Large Scale Learning with String Kernels

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joint work with
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1. Introduction

2. Linadd Algorithm

3. Experiments
Outline

1. Introduction
2. Linadd Algorithm
3. Experiments
Large Scale Problems

- **Text Classification (Spam, Web-Spam, Categorization)**
  - Task: Given $N$ documents, with class label $\pm 1$, predict text type.

- **Security (Network Traffic, Viruses, Trojans)**
  - Task: Given $N$ executables, with class label $\pm 1$, predict whether executable is a virus.

- **Biology (Promoter, Splice Site Prediction)**
  - Task: Given $N$ sequences around Promoter/Splice Site (label $+1$) and fake examples (label $-1$), predict whether there is a Promoter/Splice Site in the middle.

⇒ **Approach:** String kernel + Support Vector Machine
⇒ **Large $N$ is needed to achieve high accuracy** (i.e. $N = 10^7$)
Formally

- **Given:**
  - $N$ training examples $(x_i, y_i) \in (\mathcal{X}, \pm 1)$, $i = 1 \ldots N$
  - string kernel $K(x, x') = \Phi(x) \cdot \Phi(x')$

- **Examples:**
  - words-in-a-bag-kernel
  - k-mer based kernels (Spectrum, Weighted Degree)

- **Task:**
  - Train Kernelmachine on Large Scale Datasets, e.g. $N = 10^7$
  - Apply Kernelmachine on Large Scale Datasets, e.g. $N = 10^9$
String Kernels

- **Spectrum Kernel (with mismatches, gaps)**

  \[ K(x, x') = \Phi_{sp}(x) \cdot \Phi_{sp}(x') \]

- **Weighted Degree Kernel (with shift)**

  \[ k(s_1, s_2) = w_7 + w_1 + w_2 + w_2 + w_3 \]

For string kernels \( \mathcal{X} \) discrete space and \( \Phi(x) \) sparse
Kernel Machine Classifier:

\[ f(x) = \text{sign} \left( \sum_{i=1}^{N} \alpha_i y_i k(x_i, x) + b \right) \]

To compute output on all \( M \) examples:

\[ \forall j = 1, \ldots, M : \sum_{i=1}^{N} \alpha_i y_i k(x_i, x_j) + b \]

Computational effort:

- Single \( \mathcal{O}(NT) \) (\( T \) time to compute the kernel)
- All \( \mathcal{O}(NMT) \)

\( \Rightarrow \) Costly!

\( \Rightarrow \) Used in training and testing - worth tuning.

\( \Rightarrow \) How to further speed up if \( T = \text{dim}(\mathcal{X}) \) already linear?
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Linadd Speedup Idea

Key Idea: Store $w$ and compute $w \cdot \Phi(x)$ efficiently

$$\sum_{i=1}^{N} \alpha_i y_i k(x_i, x_j) = \sum_{i=1}^{N} \alpha_i y_i \Phi(x_i) \cdot \Phi(x_j) = w \cdot \Phi(x_j)$$

When is that possible?

1. $w$ has low dimensionality and sparse (e.g. $4^8$ for Feature map of Spectrum Kernel of order 8 DNA)
2. $w$ is extremely sparse although high dimensional (e.g. $10^{14}$ for Weighted Degree Kernel of order 20 on DNA sequences of length 100)

Effort: $\mathcal{O}(MT') \Rightarrow$ Potential speedup of factor $N$
Technical Remark

Treating \( w \)

- \( w \) must be accessible by some index \( u \) (i.e. \( u = 1 \ldots 4^8 \) for 8-mers of Spectrum Kernel on DNA or word index for word-in-a-bag kernel)

- Needed Operations
  - Clear: \( w = 0 \)
  - Add: \( w_u \leftarrow w_u + v \) (only needed \(|W|\) times per iteration)
  - Lookup: obtain \( w_u \) (must be highly efficient)

- Storage
  - **Explicit Map** (store dense \( w \)); Lookup in \( \mathcal{O}(1) \)
  - **Sorted Array** (word-in-bag-kernel: all words sorted with value attached); Lookup in \( \mathcal{O}(\log(\sum_u I(w_u \neq 0))) \)
  - **Suffix Tries, Trees**; Lookup in \( \mathcal{O}(K) \)
Datastructures - Summary of Computational Costs

Comparison of worst-case run-times for operations

- clear of \( w \)
- add of all k-mers \( u \) from string \( x \) to \( w \)
- lookup of all k-mers \( u \) from \( x' \) in \( w \)

