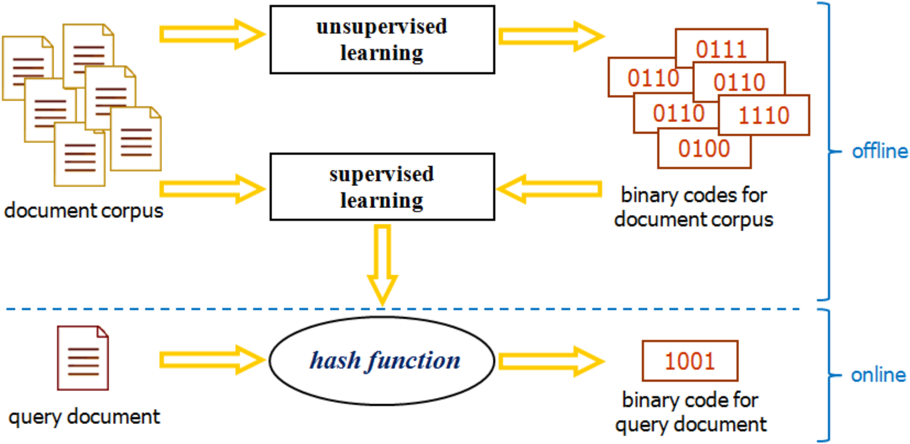


Figure: The proposed STH approach to semantic hashing.

Review of STH

Stage 1: Learning of Binary Codes

- Let $\mathbf{y}_i \in \{-1, +1\}^l$ represent the binary code for document vector $\mathbf{x}_i$
  - $-1 =$ bit off; $+1 =$ bit on.
- Let $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_n]^T$

Review of STH

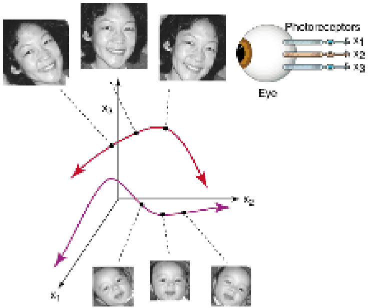
Criterion 1a: Similarity Preserving

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

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

$$W_{ij} = \begin{cases} \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right) & \text{if } \mathbf{x}_i \in N_k(\mathbf{x}_j) \text{ or } \mathbf{x}_j \in N_k(\mathbf{x}_i) \\ 0 & \text{otherwise} \end{cases}$$

Review of STH



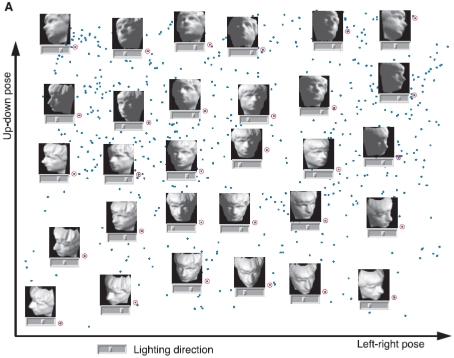


Figure: The local structure of data in a high-dimensional space.

Review of STH

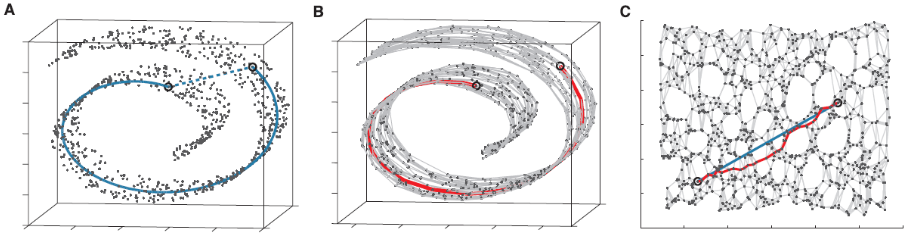


Figure: Manifold analysis: exploiting the local structure of data.

