Two Algorithms for Finding $k$ Shortest Paths of a Weighted Pushdown Automaton

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1 Introduction

Weighted pushdown automata (WPDA) have recently been adopted in some applications such as machine translation [Iglesias et al., 2011] as a more compact alternative to weighted finite-state automata (WFSAs) for representing a weighted set of strings. Allauzen and Riley [2012] introduce a set of basic algorithms for construction and inference of WPDA, and the corresponding implementation as an extension of the open source finite-state transducer toolkit OpenFst\textsuperscript{1}.

Although a shortest-path algorithm for WPDA with bounded stack is described in Allauzen and Riley [2012], it does not give a $k$-shortest-path algorithm, which finds the $k$ shortest accepting paths of the given automaton. Other than just the single shortest path, $k$ shortest paths are useful for many purposes such as reranking the output in parsing [Collins and Koo, 2005] or tuning feature weights in machine translation [Chiang et al., 2009]. One existing work-around is to first expand the WPDA into an equivalent WFSA and then find the $k$ shortest paths of the WFSA using the $k$-shortest-path algorithm for WFSAs (the expansion approach). Since the WPDA expansion has an exponential time and space complexity with respect to the size of the automaton, one usually has to prune the WPDA before expansion (the pruned expansion approach), i.e. remove those transitions and states that are not on any accepting path with a weight at most a given threshold greater than the shortest distance. However, setting an adequate threshold that neither prunes nor keeps too many states or transitions a priori is almost impossible in practice.

In this paper, we introduce two efficient algorithms for finding the $k$ shortest paths of a WPDA, both derived from the same weighted deductive logic description of the execution of a WPDA using different search strategies.

2 Weighted pushdown automata

2.1 Formal definitions

Following Allauzen and Riley [2012], we represent a WPDA as directed graph with labeled and weighted arcs (transitions).

Definition 1. A WPDA $M$ over a semiring $(\mathbb{K}, \oplus, \otimes, 0, 1)$ is a tuple $(\Sigma, \Pi, \hat{\Pi}, Q, E, s, f)$, where
\footnote{1http://www.openfst.org/twiki/bin/view/FST/FstExtensions}
Figure 1: A WPDA of \(a^n b^n | n > 0\)

- \(\Sigma, \Pi, \hat{\Pi}\) are disjoint finite sets of symbols;
- \(\Sigma\) is the alphabet of input symbols;
- \(\Pi, \hat{\Pi}\) are the alphabets of respectively opening and closing parentheses; there exists a bijection between them that pairs the parentheses; for any \(a \in \Pi \cup \hat{\Pi}\), we represent its counterpart in the other alphabet as \(\hat{a}\);
- \(Q\) is a finite set of states; \(s \in Q\) is the start state and \(f \in Q\) is the final state;
- \(E \subseteq Q \times (\Sigma \cup \Pi \cup \hat{\Pi} \cup \{e\}) \times K \times Q\) is a finite set of transitions; \(e = \langle p[e], i[e], w[e], n[e] \rangle \in E\) denotes a transition from state \(p[e]\) to state \(n[e]\) with label \(i[e]\) and weight \(w[e]\), where \(w[e] \neq \emptyset\).

A path \(\pi\) is a sequence of transitions \(\pi = e_1 e_2 \ldots e_m\), such that \(n[e_i] = p[e_{i+1}]\) for all \(1 \leq i < m\). \(p[\cdot], i[\cdot], w[\cdot]\) and \(n[\cdot]\) can all be generalized to paths. For a given path \(\pi = e_1 e_2 \ldots e_m\), define \(p[\pi] = p[e_1], n[\pi] = n[e_m], i[\pi] = i[e_1] i[e_2] \ldots i[e_m]\), and \(w[\pi] = w[e_1] \otimes w[e_2] \otimes \ldots \otimes w[e_m]\). Unlike a WFSA, not all paths from \(s\) to \(f\) in a WPDA are accepting paths. For a set of symbols \(S\), let \(c_{\Sigma, \Pi}[\pi]\) be the substring of \(i[\pi]\) consisting of all and only the symbols from set \(S\). For example, \(c_{\Sigma, \Pi}[\pi]\) is the substring of \(i[\pi]\) consisting of all and only the opening and closing parentheses. Then,

**Definition 2.** The Dyck language on finite parenthesis alphabets \(\Pi, \hat{\Pi}\) consists of strings of balanced parentheses. A path \(\pi\) is balanced if \(c_{\Sigma, \Pi}[\pi]\) belongs to the Dyck language on \(\Pi\) and \(\hat{\Pi}\).

For example, when \(\Pi = \{\text{(', '}\}\) and \(\hat{\Pi} = \{\text{', '}'\}\) with normal pairing by appearance, strings such as \((\), \((()\))\) are members of the Dyck language while \((\) or \((\))\) are not.

Finally,

**Definition 3.** A path \(\pi\) is an accepting path if and only if \(p[\pi] = s, n[\pi] = f\) and \(\pi\) is balanced.

This representation of WPDA is slightly different from the classical representation of PDAs, where a stack alphabet is defined with optional push or pop operations at each transition. Here the stack alphabet is essentially \(\Pi\) and \(\hat{\Pi}\), paired by the bijection between them. Whenever a symbol from \(\Pi\) is consumed, it is equivalent to pushing the particular symbol onto the stack in the classical representation; and whenever a symbol from \(\hat{\Pi}\) is consumed, it is equivalent to popping a symbol off the stack and checking if the symbol is its counterpart from \(\Pi\). As discussed in [Allauzen and Riley, 2012], such representation leads to easy adaptation of some WFSA algorithms for similar purposes on a WPDA.

Following [Allauzen and Riley, 2012], we limit our effort in finding \(k\) shortest paths to WPDA with a bounded stack in both pushing and popping.

