Fast Locality Sensitive Hashing for Beam Search on GPU

Xing Shi\textsuperscript{1}, Shizhen Xu\textsuperscript{2} and Kevin Knight\textsuperscript{1}

\textsuperscript{1}Department of Computer Science, University of Southern California
\{xingshi, knight\}@isi.edu
\textsuperscript{2}Department of Computer Science and Technology, Tsinghua University
xsz12@mails.tsinghua.edu.cn

\section*{Abstract}

We present a GPU-based Locality Sensitive Hashing (LSH) algorithm to speed up beam search for sequence models. We utilize the winner-take-all (WTA) hash, which is based on relative ranking order of hidden dimensions and thus resilient to perturbations in numerical values. Our algorithm is designed by fully considering the underling architecture of CUDA-enabled GPUs (Algorithm/Architecture Co-design): 1) A parallel Cuckoo hash table is applied for LSH code lookup (guaranteed $O(1)$ lookup time); 2) Candidate lists are shared across beams to maximize the parallelism; 3) Top frequent words are merged into candidate lists to improve performance. Experiments on 4 large-scale neural machine translation models demonstrate that our algorithm can achieve up to 4x speedup on softmax module, and 2x overall speedup without hurting BLEU on GPU.

\section{Introduction}

Beam search has been widely applied as the decoding technique of choice for Recurrent Neural Network (RNN) based text generation tasks, such as machine translation (Wu et al., 2016), summarization (Rush, Chopra, and Weston, 2015), image captioning (Xu et al., 2015) and poetry generation (Ghazvininejad et al., 2016). Decoding can be time consuming: 1) Most tasks generate target sentences in an on-line fashion, one token at a time, unlike batch mode used during training; 2) Decoding time is proportional to the beam size $B$, which is usually around 10 in machine translation and 50 in poetry generation; 3) Vocabulary size $V$ can be very large (tens of thousands), and the computational complexity of the two major components, Softmax andBeam expansion, are proportional to $V$. As Table 1 shows, these two parts occupy 46% and 30% of the decoding time respectively.

The major bottleneck for Softmax is the matrix multiplication between hidden states $H \in \mathbb{R}^{B \times d}$ and the word embedding matrix $E \in \mathbb{R}^{d \times |V|}$. As for Beam expansion, tremendous time is spent on transferring the output of Softmax $P \in \mathbb{R}^{B \times |V|}$ from device memory to host memory and the following heap-sort on CPU, with complexity $O(\log(B) \times |V|)$.

\begin{itemize}
\item[1.] The LSH schema used by Vijayanarasimhan et al. is not GPU-friendly: a) It uses a hash table on CPU to store the bucket key and word list, and the underlying data structure is usually a balanced binary search tree or linked list, both of which are hard to transport to GPU. b) It requires sorting to get the candidate lists, which can not easily parallelize on GPU. c) It processes each hidden vector in the batch one by one, whereas the matrix dot-product on GPU is calculated across the whole batch to fully take advantage of the GPU parallelism.
\item[2.] Beam search generally requires high recall of the top words according to the actual dot-product, because the error will accumulate fast as the sentence is built up. Whereas in practice, we find LSH alone does not delivery an adequate recall/speedup trade-off.
\end{itemize}

Our main contribution is to re-design the LSH algorithm on GPU for beam search to address the above-
| Device | Percent | Full Vocab | LSH | Speedup |
|--------|---------|------------|-----|---------|
| Total  | GPU+CPU | 100 %      | 1178.5 s | 574.3 s | 2.05   |
| Source side | GPU | 7 %       | 88 s     | 88.1 s  | 1.00   |
| Target side | GPU | 63 %      | 735.5 s  | 387.2 s | 1.90   |
| – Softmax | GPU | 43 %      | 505.3 s  | 157 s   | 3.22   |
| – 2nd layer | GPU | 10 %      | 113.7 s  | 113.7 s | 1.00   |
| – 1st layer | GPU | 10 %      | 115.2 s  | 115.2 s | 1.00   |
| Beam Expansion | GPU+CPU | 30 % | 352.4 s | 96.4 s  | 3.66   |
| – Device2Host data transfer | GPU+CPU | 12 % | 138.1 s | 25.8 s  | 5.35   |
| – Heapsort | CPU | 15 %      | 176 s    | 31.9 s  | 5.52   |
| – Hidden states reorder | GPU | 3 %       | 38.3 s   | 38.7 s  | 0.99   |
| Runtime vocab size | - | -         | 40,000   | 5,792   | 6.91   |
| BLEU   | -       | -         | 28.12    | 27.81   | -      |