Review of STH

Criterion 1a: Similarity Preserving

- The Hamming distance between two codes y_i and y_j is

$$\frac{\|\mathbf{y}_i - \mathbf{y}_j\|^2}{4}$$

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

$$\sum_{i=1}^{n} \sum_{j=1}^{n} W_{ij} \frac{\|\mathbf{y}_i - \mathbf{y}_j\|^2}{4}$$

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

Review of STH

Spectral Methods for Manifold Analysis
— Minimising Cut-Size

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

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

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

Spectral Methods for Manifold Analysis
— Minimising Cut-Size

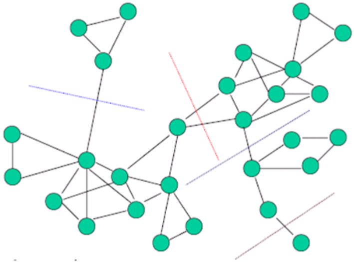


Figure: Spectral graph partitioning through *Normalised Cut*.

Review of STH

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
- $\mathbf{L}$ is positive semi-definite
  - eigenvalues: $0 = \lambda_1 = \ldots = \lambda_z < \lambda_{z+1} \leq \ldots \leq \lambda_n$
  - eigenvectors: $\mathbf{u}_1, \ldots, \mathbf{u}_z, \mathbf{u}_{z+1}, \ldots, \mathbf{u}_n$
- Optimal non-trivial division: $\mathbf{f} = \mathbf{u}_{z+1}$
  - The number of edges across clusters is small

Review of STH

Spectral Methods for Manifold Analysis
— Minimising Cut-Size

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

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

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

Review of STH

Spectral Methods for Manifold Analysis
— Minimising Cut-Size

- Laplacian Eigenmap (LapEig)

$$
\begin{aligned}
\arg\min_{\tilde{\mathbf{Y}}} \quad & \mathrm{Tr}(\tilde{\mathbf{Y}}^T \mathbf{L} \tilde{\mathbf{Y}}) \\
\text{subject to} \quad & \tilde{\mathbf{Y}}^T \mathbf{D} \tilde{\mathbf{Y}} = \mathbf{I} \\
& \tilde{\mathbf{Y}}^T \mathbf{D} \mathbf{1} = \mathbf{0}
\end{aligned}
$$

- Generalised Eigenvalue Problem

$$
\mathbf{L}\mathbf{v} = \lambda \mathbf{D}\mathbf{v} \tag{1}
$$

$$
\tilde{\mathbf{Y}} = [\mathbf{v}_1, \ldots, \mathbf{v}_l]
$$

Review of STH

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

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

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

Review of STH

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)

Review of STH

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 $\mathbf{x}_i$ as a binary class label (class-"on" or class-"off") for that document
  - Train a binary classifier $y^{(p)} = f^{(p)}(\mathbf{x})$ 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 $\mathbf{x}$

Review of STH

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

$$\begin{aligned} \underset{\mathbf{w},\xi_i \geq 0}{\arg\min} \quad & \frac{1}{2}\mathbf{w}^T\mathbf{w} + \frac{C}{n}\sum_{i=1}^{n} \xi_i \\ \text{subject to} \quad & \forall_{i=1}^{n} : y_i^{(p)} \mathbf{w}^T \mathbf{x}_i \geq 1 - \xi_i \end{aligned} \tag{2}$$

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

Review of STH

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

Review of STH

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

Outline

Extension I: Kernelisation

In the second stage of STH, we rewrite the SVM quadratic optimisation problem (2) into its dual form

$$\begin{aligned} \arg\min_{\alpha} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y_i^{(p)} y_j^{(p)} \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j \qquad (3) \\ \text{subject to} \quad & 0 \leq \alpha_i \leq C, \quad i = 1, \ldots, n \\ & \sum_{i=1}^{n} \alpha_i y_i^{(p)} = 0 \end{aligned}$$

and replace the inner product between $\mathbf{x}_i$ and $\mathbf{x}_j$ by a nonlinear kernel such as the Gaussian kernel:

