SketchSort: An Efficient Nearest Neighbor Graph Construction Method

Tabei, Yasuo

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SketchSort: An Efficient Nearest Neighbor Graph Construction Method

Yasuo Tabei
JST Minato Project, Sapporo, Japan

Outline

• Motivation
• Method
• Experiments and Results

Data represented as vector

Text
Vector

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

Chemical Compound, Protein, DNA/RNA etc

Vector

Image

"x_i = (0.2, -0.3, -1.3, 1.2, 2.2, ...)

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
    \( x = (0.2, -0.3, -1.3, 1.2, 2.2, ...) \)
    \( s = 10101011101010101 \)

All Pairs Similarity Search

• Finding all neighbor pairs from sketches
  - Find all pairs \((i, j), i < j, \Delta(x_i, x_j) \leq \epsilon\)
• 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

<table>
<thead>
<tr>
<th>(a) Input data</th>
<th>(b) Sort</th>
<th>(c) Scan neighbors</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:101111</td>
<td>7:000000</td>
<td>4:000000</td>
</tr>
<tr>
<td>2:110101</td>
<td>4:000000</td>
<td>8:010110</td>
</tr>
<tr>
<td>3:110010</td>
<td>8:010110</td>
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<tr>
<td>6:111100</td>
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<td>9:110110</td>
</tr>
<tr>
<td>10:100100</td>
<td>6:111100</td>
<td>6:111100</td>
</tr>
</tbody>
</table>
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!
- Still linear to the number of strings!!
- Ex) $d=2$

Blockwise masking

- Mask $d$ blocks in all possible ways
- The number of sorting operations reduced
- Non-neighbors might be detected
  - Filtered out by calculating actual Hamming distances
  - 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 \( \epsilon \)
    \[
    \Delta(x_i, x_j) \leq \epsilon
    \]

Duplication Checks

- Block-level duplication check
  - Define dictionary order of blocks, and take only minimum combinations of blocks. 
    \( \text{ex) } d=2 \)
    \( (1,2)<(1,3)<(1,4)<(2,3)<(2,4)<(3,4) \)
- 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

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/](http://code.google.com/p/sketchsort/)