Table 1: Time breakdown, runtime vocabulary size, and BLEU score of full vocabulary decoding and LSH decoding. The model is a 2-layer, 1000-hidden dimension, 40000 target vocabulary LSTM seq2seq model trained on a French to English corpus (Bojar et al., 2014). The experiments are conducted on a Nvidia K20 GPU and a single-core 2.4GHz Intel Xeon CPU. The code is compiled against CUDA 8.0.

Related Work

Several approaches have been proposed to speed up beam search for RNN-based generation tasks. The first line of research is to use specialized hardware, like Tensor Processing Unit (TPU) and low precision (Low-p) calculation (Wu et al., 2016). This method will usually speedup all parts of the neural models.

The second line tries to compress the original large model to a small model by weight pruning (WP) (See, Luong, and Manning, 2016) or sequence-level knowledge distillation (KD) (Kim and Rush, 2016). These methods require additional fine-tuning.

The third line is to modify the Softmax layer to speed up the decoding. Noise-contrastive estimation (NCE) (Gutmann and Hyvärinen, 2010) discriminates between the gold target word and $k (k << |V|)$ other sampled words. It has been successfully applied on several NLP tasks (Mnih and Teh, 2012; Vaswani et al., 2017; Williams et al., 2015; Zoph et al., 2016). Morin and Bengio introduces hierarchical softmax (H-softmax) where $\log_2 |V|$ binary classifications are performed rather than a single $|V|$-way classification. However, these two methods can only speedup training and still suffer at the decoding phase. Chen, Grangier, and Auli propose differentiated softmax (D-softmax) based on the idea that more parameters should be assigned for embeddings of frequent words and fewer for rare words. It can achieve speedups on both training and decoding.

The fourth line of research uses word alignments (WA) trained on the parallel corpus to construct a small runtime vocabulary for each sentence (Jean et al., 2015; Mi, Wang, and Ittycheriah, 2016; L’Hostis, Grangier, and Auli, 2016; Shi and Knight, 2017). However, this approach is only suitable for tasks where sensible alignments can be extracted, such as machine translation and summarization, and do not benefit tasks like image caption or poem generation.

Table 2 compares different speed up methods. Compared to these existing methods, LSH has the following advantages:

1. It is orthogonal to the first two lines of research. The first two lines of approaches do not decrease the ratio of the number of word embedding parameters to the number of the rest parameters. Thus, LSH can be applied for further speedup.

2. It is a machine learning free (ML-free) method, which means it can be used in plug-and-play style, without requiring additional tuning processes or alignment information, once the original model is done training.
|               | Speedup Train | Speedup Decode | ML Free |
|---------------|---------------|----------------|---------|
| TPU           | X             | X              | X       |
| Low-p         | X             | X              | X       |
| WP            |               | X              |         |
| KD            |               | X              |         |
| NCE           | X             | n/a            |         |
| D-softmax     | X             | X              |         |
| H-softmax     | X             | n/a            |         |
| WA            | X             | X              |         |
| LSH           | X             | X              |         |

Table 2: Comparison of speedup methods.

3 GPU Computing Concept

In this section, we describe the basic concepts of CUDA-enabled GPU computing to better motivate our decisions in re-designing the LSH algorithm.

3.1 Warp

Kernels are functions executed on GPU. Each kernel will be executed by many GPU threads in parallel. These threads are further grouped into warps, where each warp consists of 32 threads. All 32 threads in a warp will execute the same instruction concurrently. However, due to the branches inside the code, some threads in a warp will be diverged and the rest of the threads in the same wrap will have to idle in that cycle. We should make every effort to avoid warp divergence to maximize GPU usage. Figure 1 shows an example of warp divergence.

![Figure 1: Illustration of kernel, warp and warp divergence.](image)

Figure 1: Illustration of kernel, warp and warp divergence. The solid line means the thread is active, and the dashed line means the thread is idle. Because of the branch, the first half of the warp will execute instruction A and be idle when the other half executes instruction B.