**Definition 4.** A WPDA has a bounded stack if there exists an integer \(K\) such that for any path \(\pi\), the number of unmatched parenthesis in \(c_{\Sigma, \Pi}[\pi]\) is no greater than \(K\).

Although this rules out all WPDA with recursion, the ones found in applications that need to find the \(k\) shortest paths usually do not have recursion [Iglesias et al., 2011]. Thus an algorithm that only works on WPDA with a bounded stack is already very useful.

[Allauzen and Riley, 2012] give a general algorithm for converting a context free grammar into an equivalent WPDA. Figure 1 is an example WPDA representing the classical context free language \(\{a^n b^n | n > 0\}\) constructed.

\(^2\)This definition is slightly different from [Allauzen and Riley, 2012], which only bounds pushing.
following their algorithm. It is easy to see this WPDA does not have a bounded stack. However, considering this as a “grammar”, one can then “parse” strings with the grammar by encoding the input as a WFSA and intersecting the WPDA with it. For example, Figure 3 is the result of intersecting Figure 2 with Figure 1, which now has a bounded stack.

2.2 Automata execution as weighted deduction

A deductive logic defines a space of weighted items, some of which are axioms or goals (items to prove), and a set of inference rules of the form,

\[
\frac{A_1 : w_1 \quad A_2 : w_2 \quad \ldots \quad A_m : w_m}{B : g(w_1, w_2, \ldots, w_m)} \phi
\]

which means if items \( A_1, A_2, \ldots, A_m \) are provable respectively with weights \( w_1, w_2, \ldots, w_m \), then item \( B \) is also provable with weight \( g(w_1, w_2, \ldots, w_m) \) given the side condition \( \phi \) is satisfied. We also call \( B \) proved this way an instantiation of \( B \) with weight \( g(w_1, w_2, \ldots, w_m) \). This style of system has been commonly used to express parsing strategies since Shieber et al. [1995].

The execution of a WPDA \( M \) can be described using the following weighted deductive logic \( L_M \).

- The items are of the form \( q_1 \sim q_2 \), where \( q_1, q_2 \in Q \). An instantiation \( q_1 \sim q_2 : u \) for some \( u \in K \) intuitively means there is a balanced path from \( q_1 \) to \( q_2 \) with weight \( u \).

- Axioms are

\[
q = s \text{ or there exists } e \in E \text{ such that } n[e] = q \text{ and } i[e] \in \Pi
\]

Furthermore, we call any state \( q \) an entering state if \( q \sim q : \top \) is an axiom.

- There are two inference rules,
  1. Scan

\[
q \sim p[e] : u \quad q \sim n[e] : u \otimes w[e] \quad e \in E \text{ such that } i[e] \in \Sigma \cup \{e\}
\]

  2. Complete

\[
q \sim p[e_1] : u_1 \quad n[e_1] \sim p[e_2] : u_2 \quad e_1, e_2 \in E \text{ such that } i[e_1] \in \Pi, i[e_2] \in \hat{\Pi}, i[e_1] = \hat{i}[e_2]
\]
Theorem 3

For any $a \oplus b \in \mathbb{K}$, $a \leq b$ if and only if $a \oplus b = a$.

For the problem to be well-defined, the natural ordering also has to be total, which is equivalent to requiring the $\oplus$ operator to have the following path property: for any $a, b \in \mathbb{K}$, $a \oplus b = a$ or $a \oplus b = b$. An example meeting these conditions is the tropical semiring $\langle \mathbb{R} \cup \{\infty\}, \min, +, \infty, 0 \rangle$, one of the most commonly used as weights in parsing and machine translation. Its natural ordering is simply the ordering of real numbers and infinity.

3 Computing the Shortest Distance

One of the benefits of the above weighted deduction representation is that many properties can be computed by carrying out the deductions in a uniform style. As a starting point, we are interested in finding the smallest-weight instantiation of some item $q_1 \leadsto q_2$. For reasons which will become clear later, we call the weight of that

Figure 4: A proof of the accepting path of “aabb”

- The only goal item is $s \leadsto f$

Any valid proof forms a tree that induces a path. The induced path can be obtained by reading off the transitions in side conditions through a left-to-right post-order traversal of the proof tree. Take the WPDA in Figure 1 for example; Figure 4 is a proof of the accepting path of the string “aabb”. The accepting path is thus $q_1 \rightarrow q_2 (1), q_3 \rightarrow q_4 (2), q_2 \rightarrow q_1 (3), q_3 \rightarrow q_4 ; q_4 \rightarrow q_3 (4), q_3 \rightarrow q_4 (5), q_1 \rightarrow q_2 (7), q_3 \rightarrow q_4 (8)$

One can easily prove the following by induction for any WPDA $M$ (see the appendix)\(^5\)

Theorem 1 (Soundness). Any valid proof of an instantiation $q_1 \leadsto q_2 : u$ in $L_M$ induces a balanced path from $q_1$ to $q_2$ with weight $u$ in $M$.

Theorem 2 (Completeness). Any balanced path from an entering state $q_1$ to some state $q_2$ with weight $u$ in $M$ has a valid proof of an instantiation $q_1 \leadsto q_2 : u$ in $L_M$ whose induced path is that path.

Theorem 3 (In-ambiguity). Any balanced path from an entering state in $M$ has a unique proof in $L_M$\(^4\)

The three properties together essentially state that there is a one-to-one correspondence between proofs of goal items in $L_M$ and accepting paths in $M$.

2.3 The $k$-shortest-path problem

The $k$-shortest-path problem on a WPDA $M$ with a bounded stack is to find $k$ accepting paths from $M$ with the smallest weights with respect to the natural ordering of $M$’s weight semiring $\mathbb{K}$\(^5\).

