SketchSort: An Efficient Nearest Neighbor Graph Construction Method

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Outline

• Motivation
• Method
• Experiments and Results
Data represented as vector

Text

Vector

$x_t=(1, 0, 1, 0, 0, ...)$

Image

$\mathbf{x}_i=(0.2, -0.3, -1.3, 1.2, 2.2, ...)$

Chemical Compound, Protein, DNA/RNA etc
Locality Sensitive Hashing
(Gionis et al,99)

- Mapping vector to binary string (sketch)
- Conserve the distance in the original space
  - Enable to store gigascale data in main memory
  - Speed up learning algorithms

\[
x=(0.2, -0.3, -1.3, 1.2, 2.2, \ldots)
\]

\[
s=10101011101010101
\]
All Pairs Similarity Search

- Finding all neighbor pairs from sketches
  - Find all pairs \((i, j), i < j, \quad \Delta(x_i, x_j) \leq \epsilon\)
- Enable to build a neighborhood graph
  - semi-supervised learning, spectral clustering, ROI detection in images, retrieval of protein sequences
Single Sorting Method (SSM)

- Find neighbors by sorting sketches
  - Various applications ex) google news

(a) Input data
1: 101111
2: 110101
3: 110010
4: 010000
5: 101000
6: 101000
7: 111100
8: 010110
9: 110110
10: 100100

(b) Sort
7: 000000
4: 010000
8: 010110
10: 100100
5: 101000
1: 101111
3: 110010
2: 110101
9: 110110
6: 111100

(c) Scan neighbors
7: 000000
4: 010000
8: 010110
10: 100100
5: 101000
1: 101111
3: 110010
2: 110101
9: 110110
6: 111100
Drawbacks of Single Sorting

• Need a large number of distance calculation for achieving reasonable accuracy.

• Can not derive an analytic estimate of the fraction of missing neighbors.
Overview of SketchSort

- Employ the multiple sorting method (MSM) as a building block
  - Enumerate all pairs within Hamming distance $d$ from a string pool $S=\{s_1,\ldots,s_n\}$
- A number of distance calculation is significantly reduced
- A bound of the expected fraction of missing neighbors can be obtained.
Special case: Finding identical strings (d=0)

- Radix sort, and partition the strings into equivalence classes: \( O(n) \)
- Build edges between all pairs in equivalent classes: \( O(m) \)
- Complexity: \( O(n+m) \)
Multiple sorting method (d > 0)

- Mask d characters in all possible ways
- Perform radix sort $\binom{l}{d}$ times
- Time exponential to $d$, polynomial to the string length $l$
- Still linear to the number of strings!!

Ex) $d=2$

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<tr>
<th>7:000</th>
<th>0001 0011 1110</th>
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<tbody>
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<td>0001 1101 1100</td>
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<tr>
<td>8:010</td>
<td>1001 0111 1000</td>
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<tr>
<td>10:100</td>
<td>0011 1001 0111</td>
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<tr>
<td>5:101</td>
<td>0010 1110 1000</td>
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<tr>
<td>1:101</td>
<td>1111 0011 1110</td>
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<tr>
<td>2:110</td>
<td>0111 0111 0011</td>
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<tr>
<td>3:110</td>
<td>1000 1101 1110</td>
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<tr>
<td>9:110</td>
<td>1000 1101 1110</td>
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<tr>
<td>6:111</td>
<td>0011 1001 0111</td>
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</tbody>
</table>
Blockwise masking

- Mask d blocks in all possible ways
- The number of sotring operations reduced
- Non-neighbors might be detected

- Filtered out by calculating actual Hamming distances

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Ex) d=2
Recursive Algorithm

Figure 5: Updating equivalence classes in block concatenation. Strings in a block are sorted and equivalence classes (shown as square frames) are detected. A next block is concatenated to each equivalence class and sorted again.
SketchSort

• Basic idea: Map vectors to strings and apply MSM

• Not good: Create long strings and apply MSM at once

• Replication:
  - Create $Q$ independent string pools of length $l$
  - apply MSM to each string pool
  - Report the pairs less than a threshold $\varepsilon$

$$\Delta(x_i, x_j) \leq \varepsilon$$
Duplication Checks

- Block-level duplication check
  - Define dictionary order of blocks, and take only minimum combinations of blocks.
  - ex) $d=2$
    $\{1,2\}<\{1,3\}<\{1,4\}<\{2,3\}<\{2,4\}<\{3,4\}$
- Chunk-level duplication check
  - Take only minimum chunks.
Two types of errors

• True edges $E^*$, Our results $E$

• Type-I error (false positive): A non-neighbor pair has a Hamming distance within $d$ in at least one replicate

$$F_1 = \{(i, j) \mid (i, j) \in E, (i, j) \notin E^*\}.$$ 

• Type II-error (false negative): A neighbor pair has a Hamming distance larger than $d$ in all replicates

$$F_2 = \{(i, j) \mid (i, j) \notin E, (i, j) \in E^*\}.$$
Bound of type-II error: Missing edge ratio

- Basically, type-II error is more crucial - type-I errors are filtered out by distance calculations

- Missing edge ratio (type-II error) is bounded as

$$E \left[ \frac{|F_2|}{|E^*|} \right] \leq \left( 1 - \sum_{k=0}^{[d]} \binom{\ell}{k} p^k (1-p)^{\ell-k} \right)^Q,$$

where $p$ is an upper bound of the non-collision probability of neighbors

$$p = \frac{\arccos(1 - \epsilon)}{\pi}.$$
Results for All Pairs Similarity Search

Faster and more accurate than recent methods

All pairs similarity search on MNIST and TinyImage datasets for cosine distance thresholds 0.10\(\pi\) (top) and 0.15\(\pi\) (bottom).
Results for 5-nearest neighbor search

Error rate for 5-nearest neighbor search on MNIST and TinyImage datasets
All Pairs Similarity Search in 1.6 Million Images

- Set parameters so as to keep missing edge ratio no more than $1.0 \times 10^{-6}$
- Enable to detect similar pairs nearly exactly
- Take only 4.3 hours for 1.6 million images

Near duplication detection in up to 1.6 million images at threshold $0.05\Pi$ (left), $0.10\Pi$ (middle) and $0.15\Pi$ (right)
A C++ implementation of SketchSort is available from http://code.google.com/p/sketchsort/

Introduction
SketchSort is a software for all pairs similarity search. It takes as an input data points and outputs approximately nearest neighbor pairs within a distance. First, the input data points are mapped to binary bit strings by locality sensitive hashing, and then nearest neighbor pairs of strings within a Hamming distance are enumerated by the multiple sorting method (3). Finally, the cosine distances for such nearest neighbor pairs are calculated. If the cosine distance for a nearest neighbor pair is no more than a user-specified threshold, the nearest neighbor pair is outputted. One might worry about missed nearest neighbor pairs by our method. A theoretical bound of the expectation of missing edge ratio is derived. It enables us to set parameters so as to limit the empirical missing edge ratio as small as possible.

Quick Start
To compile SketchSort, please type the followings:

```
tar -zxf sketchsort-0.0.tar.gz
cd sketchsort-0.0/
make
```
```
./sketchsort -hamdist 3 -numblocks 6 -cosdist 0.01 -numchunks 10 sample.txt outputfile
```

Usage
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