3.2 Memory Hierarchy

The bandwidth of GPU global memory is 208 GB/s for Tesla K20 GPU, and it takes 400-800 cycles for global memory access. Another faster but limited memory is shared memory, whose bandwidth is more than 2 TB/s and only takes 3-4 cycles for each access.

The way to access the global memory also strongly affects the speed. Coalesced access, where threads in the same wrap will access consecutive address, can take the full bandwidth, i.e. around 200 GB/s. Whereas the bandwidth of random access can be as low as 20 GB/s.

In practice, we will load data from global memory in a coalesced way to shared memory, then manipulate the data on shared memory, and finally write back to global memory in a coalesced way again.

3.3 Latency Hiding

The global memory access can lead to a large latency (400-800 cycles). However, the GPU scheduler has a smart strategy to hide the latency: when a warp needs to access global memory, GPU will put it into wait, and switch to another warp to execute. In order to hide the latency completely, each kernel should launch enough threads (more than 1000) in parallel.

4 Locality Sensitive Hashing

At each step during beam search with beam size $B$, given the hidden state $H \in \mathbb{R}^{B \times d}$ from the top RNN layer, the probability distribution $P \in \mathbb{R}^{B \times |V|}$ over $V$ will be calculated by softmax:

$$P[i, j] = p(y = j | H_i) = \frac{e^{Logit[i, j]}}{\sum_{k=1}^{V} e^{Logit[i, k]}}$$

(1)

$$Logit = H \ast E$$

(2)

where $H_i$ is the $i$th row of $H$ and $E \in \mathbb{R}^{d \times |V|}$ is the word embedding matrix. The computational intensive part is the matrix product in 2, whose complexity is $O(dB|V|)$.

For each beam entry, we are only interested in the top $B$ words according to the probability/logit. We can reduce the complexity down to $O(dBV)(|V'| \ll |V|)$ if we can inexpensively construct a much smaller vocabulary set $V'$ that also contains the top $B$ words.

$$p(y = j | H_i) \propto e^{Logit[i, j]}$$

is proportional to the dot-product between $H_i$ and $E_j$. Thus, finding the top $B$ words with highest probability is equivalent to finding the nearest neighbors of $H_i$ from all embedding vectors $E_k, \forall k = 1, \ldots, |V|$ under the dot-product distance measure. LSH (Gionis et al., 1999) is an efficient tool for the nearest neighbor problem. LSH will construct a small candidate vocabulary set $V_{LSH}$ which will contains the top $B$ words with a high expectation.

4.1 LSH on CPU

Vijayanarasimhan et al. successfully utilize winner-take-all (WTA) LSH to speed up the softmax calculation on CPU:

1. Hash every word embedding $E_j \in \mathbb{R}^d$ into hash code $WTA(E_j) \in Z^W$ where $W$ is the dimension of the hash space. Organize these hash codes in hash tables.

2. For each hidden vector $H_i \in \mathbb{R}^d$, apply the same hash function to get $WTA(H_i)$. 

3. The hash codes in $WTA(H_i)$ are searched for the nearest neighbors from $WTA(E_j)$. The vector $E_j$ that is the closest to $H_i$ will be the winning candidate.
3. Given $WTA(H_i)$, select the top $K$ collisions in the hash table, to construct the candidate vocabulary set $V_{LSH,i}$.

4. Calculate the dot-product $H_i * E_k, \forall k \in V_{LSH,i}$.

5. Repeat step 2-4 for each entry in the batch.

Figure 2 illustrates the detailed pipeline of our LSH algorithm on GPU. Table 4 shows the time breakdown of each step in LSH softmax. Although every step is running nicely in batch mode, we still need to carefully design each step as a naive implementation leads to large overhead on GPU.

4.2 LSH on GPU

A similar reduction in speedup will also happen on GPU, especially because GPUs prefer large-scale calculation to hide latency, as described in Section 3.3. Table 3 shows a comparison of matrix multiplications at different scales. Even though calculation is reduced to 1/12th, the time spent is only shrunk to one third.