The natural ordering $\leq \subseteq \mathbb{K} \times \mathbb{K}$ is defined as

Definition 5. For any $a, b \in \mathbb{K}$, $a \leq b$ if and only if $a \oplus b = a$.

Note especially that a bounded stack is not required.

Up to the tree structure with side conditions.

In the rest of this paper, we always assume the WPDA $M$ has a bounded stack.
instantiation the inside weight of $q_1 \leadsto q_2$. Let $R$ be the set of all instantiations of provable items. Because of the path property, computing the inside weight of $q_1 \leadsto q_2$ is equivalent to computing

$$a(q_1 \leadsto q_2) = \bigoplus_{u} u \in \{u | q_1 \leadsto q_2; w \in R\}$$

The sum can be further grouped by the last step taken in a proof of $q_1 \leadsto q_2 : u$. Define $A(q_1 \leadsto q_2)$ to be the following,

$$A(q_1 \leadsto q_2) = \begin{cases} 1 & q_1 \leadsto q_2 \text{ is an axiom} \\ 0 & \text{otherwise} \end{cases}$$

Define $S_{q_1 \leadsto q_2} \subseteq E$ be the set of “last steps taken” to prove $q_1 \leadsto q_2$ with a Scan, i.e. $e$ is in $S_{q_1 \leadsto q_2}$ if and only if some instantiation $q_1 \leadsto p[e] : u$ with $e$ as the side condition can prove $q_1 \leadsto q_2$ with the Scan rule. Similarly, define $C_{q_1 \leadsto q_2} \subseteq E \times E$ be the set of “last steps taken” to prove $q_1 \leadsto q_2$ with a Complete, i.e. $(e_1, e_2)$ is in $C_{q_1 \leadsto q_2}$ if and only if some instantiations $q_1 \leadsto p[e_1] : u_1$ and $u[e_1] \leadsto p[e_2] : u_2$ can prove $q_1 \leadsto q_2$ with the Complete rule. Then, $a(q_1 \leadsto q_2)$ can be rewritten as

$$a(q_1 \leadsto q_2) = A(q_1 \leadsto q_2) + \left( \bigoplus_{e \in S_{q_1 \leadsto q_2}} \bigoplus_{u} u \otimes w[e] \right) \bigoplus \left( \bigoplus_{(e_1, e_2) \in C_{q_1 \leadsto q_2}} \bigoplus_{u_1} u_1 \otimes w[e_1] \otimes u_2 \otimes w[e_2] \right)$$

This recursive formulation allows us to compute the shortest distance of an item using the shortest distance of its component sub-items. When the WPDA $M$ has a bounded stack, one can easily derive an algorithm that computes the shortest distance using $L_M$. Figure 5 is a simple example of such an algorithm. This algorithm carries out a standard agenda-based reasoning with the relaxation technique [Cormen et al. 2009], where $Q$ is the agenda. The map $\alpha$ maintains the current estimate of each proven item’s inside weight. Lines 4-7 seed the axioms as the starting point of reasoning. Then lines 8-26 try to prove new items by applying the Scan rule (lines 12-13) and the Complete rule (lines 14-24). Any item that is newly proven or proven with a smaller weight is added back to the agenda in the Relax function.

The above algorithm is conveniently derived from the weighted deduction system using standard techniques. Nevertheless, there are other strategies that can also be used; for example, the shortest path algorithm in [Allauzen and Riley 2012] is essentially computing the inside weights with a multi-agenda strategy.

4 Algorithm 1

Having discussed the shortest distance problem in a WPDA, we now move on to the $k$-shortest-path problem. The key idea of our first algorithm is similar to the $A^*$ $k$-best parsing algorithm in [Pauls and Klein 2009]. As we have shown in Section 2.2 similar to parsing, the execution of a WPDA can be described as a weighted deductive logic. The generalized $A^*$ search algorithm from [Felzenszwalb and McAllester 2007] can then be applied with a monotonic and admissible heuristic function to find the $k$ instantiations of the goal item with smallest weights, from which we get the $k$ shortest paths. The outside weight of items can be defined with similar meanings to parsing and used as an exact heuristic. Another, inexact heuristic will also be discussed, which will eventually lead to our second algorithm.
function Inside
    $\alpha \leftarrow \text{empty map}$
    $Q \leftarrow \text{empty queue}$
    for all entering state $q$ do
        $\text{Push}(q \sim q, Q)$
        $\alpha[q \sim q] \leftarrow \top$
    end for
    while $Q$ is not empty do
        $q_1 \sim q_2 \leftarrow \text{Pop}(Q)$
        for all transition $e$ such that $p[e] = q_2$ do
            if $i[e] \in \Sigma \cup \{\epsilon\}$ then
                $\text{Relax}(q_1 \sim n[e], u \otimes w[e])$
            else if $i[e] \in \Pi$ then
                $\text{Complete; as the left antecedent}$
                for all $e'$ such that $i[e'] = i[e]$ and $n[e] \sim p[e']$ is in $\alpha$ do
                    $\text{Relax}(q_1 \sim n[e'], u \otimes w[e] \otimes n[e] \sim p[e'] \otimes w[e'])$
                end for
            else if $i[e] \in \hat{\Pi}$ then
                $\text{Complete; as the right antecedent}$
                for all $q_3$ such that $q_3 \sim p[e']$ is in $\alpha$ do
                    $\text{Relax}(q_3 \sim n[e], \alpha[q_3 \sim p[e']] \otimes w[e'] \otimes u \otimes w[e])$
                end for
            end if
        end for
    end while
end function

function Relax($q_1 \sim q_2, w$)
    if $q_1 \sim q_2$ is in $\alpha$ then
        $u \leftarrow \alpha[q_1 \sim q_2] \oplus w$
        if $u \neq \alpha[q_1 \sim q_2]$ then
            $\alpha[q_1 \sim q_2] \leftarrow u$
            $\text{Push}(q_1 \sim q_2, Q)$ if $q_1 \sim q_2$ not already in $Q$
        end if
    else
        $\alpha[q_1 \sim q_2] \leftarrow u$
        $\text{Push}(q_1 \sim q_2, Q)$ if $q_1 \sim q_2$ not already in $Q$
    end if
end function

Figure 5: A simple Inside algorithm
4.1 A* search on a deductive logic

Felzenszwalb and McAllester [2007] introduce the generalized A* search algorithm on a deductive logic. Although the original algorithm assumes the weights are from a positive tropical semiring, this is not a necessary requirement in our problem, as we show next.