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right) \qquad (4)$$

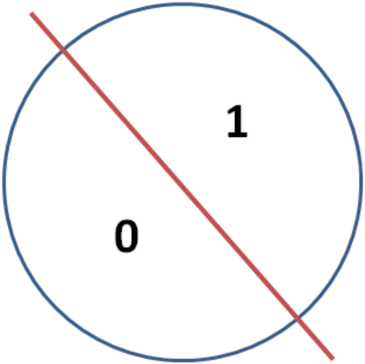
Extension I: Kernelisation

Then the p-th bit (i.e., binary feature) of the binary code for a query document $\mathbf{x}$ would be given by

$$f^{(p)}(\mathbf{x}) = \mathrm{sgn}\left(\sum_{i=1}^{n} \alpha_i y_i^{(p)} K(\mathbf{x}, \mathbf{x}_i)\right) \tag{5}$$

which is a nonlinear mapping.

Extension I: Kernelisation



- For example, using 16-bit binary codes,
  - linear hashing: $2l = 2 \times 16 = 32$ sectors
  - nonlinear hashing: $2^l = 2^{16} = 65536$ pieces

Extension I: Kernelisation

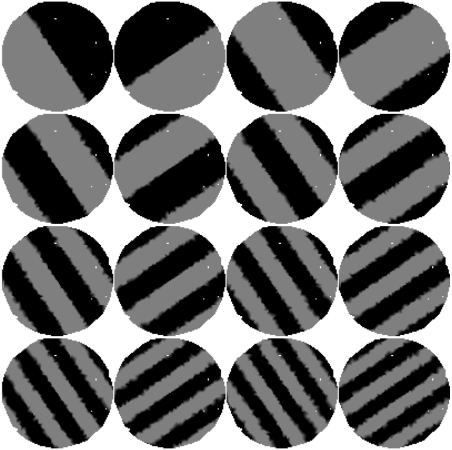


Figure: The 16-bit hash function for the pie dataset using SpH.

Extension I: Kernelisation

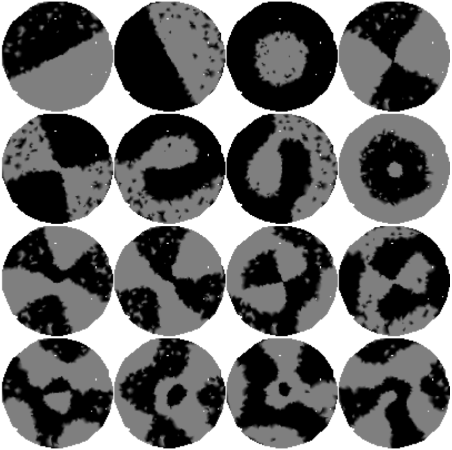


Figure: The 16-bit hash function for thepie dataset using STH.

Extension I: Kernelisation

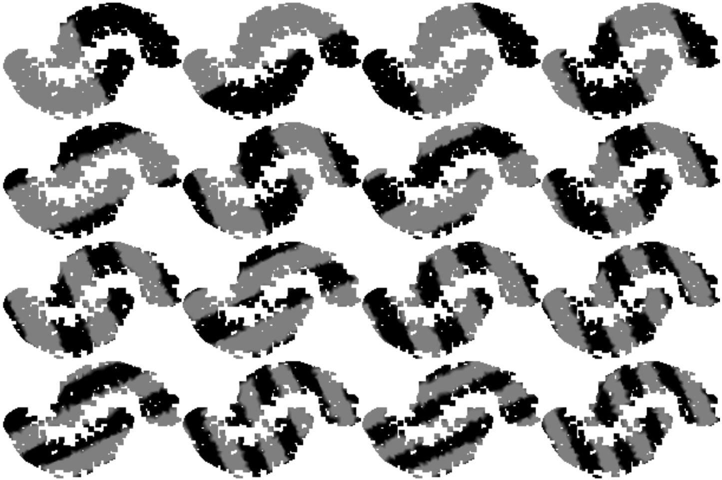


Figure: The 16-bit hash function for the two-moon dataset using SpH.