Table 3: The time consumption and floating point operations per second (Gflop/s) of matrix multiplication on GPU at different scales.

| (m,k,n): $A^{m,k} * B^{k,n}$ | Time (ms) | Gflop/s |
|-----------------------------|-----------|--------|
| (12,1000,500000)           | 5.12      | 234.58 |
| (1,1000,500000)            | 1.63      | 61.27  |

Following Vijayanarasimhan et al., we use the winner-take-all (WTA) (Yagnik et al., 2011) hashing function, $V_{LSH} = V_T \cup (\cup_{i=1}^{B} V_{LSH,i})$. (3)
Table 4: The runtime vocabulary size and time breakdown of each step of full vocabulary decoding and our LSH decoding on translating a French sentence to an English sentence with beam size 12. The last column means the slowdown if the corresponding optimized step is replaced by a naive implementation.

|                      | Full Vocab (ms) | Percent | LSH (ms) | Percent | Naive slowdown |
|----------------------|----------------|---------|----------|---------|----------------|
| Softmax              | 120.97         | 100.0%  | 44.09    | 100.0%  |                |
| LSH overhead         | -              | -       | 16.53    | 37.5%   |                |
| WTA-hash             | -              | -       | 3.72     | 8.4%    | 3.4x           |
| Cuckoo lookup        | -              | -       | 7.29     | 16.5%   | 1.7x           |
| Construct candidate list | -         | -       | 2.51     | 5.7%    |                |
| Construct $E_{L,SH}$ | -              | -       | 3.01     | 6.8%    |                |
| Matrix multiply      | 108.16         | 89.4%   | 22.43    | 50.9%   |                |
| Normalization        | 12.33          | 10.2%   | 2.74     | 6.2%    |                |
| Runtime vocab size   | 40,000         |         | 6,177    |         |                |

which can be formally defined in the following equations:

$$WTA(H \in \mathbb{R}^d) = [I_1; \ldots; I_p; \ldots; I_P]$$  \hspace{1cm} (4)

$$I_p = \arg \max_{k=1}^K \text{Permute}_p(H)[k]$$  \hspace{1cm} (5)

WTA will convert a $d$-dimension real value hidden vector into a $P$-dimension int value hash code. Each $I_p$ is the index of the maximum value of the first $K$ elements of the permuted $H$. Thus, the hash code is actually an ordinal embedding of the original hidden vector, and we use the ordinal similarity as a proxy for the dot-product similarity. We can further group these hash codes into bands, and convert into a $W$-dimension band code:

$$WTA_{\text{band}}(H) = [B_1; \ldots; B_w; \ldots; B_W]$$  \hspace{1cm} (6)

$$B_w = [I_{w-1}+u+1; \ldots; I_{w-1}+u+i; \ldots; I_{w+u}]$$  \hspace{1cm} (7)

$$u = P/W$$  \hspace{1cm} (8)

where each band code $B_w$ is the concatenation of $u$ hash codes. Table 5 shows an example of WTA hash. We can represent $B_w$ in $u \times \log_2(K)$ bits, and we make sure $u \times \log_2(K) < 31$ so that we can store each band code using an int32 on GPU. The hyper parameters for WTA hash are $\{K, u, W\}$.

![Figure 3: Example of cuckoo lookup. The beam size is 1, $W = 2$ and $|V| = 6$.](image)

| $H$      | 0.32 | 0.48 | -0.57 | 0.63 |
|----------|------|------|-------|------|
| $\text{Permute}_0$ | 1    | 2    | 4     | 3    |
| $\text{Permute}_1$ | 1    | 3    | 2     | 4    |
| $\text{Permute}_2$ | 3    | 2    | 4     | 1    |
| $\text{Permute}_3$ | 4    | 1    | 2     | 3    |

| $I_1$ | 0 (00) |
|-------|--------|
| $I_2$ | 0 (01) |
| $I_3$ | 0 (01) |
| $I_4$ | 0 (00) |

| $B_1$ | 0 (0001) |
|-------|----------|
| $B_2$ | 0 (0100) |

Table 5: The running example of WTA hash with $W = 2$, $u = 2$ and $K = 2$.