Similar to the original A* algorithm on graphs [Hart et al., 1968], we need a heuristic function $H$ to estimate the final weight continuing from the current search state (an instantiation in this case) to the closest goal item. More formally, for a weighted logic $L$ with (unweighted) item space $I$ on semiring $\langle K, \oplus, \otimes, 0, 1 \rangle$, a heuristic function $H : \langle I, K \rangle \rightarrow K$ is any function satisfying the following,

**Admissibility** For any provable instantiation of the goal item $G : w$,

$$H(G : w) = w$$

**Monotonicity** For any provable instantiations $A_1 : w_1, A_2 : w_2, \ldots, A_m : w_m$ and an inference rule

$$\begin{align*}
A_1 : w_1 & \quad \quad A_2 : w_2 & \quad \quad \ldots & \quad \quad A_m : w_m \\
\hline
B : g(w_1, w_2, \ldots, w_m)
\end{align*}$$

and $1 \leq i \leq n$,

$$H(A_i : w_i) \leq H(B : g(w_1, w_2, \ldots, w_m))$$

where $\leq$ is the natural ordering of the semiring.

With such an $H$, the A* algorithm on a deductive logic can then be described as in Figure 6.

Similar to the original A* algorithm, the following property holds for the generalized A* algorithm as well:

**Theorem 4.** If a monotonic $H$ is used, the generalized A* algorithm pops instantiations in increasing order of their $H$ value.

The proof of the tropical semiring case can be found in Felzenszwalb and McAllester [2007]. We include the proof simply to show this is the case with any monotonic heuristic function and any semiring with the path property; not just the tropical semiring.
Proof. Suppose some instantiation is not popped in order of the $H$ value. Let the instantiations popped in order be $A_1 : w_1, A_2 : w_2, \ldots$ and let $i$ be the smallest index such that $H(A_{i-1} : w_{i-1}) > H(A_i : w_i)$. Right before $A_{i-1} : w_{i-1}$ is popped, $A_i : w_i$ cannot be inside $Q$, otherwise it will be popped instead. This means $A_i : w_i$ is added into $Q$ after popping $A_{i-1} : w_{i-1}$ by applying some inference rule with $A_{i-1} : w_{i-1}$. The application is of the form

$$\ldots A_{i-1} : w_{i-1} \quad \ldots$$

$$A_i : g(\ldots, w_{i-1}, \ldots)$$

Because $H$ is monotonic,

$$H(A_{i-1} : w_{i-1}) \leq H(A_i : g(\ldots, w_{i-1}, \ldots)) = H(A_i : w_i)$$

This contradicts the assumption $H(A_{i-1} : w_{i-1}) > H(A_i : w_i)$.

If $H$ is also admissible, then for any instantiation of a goal item $G : w$, $H(G : w)$ is just $w$. Thus such instantiations are popped in increasing order of their weights and the first $k$ such instantiations popped are the ones with the smallest weight.

4.2 Outside weight as an exact heuristic

For a given instantiation $q_1 \sim q_2 : u$, we want the heuristic to tell us the weight of the shortest accepting path continuing from this instantiation. Such a heuristic is trivially monotonic and admissible. Let $\pi$ be the path induced by $q_1 \sim q_2 : u$, and define

$$H_1(q_1 \sim q_2 : u) = \bigoplus_{\mu, \nu} w[\mu] \otimes u \otimes w[\nu]$$

where the sum is over all pairs of prefixes and suffixes of transitions such that $\mu \pi \nu$ forms an accepting path. When the semiring is commutative, the heuristic has a simple form. Define $\beta(q_1 \sim q_2) = \bigoplus_{\mu, \nu} w[\mu] \otimes w[\nu]$; then

$$H_1(q_1 \sim q_2 : u) = \beta(q_1 \sim q_2) \otimes u$$

We call $\beta(q_1 \sim q_2)$ the outside weight of $q_1 \sim q_2$, because on the shortest accepting path going through $q_1 \sim q_2$, $\beta(q_1 \sim q_2)$ is the weight of the partial path “outside” of $q_1 \sim q_2$, as illustrated in Figure 7. This can be easily computed by applying the Scan and Complete rules in reverse, starting from the goal after the inside weights have been computed. See Figure 8 for a simple algorithm. Very similar to the inside algorithm in Figure 5, we use agenda-based reasoning, but with the goal item as the starting point (lines 5-6). Then lines 7-20 try to propagate the estimates to inner items by applying inference rules in reverse.
function Outside
    α ← the inside weights from Inside
    β ← empty map
    Q ← empty queue
5:  β[s ↼ f] ← T
    Push(s ↼ f, Q)
while Q is not empty do
    q₁ ↼ q₂ ← Pop(Q)
    u ← β[q₁ ↼ q₂]
10: for all incoming e of q₂ do
    if i[e] ∈ Σ ∪ {e} then ▷ Scan in reverse
        Relax(q₁ ↼ p[e], u ⊗ w[e])
    else if i[e] ∈ Π then ▷ Complete in reverse
        for all e′ such that i[e′] = i[e] and q₁ ↼ p[e′] and n[e′] ↼ p[e] both in α do
            Relax(q₁ ↼ p[e′], u ⊗ w[e′] ⊗ α[n[e′] ↼ p[e]] ⊗ w[e])
            Relax(n[e′] ↼ p[e], u ⊗ w[e′] ⊗ α[q₁ ↼ p[e′]] ⊗ w[e])
        end for
    end if
end for
15: end while
end function