Extension I: Kernelisation

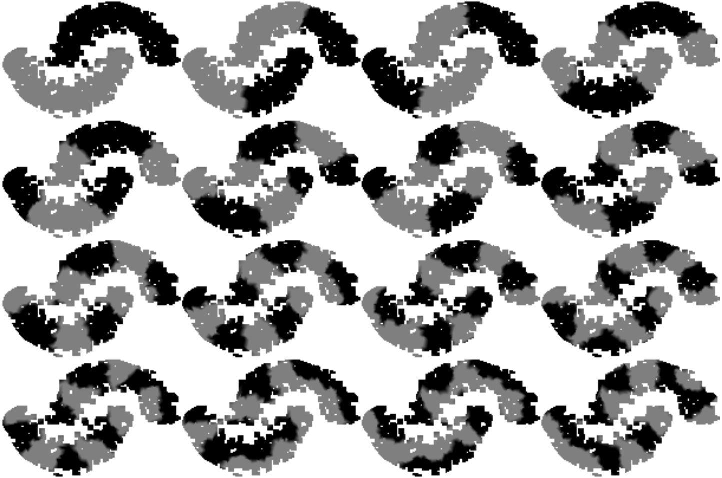


Figure: The 16-bit hash function for the two-moon dataset using STH.

Extension II: Supervision

In the first stage of STH, we make use of the class label information in the construction of k-nearest-neighbour graph for LapEig: a training document $\mathbf{x}$'s k-nearest-neighbourhood $N_k(\mathbf{x})$ would only contain k documents in the same class as $\mathbf{x}$ that are most similar to $\mathbf{x}$.

Let **STHs** denote such a supervised version of STH to distinguish it from the standard unsupervised version of STH.

Extension II: Supervision

Why not use SVMs directly?

kNN still has its advantages over SVMs in some aspects.

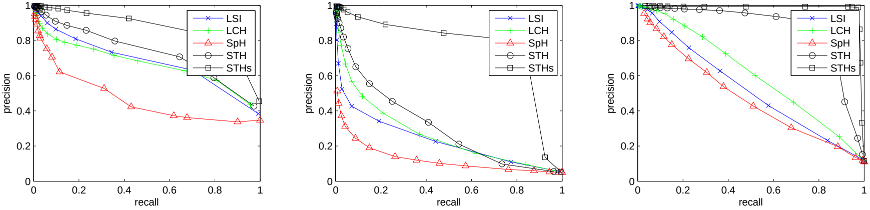
- For example, if there are 1000 classes,
  - the multi-class SVM approach may need 1000 binary SVM classifiers using the one-vs-rest ensemble scheme
  - the kNN (on top of STH) approach using 16-bit binary codes would only require 16 binary SVM classifiers

Extension II: Supervision

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

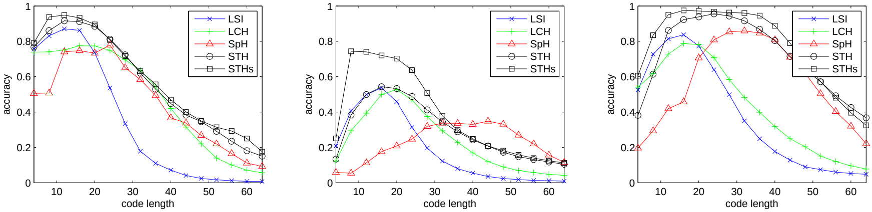
Extension II: Supervision



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

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

Extension II: Supervision



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

Figure: The accuracy of approximate kNN classification (via hashing).

Outline

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

Question Time

Thanks!

8-)