4.2.2 Cuckoo lookup

Given $WTA_{\text{band}}(H) \in \mathbb{Z}^{B \times W}$, this step will calculate the hit matrix $L \in \mathbb{Z}^{B \times |V|}$, where

$$L[i, j] = \sum_{w=1}^W I(WTA_{\text{band}}(H_i)[w] = WTA_{\text{band}}(E_j)[w])$$  \hspace{1cm} (9)

$L[i, j]$ counts how many band codes are the same between $WTA_{\text{band}}(H_i)$ and $WTA_{\text{band}}(E_j)$, which estimates the dot-product similarity between $H_i$ and $E_j$.

First, we hash all word embeddings $WTA_{\text{band}}(E_j)$. For each band, we will build a hash table:

$$T_w = \{\text{band code : [word id}_1, \ldots, \text{word id}_n]\}$$

where the key is the band code and the value is a list containing all the words whose band code is equal to the key. We re-organize $T_w$ into an flat array on GPU: word ids with same band code are stored in continuous span, and we build a cuckoo hash table for each $T_w$ to store the starting position and corresponding length of each span:

$$\text{CuckooT}_w = \{\text{band code : [start, length]}\}$$

Second, we launch a total of $B \times W$ GPU threads to calculate $L$, and each thread follows Algorithm 1. To look up certain key in cuckoo hash table, it hashes and
compares the key at most twice. Thus the warp (a group of 32 threads) won’t diverge at line 2.

However, at line 3, because different threads will have different length values, the execution time of the warp will depend on the largest length. There will be a serious warp divergence at line 3-6. To solve this problem, we re-arrange the execution order so that the 32 threads will first process the for-loop of thread0 together, then the for-loop of thread1 together, until that of thread31. Such re-arrangement will speed up this step by 3.4x. Figure 4 illustrates the two different thread arrangements.

Algorithm 1 Cuckoo lookup

Inputs: $T, CuckooT, WTA_{band}(H)$

beam index $i$, band index $w$

Output: $L$

1: code = $WTA_{band}(H_i)[w]$
2: start, length = $CuckooT_w[code]$
3: for pos = start to start + length do
4: word_id = $T_w[pos]$
5: $L[i,\text{word}_id] += 1$
6: end for

Figure 4: Illustration of naive implementation and optimized implementation of line 3-6 in Algorithm 1. We assume each warp contains 4 threads, and their for-loop lengths are 1, 7, 3, and 2. The round grey rectangle represents one step of a warp. (a) The naive implementation, which takes the warp 7 steps to finish. (b) The optimized implementation, which takes only 5 steps.

4.2.3 Construct candidate list

Given the hit matrix $L \in \mathbb{Z}_+^{B \times |V|}$ and a threshold $t$, this step selects the final candidate vocabulary set $V_{LSH}$, where:

$$j \in V_{LSH} \iff \exists i, s.t. L[i,j] >= t$$  (10)

We use threshold to avoid the inefficient sorting on GPU. $L$ is a sparse matrix after filtering with $t$, whereas $V_{LSH}$ should be a dense array. This is the canonical Stream Compaction problem, and one can simply use $\text{copy_if}$ function provided in thrust library. To further improve the efficiency, we re-design the algorithm by taking advantage of shared memory and coalesced access. The new algorithm is illustrated in Figure 5.

Figure 5: Illustration of optimized stream compaction algorithm. We assume each warp contains 4 threads here. 2 warps will first load $L$ into shared memory in a coalesced read. Then only the first thread of each warp will scan the 4 values and filter out the valid word ID. Then each warp will write the valid word ID back in a coalesced write. The start position in $V_{LSH}$ for each warp is maintained in global memory, omitted here.

Hyper-parameters that define a WTA LSH beam search are \{K, u, W; B, T, t\}, where $B$ is beam size, $T$ is the number of top frequent words to merge and $t$ is the threshold to select $V_{LSH}$.

5 Experiment

We conduct our experiment on 4 machine translation models: Japanese to English (J2E), English to Japanese (E2J), French to English (F2E) and Uzbek to English (U2E). The statistics and training parameters are shown in Table 6.