function Relax(q₁ ↼ q₂, w)
    if q₁ ↼ q₂ is in β then
25:        u ← β[q₁ ↼ q₂] ⊕ w
        if u ≠ β[q₁ ↼ q₂] then
            β[q₁ ↼ q₂] ← u
            Push(q₁ ↼ q₂, Q) if q₁ ↼ q₂ not already in Q
        end if
    else
        β[q₁ ↼ q₂] ← u
        Push(q₁ ↼ q₂, Q) if q₁ ↼ q₂ not already in Q
    end if
end function

Figure 8: A simple Outside algorithm
4.3 An inexact heuristic and its problems

The above heuristic is very effective in the search because the outside weight gives an exact estimate. However, pre-computation of the outside weight requires two passes traversing the automaton. A natural question is whether there is an inexact heuristic, yet still monotonic and admissible, which takes less time to compute.

When the multiplication does not decrease the weight, one may use the weight of only part of the final shortest accepting path as an estimate. This can produce a heuristic that is less expensive to compute, possibly at the cost of increasing the search time. In particular, define $D(q_1, q_2)$ to be the shortest distance between any pair of states $q_1$ and $q_2$, and $\gamma(q_1 \leadsto q_2) = \bigoplus_{q_3} D(q_2, q_3)$, where the summation is over all states reachable from $q_2$ that have a closing parenthesis or simply $f$ when $q_1$ is $s$ (call such a state an exiting state, in contrast with an entering state). $\gamma(q_1 \leadsto q_2)$ is roughly how far away $q_1 \leadsto q_2$ is to a pair of immediate enclosing parenthesis. For example, in Figure 9, $\gamma(q_1 \leadsto q_2) = D(q_2, q_3) \oplus D(q_2, q_4)$ is the shortest distance from $q_2$ to exiting states $q_3$ and $q_4$. All the relevant values of $D$ are in fact the inside weights of the reversed WPDA of $M$ (for example, see Figure 10), therefore we call it the reverse inside weight.

Figure 9: $\gamma(q_1 \leadsto q_2) = D(q_2, q_3) \oplus D(q_2, q_4)$ is the shortest distance from $q_2$ to an “exit”

Figure 10: The reversed WPDA of Figure 9

Then, we can define the following heuristic,

$$H_2(q_1 \leadsto q_2 : u) = u \otimes \gamma(q_1 \leadsto q_2)$$

6For example, the tropical semiring with only non-negative weights in the setting of the classical shortest path problem on a graph, where real valued weights are summed within the path and the minimum is taken (i.e. use $+$ as $\otimes$ and $\min$ as $\oplus$).

7This is only a rough estimate since there may not be a opening parenthesis going to $q_1$ that matches the closing parenthesis of the selected exiting state. However, the actual shortest distance is never smaller than this, which means the estimate is still admissible.

8That is, reverse the direction of transitions; swap $s$ and $f$; and swap $\Pi$ and $\hat{\Pi}$. 

Figure 11: A problematic WPDA for $H_2$, weights are in the tropical semiring

This gives us the weight of the shortest path starting at the induced path of $q_1 \sim q_2 : u$ to any exiting state, which may be a part of an accepting path. It is trivially admissible because $\gamma(s \sim f) = D(f,f) = 1$. When multiplication does not decrease the weight, the weight of part of a path is always smaller than or equal to the weight of the whole path. Therefore, the heuristic is monotonic. Unlike the outside weight, the semiring does not need to be commutative for this heuristic to be well-defined.

Unfortunately, though we now spend less time in pre-computing the heuristic, the actual A* search usually ends up taking much longer because of the inexactness. To see why, notice that any instantiation of an item with a weight smaller than the shortest accepting path has to be visited, even if it will only be used in an accepting path far longer than the $k$ shortest ones. For example, consider the WPDA in Figure 11 with the relevant values of $\beta$ and $\gamma$ listed in Table 1. When using $H_1$, the following are instantiated before reaching the 1-shortest path:

| Item       | $\beta$ | $\gamma$ |
|------------|---------|----------|
| $s \sim s$ | 3       | 3        |
| $s \sim q_6$ | 1     | 1        |
| $s \sim f$ | 0       | 0        |
| $q_1 \sim q_1$ | 3   | 0        |
| $q_1 \sim q_2$ | 2   | 1        |
| $q_1 \sim q_3$ | 4   | 0        |
| $q_1 \sim q_4$ | 1   | 0        |
| $q_1 \sim q_5$ | 4   | 0        |
| $q_1 \sim q_7$ | 4   | 0        |
| $q_1 \sim q_8$ | 4   | 0        |

Table 1

When using $H_1$, the following are instantiated before reaching the 1-shortest path:

- $s \sim s : 0 \quad (H_1 = 0 + 3 = 3, Q = \{q_1 \sim q_1 : 0\})$
- $q_1 \sim q_1 : 0 \quad (H_1 = 0 + 3 = 3, Q = \{q_1 \sim q_2 : 1, q_1 \sim q_3 : 0\})$
- $q_1 \sim q_2 : 1 \quad (H_1 = 1 + 2 = 3, Q = \{q_1 \sim q_4 : 2, q_1 \sim q_3 : 0\})$
- $q_1 \sim q_4 : 2 \quad (H_1 = 2 + 1 = 3, Q = \{s \sim q_6 : 2, q_1 \sim q_3 : 0\})$
- $s \sim q_6 : 2 \quad (H_1 = 2 + 1 = 3, Q = \{s \sim f : 3, q_1 \sim q_3 : 0\})$
- $s \sim f : 3 \quad (H_1 = 3 + 0 = 3, Q = \{q_1 \sim q_3 : 0\})$
However, when $H_2$ is used, the following are instantiated before the 1-shortest,

\[
q_1 \sim q_1 : 0 \quad (H_2 = 0 + 0 = 0, Q = \{q_1 \sim q_3 : 0, q_1 \sim q_2 : 1, s \sim s : 0\})
\]
\[
q_1 \sim q_3 : 0 \quad (H_2 = 0 + 0 = 0, Q = \{q_1 \sim q_5 : 0, q_1 \sim q_2 : 1, s \sim s : 0\})
\]
\[
q_1 \sim q_5 : 0 \quad (H_2 = 0 + 0 = 0, Q = \{q_1 \sim q_7 : 0, q_1 \sim q_2 : 1, s \sim s : 0\})
\]
\[
q_1 \sim q_7 : 0 \quad (H_2 = 0 + 0 = 0, Q = \{q_1 \sim q_8 : 0, q_1 \sim q_2 : 1, s \sim s : 0\})
\]
\[
q_1 \sim q_8 : 0 \quad (H_2 = 0 + 0 = 0, Q = \{q_1 \sim q_2 : 1, s \sim s : 0, s \sim f : 4\})
\]
\[
q_1 \sim q_2 : 1 \quad (H_2 = 1 + 1 = 2, Q = \{q_1 \sim q_4 : 2, s \sim s : 0, s \sim f : 4\})
\]
\[
q_1 \sim q_4 : 2 \quad (H_2 = 2 + 0 = 2, Q = \{s \sim s : 0, s \sim f : 4\})
\]
\[
s \sim s : 0 \quad (H_2 = 0 + 3 = 3, Q = \{s \sim q_6 : 0, s \sim f : 4\})
\]
\[
s \sim q_6 : 2 \quad (H_2 = 2 + 1 = 3, Q = \{s \sim f : 3, s \sim f : 4\})
\]
\[
s \sim f : 3 \quad (H_2 = 3 + 0 = 3, Q = \{s \sim f : 4\})
\]

$H_2$ ends up visiting more instantiations along the path from $q_1$ to $q_8$ because that path is shorter in the scope of the enclosing parentheses. The following closing parenthesis completely flips the position, but this is some information $H_1$ “knows” while $H_2$ does not. In practice, we find this happens so frequently that $H_2$ fails to output the shortest path within a reasonable amount of time.

Another problem with $H_2$ is that when multiplication may increase the weight (for example, in the tropical semiring with negative weights, which is commonly used in applications such machine translation), the heuristic is no longer monotonic.

## 5 Algorithm 2

We can adopt a new search strategy to address the problems with $H_2$. Before describing the algorithm, we take a brief excursion to introduce a technique from Huang and Chiang [2005]. Consider the following problem:

Let $A$ and $B$ be two (possibly infinite) ordered sequence of real numbers (i.e. for any $i$, $A_i \leq A_{i+1}$ and $B_i \leq B_{i+1}$). Find the $k$ smallest elements in $A \times B$, ordered by the sum of the pair.

For example, when $A = \{0, 2, 2\}$ and $B = \{1, 2, 4\}$, the 3 smallest elements are $\{0, (0, 1), (0, 2), (2, 1)\}$. A naive solution is to compute the first $k$ elements in both $A$ and $B$ and then sort all the $k^2$ combinations. The technique from Huang and Chiang [2005], described in Figure 12, visits at most $2k$ combinations and usually a lot fewer in practice. The key insight is that there is no need to explore $(A_{i+1}, B_j)$ or $(A_i, B_{j+1})$ before $(A_i, B_j)$ is popped because both of them are guaranteed to be sub-optimal compared with $(A_i, B_j)$. When computing elements in $A$ and $B$ is expensive, this technique is substantially faster than the naive solution.
Table 2

| Pair of states | D |
|----------------|---|
| s, f           | 3 |
| q1, q4         | 2 |
| q2, q4         | 1 |
| q4, q4         | 0 |
| q1, q8         | 0 |
| q3, q8         | 0 |
| q5, q8         | 0 |
| q7, q8         | 0 |
| q8, q8         | 0 |

The same idea can be applied in our problem. For any pair of entering and exiting states \((p, q)\), let \(G_{pq}\) be the sequence of balanced paths from \(p\) to \(q\) ordered by their weight and let \(G_{pq}^i\) be the \(i\)-th path. Following similar reasoning, we know there is no need to compute the actual value of \(G_{pq}^{i+1}\) before \(G_{pq}^i\) is ever used as part of a larger path, in search of the \(k\) shortest accepting path. Furthermore, \(G_{pq}\) can be incrementally computed, as we show next in Figure 13.

The algorithm operates as follows. First of all, instead of having a single priority queue, now for every relevant \(G_{pq}\), we have a corresponding priority queue \(Q_{pq}\). \(Q_{pq}\) is only responsible for finding the intermediate “goal”, i.e. balanced paths from \(p\) to \(q\), in increasing order of their weights. Further, only items of the form \(p \sim r\) are pushed into \(Q_{pq}\), which allows us to use the following heuristic that only requires the reverse inside weights,

\[
H_{pq}(p \sim r : u) = u \otimes D(r, q)
\]

Items are then proved in a top-down fashion, starting with \(G_{sf}\). The search process can be described recursively (Figure 13). Let the sequence in consideration be \(G_{pq}\),

- If there is no balanced path from \(p\) to \(q\) using any parenthesis, all proofs only involve the Scan rule. As a result, \(G_{pq}\) can be incrementally computed without consulting any other sequence (lines 23-27).
- Otherwise, let \(e\) and \(e'\) be the pair of parentheses encountered during the search. Simply query \(G_{n[e]p[e']}\) to get the shortest path (line 30), and only use the \((k + 1)\)-th shortest path after an instantiation proved with the \(k\)-th one is popped (lines 14-18).