<table>
<thead>
<tr>
<th></th>
<th>Explicit map</th>
<th>Sorted arrays</th>
<th>Tries</th>
<th>Suffix trees</th>
</tr>
</thead>
<tbody>
<tr>
<td>clear</td>
<td>( \mathcal{O}(</td>
<td>\Sigma</td>
<td>^d) )</td>
<td>( \mathcal{O}(1) )</td>
</tr>
<tr>
<td>add</td>
<td>( \mathcal{O}(l_x) )</td>
<td>( \mathcal{O}(l_x \log l_x) )</td>
<td>( \mathcal{O}(l_xd) )</td>
<td>( \mathcal{O}(l_x) )</td>
</tr>
<tr>
<td>lookup</td>
<td>( \mathcal{O}(l_{x'}) )</td>
<td>( \mathcal{O}(l_x + l_{x'}) )</td>
<td>( \mathcal{O}(l_{x'}d) )</td>
<td>( \mathcal{O}(l_{x'}) )</td>
</tr>
</tbody>
</table>

Conclusions

- Explicit map ideal for small \( |\Sigma| \)
- Sorted Arrays for larger alphabets
- Suffix Arrays for large alphabets and order (overhead!)
Support Vector Machine

Linadd **directly applicable** when applying the classifier.

\[
f(x) = \text{sign}\left(\sum_{i=1}^{N} \alpha_i y_i k(x_i, x) + b\right)
\]

**Problems**

- \(w\) may still be huge \(\Rightarrow\) fix by not constructing whole \(w\) but only blocks and computing batches

**What about training?**

- general purpose QP-solvers, Chunking, SMO
- optimize kernel (i.e. find \(O(L)\) formulation, where \(L = \text{dim}(\mathcal{X})\))
- **Kernel Caching infeasable**
  (for \(N = 10^6\) only 125 kernel rows fit in 1GiB memory)

\(\Rightarrow\) **Use linadd again: Faster + needs no kernel caching**
Analyzing Chunking SVMs (GPDT, SVM$^\text{light}$):

Training algorithm (chunking):

\[
\text{while optimality conditions are violated do} \\
\quad \text{select } q \text{ variables for the working set.} \\
\quad \text{solve reduced problem on the working set.} \\
\text{end while}
\]

- At each iteration, the vector \( f \), \( f_j = \sum_{i=1}^{N} \alpha_i y_i k(x_i, x_j) \), \( j = 1 \ldots N \) is needed for checking termination criteria and selecting new working set (based on \( \alpha \) and gradient w.r.t. \( \alpha \)).
- Avoiding to recompute \( f \), most time is spend computing “linear updates” on \( f \) on the working set \( W \)

\[
f_j \leftarrow f_j^{\text{old}} + \sum_{i \in W} (\alpha_i - \alpha_i^{\text{old}}) y_i k(x_i, x_j)
\]
Use \textit{linadd} to compute updates.

Update rule: \( f_j \leftarrow f_j^{old} + \sum_{i \in W} (\alpha_i - \alpha_i^{old}) y_i k(x_i, x_j) \)

Exploiting \( k(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j) \) and \( w = \sum_{i=1}^{N} \alpha_i y_i \Phi(x_i) \):

\[
  f_j \leftarrow f_j^{old} + \sum_{i \in W} (\alpha_i - \alpha_i^{old}) y_i \Phi(x_i) \cdot \Phi(x_j) = f_j^{old} + w^W \cdot \Phi(x_j)
\]

\((w^W \text{ normal on working set})\)

Observations

\begin{itemize}
  \item \( q := |W| \) is very small in practice \( \Rightarrow \) can effort more complex \( w \) and clear, add operation
  \item lookups dominate computing time
\end{itemize}
Recall we need to compute updates on $f$ (effort $c_1|W|LN$):

$$f_j \leftarrow f_j^{old} + \sum_{i \in W} (\alpha_i - \alpha_i^{old}) y_i k(x_i, x_j) \text{ for all } j = 1 \ldots N$$

Modified SVM$^\text{light}$ using “LinAdd” algorithm (effort $c_2\ell LN$, $\ell$ Lookup cost)

$$f_j = 0, \quad \alpha_j = 0 \text{ for } j = 1, \ldots, N$$

for $t = 1, 2, \ldots$ do

- Check optimality conditions and stop if optimal, select working set $W$ based on $f$ and $\alpha$, store $\alpha^{old} = \alpha$
- solve reduced problem $W$ and update $\alpha$
- clear $w$
- $w \leftarrow w + (\alpha_i - \alpha_i^{old}) y_i \Phi(x_i)$ for all $i \in W$
- update $f_j = f_j + w \cdot \Phi(x_j)$ for all $j = 1, \ldots, N$

end for

Speedup of factor \( \frac{c_1}{c_2 \ell} |W| \)
Parallelization

\[ f_j = 0, \alpha_j = 0 \text{ for } j = 1, \ldots, N \]

for \( t = 1, 2, \ldots \) do

Check optimality conditions and stop if optimal, select working set \( W \) based on \( f \) and \( \alpha \), store \( \alpha^{old} = \alpha \)

solve reduced problem \( W \) and update \( \alpha \)

clear \( w \)

\[ w \leftarrow w + (\alpha_i - \alpha_i^{old})y_i\Phi(x_i) \text{ for all } i \in W \]

update \( f_j = f_j + w \cdot \Phi(x_j) \) for all \( j = 1, \ldots, N \)

end for

Most time is still spent in update step \( \Rightarrow \) Parallize!