Table 6: Training configurations of different language pairs. The attention model is based on Luong, Pham, and Manning. Data sources: ASPEC Japanese-English Corpus (Nakazawa et al., 2016), French-English Corpus from WMT2014 (Bojar et al., 2014), and Uzbek-English Corpus (Linguistic Data Consortium, 2016).

| Language Pair | J2E | E2J | F2E | U2E |
|---------------|-----|-----|-----|-----|
| $|V_{source}|$ | 80K | 88K | 200K | 50K |
| $|V_{target}|$ | 50K | 66K | 40K | 25K |
| #Tokens       | 70.4M | 70.4M | 652M | 3.3M |
| Attention     | Yes | Yes | No  | Yes |

Table 7: The speedup of softmax module and overall pipeline of LSH decoding over full softmax decoding.

| Language Pair | J2E | E2J | F2E | U2E |
|---------------|-----|-----|-----|-----|
| Softmax Speedup | 3.95 | 2.46 | 3.22 | 2.04 |
| Overall Speedup | 2.12 | 2.05 | 1.78 |
| BLEU Loss     | 0.43 | 0.07 | 0.31 | -0.28 |
a consistent 2x overall speedup for J2E, E2J and F2E with tiny BLEU score loss. For U2E, the speedup without BLEU loss is 1.78x, due to the small original target vocabulary size (25,000).

We compare our algorithm with two other decoding acceleration methods: Decoding using only the top frequent words (TOP) and decoding with word alignments (WA) (Shi and Knight, 2017). We conduct a grid search of the LSH hyper parameters \( \{K, u, W\} \) and find that \( \{8, 3, 500\} \) and \( \{16, 3, 500\} \) generally deliver good performance/speedup trade-off. We vary other two hyper parameters \( \{T, t\} \) to get different speedup and BLEU score. Figure 6 shows the BLEU/speedup curve of the three decoding methods on 4 translation directions.

Our LSH decoding always obtain a higher BLEU with a large margin than TOP decoding at the same speedup level. Table 4 shows that the optimized LSH overhead can take up to 37.5% of the total time to calculate softmax. Thus, to achieve the same speedup with TOP decoding, the runtime vocabulary size of LSH can not exceed half of that of TOP decoding, which demonstrates that our LSH algorithm indeed selects a smaller yet more accurate vocabulary set.

The WA decoding achieves higher speedup with the same BLEU. However, this approach can only work in the context where a sensible alignment information can be provided.

The merge of top \( T \) frequent words into frequent words (TOP) and decoding with word alignment (WA), we vary the number of aligned target words of each source word. For LSH decoding, we vary both the number of top frequent words to merge \( (T) \) and the threshold \( (t) \).

**Effects of beam size** Another easy way to speed up decoding is to just reduce the beam size, which is also orthogonal to our LSH decoding. Figure 7 demonstrates that LSH decoding with reduced beam size can achieve even better speed/performance trade-off.

On the other hand, the speed and performance at larger beam size is also important because certain application, like poem generation, requires the beam size larger than 50 to work in practice. Table 8 shows the speedup and BLEU loss of our LSH decoding over the full vocabulary decoding at larger beam size (batch size). Unlike the algorithm proposed by Vijayanarasimhan et al., our algorithm will maintain or even obtain a higher speedup with the same level of BLEU when beam size (batch size) increases, which can be further explained by that large batch size will saturate the GPU and fully exploit its parallel power.

**Effects of \( T \)** The merge of top \( T \) frequent words into the candidate word list \( V_{LSH} \) is necessary to obtain good performance. Figure 8 shows the BLEU/speedup curve for different \( T \) on the French-to-English translation task. Having \( T \) too small will result in low

| Beam size | Speedup | BLEU loss |
|-----------|---------|-----------|
| 12        | 2.06    | 0.31      |
| 24        | 2.22    | 0.35      |
| 36        | 2.23    | 0.28      |
| 48        | 2.21    | 0.31      |

Table 8: The speedup and BLEU loss of LSH decoding over full softmax decoding at different beam sizes on F2E.
BLEU whereas having $T$ too large will limit the highest speedup the method can achieve.

6 Conclusion

We re-design the LSH algorithm for beam search on GPU. The candidate vocabulary set $V_{LSH}$ is shared across the beams to execute every step in batch mode. Several key functions are optimized by using a cuckoo hash table, taking advantage of shared memory, and avoiding warp divergence. Top frequent words are merged into $V_{LSH}$ to further improve the performance. Our LSH algorithm is a machine-learning-free acceleration method that achieves 2x speedup on 4 machine translation tasks, and delivers better BLEU/speedup trade-off than TOP decoding.

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