Though omitted in Figure 13 for a simpler presentation, a further optimization is essential to achieve the desired efficiency. Observe in the second case above, that the exact knowledge of the shortest path from \(n[e]\) to \(p[e']\) is not required until an item proved using that path is popped. Therefore, instead of directly calling \(FindKTh(n[e], p[e'], 1)\), one can query \(D(n[e], p[e'])\) to get the shortest distance. This is sufficient to compute the priority and “promise” an actual proof, which will be realized once the item is popped. To distinguish actual instantiations from those with a promise, we denote \(q_1 \sim q_2 : u\) as an instantiation where the last step is based on a promise.

To see the new algorithm at work, consider again the WPDA in Figure 11. Relevant values of \(D\) are listed in Table 2. Then the following are instantiated before reaching the 1-shortest path,
function $\text{FindKth}(p, q, k)$ \hspace{1em} \triangleright \text{Finds the k-th element of } G_{pq}$

if the result has been cached then
    return the cached result
end if

5: $S$ is a global variable storing proven items, initialized as empty outside the function
$Q_{pq}$ is a min-priority queue, initialized as empty outside the function

if $p \leadsto p$ not in $S$ then \hspace{1em} \triangleright \text{First time called}
    $\text{Push}(p \leadsto p : \mathbb{1}, Q_{pq})$ with priority $D(p, q)$
end if

10: while $Q_{pq}$ is not empty do
    if top of $Q_{pq}$ is proven via Scan then
        $p \leadsto r : u \leftarrow \text{Pop}(Q_{pq})$
    else \hspace{1em} \triangleright \text{Complete; further pushing is needed}
        $\langle p \leadsto r : u, v, e, e', i \rangle \leftarrow \text{Pop}(Q_{pq})$
        $n[e] \leadsto p[e'] : w \leftarrow \text{FindKth}(n[e], p[e'], j + 1)$
        $h \leftarrow v \otimes w[e] \otimes w[e'] \otimes D(n[e'], q)$
        if $h \neq \emptyset$ then
            $\text{Push}(\langle p \leadsto r : v \otimes w[e] \otimes w[e'], v, e, e', j + 1 \rangle, Q_{pq})$ with priority $h$ \hspace{1em} \triangleright \text{Store information for further pushing in the future}
        end if
    15: end if

20: end while

Add $p \leadsto r : u$ to $S$

for all transition $e$ such that $p[e] = r$ do
    if $i[e] \in \Sigma \cup \{e\}$ then \hspace{1em} \triangleright \text{Scan}
        $h \leftarrow u \otimes w[e] \otimes D(n[e], q)$
        if $h \neq \emptyset$ then
            $\text{Push}(p \leadsto n[e] : u \otimes w[e], Q_{pq})$ with priority $h$
        end if
    25: end if

else if $i[e] \in \Pi$ then \hspace{1em} \triangleright \text{Complete; as the left antecedent}
    for all transition $e'$ such that $i[e'] = \hat{i}[e]$ and $D(n[e], p[e']) \neq \emptyset$ do
        $n[e] \leadsto p[e'] : v \leftarrow \text{FindKth}(n[e], p[e'], 1)$
        $h \leftarrow u \otimes w[e] \otimes v \otimes w[e'] \otimes D(n[e'], q)$
        if $h \neq \emptyset$ then
            $\text{Push}(\langle p \leadsto n[e'] : u \otimes w[e] \otimes v \otimes w[e'], u, e, e', 1 \rangle, Q_{pq})$ with priority $h$ \hspace{1em} \triangleright \text{Store information for further pushing in the future}
        end if
    30: end for
end if

else if $p \leadsto r : w$ is a goal item then
    Cache $p \leadsto r : w$, then return $p \leadsto r : w$
end if
35: end function

Figure 13: Algorithm 2
Notice no item is ever instantiated from $G_{q_1 q_8}$, which is exactly the desired result.

Another benefit of grouping the search by the intermediate “goals” is there is not any special requirement on the semiring — multiplication neither has to be commutative nor non-decreasing.

6 Experimental Results

We tested our algorithms on WPDA\(s\) generated from the machine translation system described in Iglesias et al. [2011]. Figure 14 compares the running time of the two algorithms with two previous approaches (expansion and pruned-expansion with oracle threshold) in finding the 1000 shortest paths on sample WPDA\(s\) with various sizes. Due to the exponential time complexity of WPDA expansion, the expansion baseline is only able to finish within our time and memory limit on the 5 smallest sample inputs. For the pruned-expansion approach, we pick the oracle threshold (the exact weight difference between the shortest path and the 1000th shortest one) for each sample.

Both of our algorithms are significantly faster than the expansion baseline, and their performance is comparable on smaller input. But as the size of the WPDA grows, the advantage of the single pass pre-computation of Algorithm 2 becomes clear, resulting in a very large time improvement in this case.

The performance of Algorithm 2 is close to the pruned-expansion’s oracle best case in almost all sample inputs. However, it is worth noting that the perfect threshold varies significantly between samples — even for those generated from the same system using different inputs, the factor of the perfect threshold relative to the weight of the shortest path can vary from 0.35% to 160% while the median is 7%. This justifies our previous claim about the difficulty in picking an appropriate threshold.

Figure 15 breaks down the running time of our algorithms on a large WPDA. Both of them spend most of their time on pre-computing the heuristics and the actual search takes very little time even with $k$ as large as 10000.