- transfer \( \alpha \) (or \( w \) depending on the communication costs and size)
- update of \( f \) is divided into chunks
- each CPU computes a chunk of \( f_I \) for \( I \subset \{1, \ldots, N\} \)
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Datasets

- Web Spam
  - Negative data: Use Webb Spam corpus
    http://spamarchive.org/gt/ (350,000 pages)
  - Positive data: Download 250,000 pages randomly from the web (e.g. cnn.com, microsoft.com, slashdot.org and heise.de)
  - Use spectrum kernel $k = 4$ using **sorted arrays** on 100,000 examples train and test (average string length 30Kb, 4 GB in total, 64bit variables $\Rightarrow$ 30GB)
Web Spam results

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<tr>
<th></th>
<th>N</th>
<th>100</th>
<th>500</th>
<th>5,000</th>
<th>10,000</th>
<th>20,000</th>
<th>50,000</th>
<th>70,000</th>
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<td>Spec</td>
<td>2</td>
<td>97</td>
<td>1977</td>
<td>6039</td>
<td>19063</td>
<td>94012</td>
<td>193327</td>
<td>-</td>
<td></td>
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<tr>
<td>LinSpec</td>
<td>3</td>
<td>255</td>
<td>4030</td>
<td>9128</td>
<td>11948</td>
<td>44706</td>
<td>83802</td>
<td>107661</td>
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<table>
<thead>
<tr>
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<th>Accuracy</th>
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<td>97.03</td>
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<tr>
<td></td>
<td>94.37</td>
<td>97.82</td>
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<td>99.43</td>
<td>99.59</td>
<td>99.61</td>
<td>99.64</td>
<td></td>
</tr>
</tbody>
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Speed and classification accuracy comparison of the spectrum kernel without (Spec) and with Linadd (LinSpec)
Splice Site Recognition

- Negative Data: 14,868,555 DNA sequences of fixed length 141 base pairs
- Positive Data: 159,771 Acceptor Splice Site Sequences
- Use WD kernel $k = 20$ (using Tries) and spectrum kernel $k = 8$ (using explicit maps) on 10,000,000 train and 5,028,326 examples
Linadd for WD kernel

For linear combination of kernels:

\[
\sum_{j \in W} (\alpha_j - \alpha_j^{old}) y_j k(x_i, x_j) \left( O(Ld | W | N) \right)
\]

use one tree of depth \( d \) per position in sequence

for Lookup use traverse one tree of depth \( d \) per position in sequence

Example \( d = 3 \):

output for \( N \) sequences of length \( L \) in \( O(Ld \cdot N) \)

\( d \) depth of tree \( \Delta \) degree of WD kernel

AAAATTTATGAAATTTATTTTCAAGTGCTGATGGAAACCGGAGAAAGAA
Spectrum Kernel on Splice Data

Number of training examples (logarithmic)

SVM training time in seconds (logarithmic)

Spec−Precompute
Spec−orig
Spec−linadd 1CPU
Spec−linadd 4CPU
Spec−linadd 8CPU
Weighted Degree Kernel on Splice Data

![Graph showing SVM training time in seconds versus number of training examples (logarithmic)]
Splice Site Recognition

More data helps

<table>
<thead>
<tr>
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<th>auPRC</th>
<th>N</th>
<th>auROC</th>
<th>auPRC</th>
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<td>100,000</td>
<td>96.14</td>
<td>47.61</td>
<td>10,000,000</td>
<td>96.03*</td>
<td>44.64*</td>
</tr>
</tbody>
</table>
Conclusions

- General speedup trick (clear, add, lookup operations) for string kernels
- Shared memory parallelization, able to train on 10 million human splice sites
- Linadd gives speedup of factor 64 (4) for Spectrum (Weighted Degree) kernel and 32 for MKL
- 4 CPUs further speedup of factor 3.2 and for 8 CPU factor 5.4
- Parallelized 8 CPU linadd gives speedup of factor 125 (21) for Spectrum (Weighted Degree) kernel, up to 200 for MKL

Discussion

- State-of-the-art accuracy
- Could we do better by encoding invariances?

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- Toolboxes,
- Languages for scientific computing

and should include
- A 4 page description,
- The code,
- A recognised open source license.

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