92 CPU hours; 4 GB of memory.
7 Conclusion

In this paper, we developed two algorithms for finding \( k \) shortest paths of a WPDA. Previously, there were two approaches to this problem. The expansion approach expands the WPDA into an equivalent WFSA, which requires exponential time and space, and then finds the \( k \) shortest paths of the WFSA. Another pruned-expansion approach expands the WPDA into a WFSA with states or transitions not on a path close enough by a given threshold to the shortest path by weight removed, and then finds the \( k \) shortest paths of the pruned WFSA. This requires less time and space, but an appropriate threshold is almost impossible to set.

In contrast, our algorithms do not need any pruning or threshold picking and give the exact \( k \) shortest paths. The experimental results on real world input show that Algorithm 2 is highly efficient, adding very little overhead to the shortest distance pre-computation, whose running time is comparable to the original shortest path algorithm in [Allauzen and Riley 2012].

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David Chiang, Kevin Knight, and Wei Wang. 11,001 new features for statistical machine translation. In Proceedings of Human Language Technologies: The 2009 Annual Conference of the North American Chapter of the Association for Computational Linguistics, pages 218–226, Boulder, Colorado, June 2009. Association for Computational Linguistics. URL http://www.aclweb.org/anthology/N/N09/N09-1025
A Proof of Properties of $L_M$

**Theorem** (Soundness). Any valid proof of an instantiation $q_1 \rightsquigarrow q_2 : u$ in $L_M$ induces a balanced path from $q_1$ to $q_2$ with weight $u$ in $M$.

**Proof.** Base An axiom of the form $q_1 \rightsquigarrow q_2 : u$ must have $q_1 = q_2$ and $u = \bar{1}$. The yield of a proof using only the axiom is an empty path, thus a balanced path with weight $\bar{1}$.

Induction Assuming proofs with at most $n$ steps satisfy the above lemma. For any proof of $q_1 \rightsquigarrow q_2 : u$ in $n + 1$ steps,

- If the last step uses the Scan rule, then it must be of the following form,

$$
\begin{array}{c}
q_1 \rightsquigarrow q_3 : u_1 \\
q_1 \rightsquigarrow q_2 : u \\
\hline
q_3 \overset{a}{\rightarrow} q_2 : u_2
\end{array}
$$

where $u_1 \otimes u_2 = u$, $q_3 \overset{a}{\rightarrow} q_2 : u_2 \in E$ and $q_1 \rightsquigarrow q_3 : u_1$ is the outcome of some proof in at most $n$ steps. Let the induced path of the proof of $q_1 \rightsquigarrow q_3 : u_1$ be $\pi' = e_1e_2\ldots e_m$. The induced path of the whole proof is thus $\pi = e_1e_2\ldots e_m(q_3 \overset{a}{\rightarrow} q_2)$. By the induction hypothesis, $\pi'$ is a balanced path from $q_1$ to $q_3$ with weight $u_1$. As a result, $\pi$ is also balanced because $a \in \Sigma \cup \{\epsilon\}$ by definition of the logic; its weight is $w[\pi] = w[\pi'] \otimes u_2 = u_1 \otimes u_2 = u$.

- If the last step uses the Complete rule, then it must be of the following form,
where $u_1 \otimes u_2 \otimes u_3 \otimes u_4 = u$, $a \in \Pi$ is an opening parenthesis, and $\hat{a} \in \hat{\Pi}$ is the corresponding closing parenthesis. Similar to the Scan rule case, one can prove the induced path is a balanced path from $q_1$ to $q_2$ with weight $u$ using the associativity of $\otimes$.

Theorem (Completeness). Any balanced path from an entering state $q_1$ to some state $q_2$ with weight $u$ in $M$ has a valid proof of an instantiation $q_1 \leadsto q_2 : u$ in $L_M$ whose induced path is that path.

Proof. Base For any empty balanced path from a state $q$ such that $q \sim q : \top$ is an axiom, the proof is just the axiom itself.

Induction Assuming all balanced paths from any entering state of at most length $n$ satisfy the above lemma. For any balanced path of length $n + 1$ from an entering state $\pi = e_1 e_2 \ldots e_{n+1}$ from $q_1$ to $q_2$ with weight $u$,

- If $e_{n+1}$ is $q_3 \overset{a}{\to} q_2 : u_2$ with $a \in \Sigma \cup \{\varepsilon\}$, then $\pi' = e_1 e_2 \ldots e_m$ is a balanced of length $n$ and $w[\pi'] \otimes u_2 = u$. By induction hypothesis, there exists a proof of $\pi'$ (via item $q_1 \sim q_2 : u_1 \otimes u_2 = u$).
  
  Applying the Scan rule then gives a proof of $q_1 \leadsto q_2 : u_1 \otimes u_2 = u$.

- If $e_{n+1}$ is $q_3 \overset{a}{\to} q_2 : u_2$ with $a \in \hat{\Pi}$, then there must be a $k \leq n$ such that $e_k$ balances with $e_{n+1}$. Similar to the above case, one can prove the item by combining the proof of $e_1 \ldots e_{k-1}$ and $e_{k+1} \ldots e_m$.

- If $e_{n+1}$ is $q_3 \overset{a}{\to} q_2 : u_2$ with $a \in \Pi$, the path cannot be balanced.

Theorem (In-ambiguity). Any balanced path from an entering state in $M$ has a unique proof in $L_M$.

Proof. This is very similar to the completeness proof, thus we only give a sketch of the proof. First note all empty paths from an entering state has a unique proof (if the start state happens to have an incoming open-parenthesis transition, we consider the two inducing the same axiom). For any longer paths, if the last transition has a label from $\Sigma \cup \{\varepsilon\}$ then the last step must be using the Scan rule with antecedents with unique proof and that particular transition as the side condition; otherwise the last transition must have a closing parenthesis, which means a unique application of the Complete rule.