State-Split for Hypergraphs with an Application to Tree-Adjoining Grammars

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Abstract
In this work, we present a generalization of the state-split method to probabilistic hypergraphs. We show how to represent the derivational structure of probabilistic tree-adjoining grammars by hypergraphs and detail how the generalized state-split procedure can be applied to such representations, yielding a state-split procedure for tree-adjoining grammars.

1 Introduction
The state-split method (Petrov et al., 2006) allows the successive refinement of a probabilistic context-free grammar (PCFG) for the purpose of natural language processing (NLP). It employs automatic subcategorization of nonterminal symbols: in an iteration of a split-merge cycle, every nonterminal of the PCFG is split into two, along with the corresponding grammar rules, whose probabilities are distributed uniformly to the split rules. The resulting PCFG’s rule probabilities are then trained on an underlying treebank using the Expectation-Maximization algorithm (Dempster et al., 1977) for maximum-likelihood estimation on incomplete data. Finally, split nonterminal symbols which do not contribute to a significant increase in likelihood are merged back together. This counteracts an exponential blowup in the number of nonterminals and prevents, to some degree, the phenomenon of overfitting.

The in-house developed statistical machine translation toolkit Vanda (Büchse et al., 2012) offers state-splitting for the refinement of its language models. Vanda’s internal representation of the various weighted tree grammar, automaton and transducer formalisms utilized for translation is by means of probabilistic hypergraphs, i.e., graphs consisting of vertices and hyperedges, where each of the latter connects a (possibly empty) sequence of tail vertices to a head vertex and is assigned a probability. Hence, our implementation of state-split operates on such hypergraphs as underlying data structures. The connection between parsing and hypergraphs is well-known in the field of NLP (Klein and Manning, 2004), where a hypergraph represents the derivation forest of a certain word. In our system, however, we use such a probabilistic hypergraph to represent the whole derivational structure of a grammar, with a one-to-one correspondence between hyperpaths and grammar derivations. We apply well-known product constructions from the theory of weighted automata, going back to Bar-Hillel et al. (1961) and generalized to the case of weighted tree automata by Maletti and Satta (2009), to restrict them to the derivations of a given word.

The mildly context-sensitive generative capacity of tree-adjoining grammars (TAG) is well-suited to the purpose of NLP (Joshi and Schabes, 1991). Tree-adjoining grammars allow two basic operations to rewrite and derive trees: substitution, where a tree’s leaf node is replaced with another tree, and adjoining, which can be seen as the second-order substitution of a context (called an auxiliary tree) into another tree.

Probabilistic tree-adjoining grammars (PTAG) (Schabes, 1992; Resnik, 1992) assign to every derived tree an associated probability. They can also be incorporated into Vanda by an appropriate representation with hypergraphs. Such PTAGs can be extracted from treebank corpora, as detailed by Chen et al. (2006). The idea to refine these grammars furthermore by executing the already implemented state-split procedure on their hypergraph representations arises naturally. The main contribution of the work at hand is a formalization of this
idea. However, one should note that our proposed method does not just apply to PTAG, but should carry over to many ... \{w \mid i \in [n], w \in \text{pos}(t_i)\} \) and \( t(w) \) denotes the label of \( t \) at position \( w \).

Throughout the rest of the paper, let \( X = \{x_1, x_2, \ldots\} \) denote an infinite set of variables and, for \( n \in \mathbb{N} \), let \( X_n = \{x_1, x_2, \ldots, x_n\} \). Similarly, let \( Y = \{y_1, y_2, \ldots\}, \) let \( Y_n = \{y_1, y_2, \ldots, y_n\} \) for \( n \in \mathbb{N} \), and \( Z = \{z\}. \) Given \( k \in \mathbb{N} \), we call a tree \( t \in U_{\Sigma}(A \cup \Delta_X) \) (resp. \( t \in U_{\Sigma,\Delta_Y}(A) \)) proper in \( X_k \) (resp. \( Y_k \)) if for every \( i > k \), there is no appearance of \( \delta_{x_i} \) (resp. \( \delta_{y_i} \)) in \( t \), and for every \( i \in [k] \), there is exactly one position in \( t \) labeled with \( \delta_{x_i} \) (resp. \( \delta_{y_i} \)), for some \( \delta \in \Delta \). This unique \( \delta \in \Delta \) will be denoted by \( lb_t(x_i) \) (resp. \( lb_t(y_j) \)).

For an alphabet \( \Sigma \) and \( k \in \mathbb{N} \), we denote first-order substitution of the trees \( s_1, \ldots, s_k \in U_{\Sigma} \) into \( t \in U_{\Sigma}(X_k) \) by \( t[x_1/s_1, \ldots, x_k/s_k] \in U_{\Sigma} \), abbreviated by \( t[x/s] \). The tree \( t[x/s] \) is the result of replacing every node in \( t \) which is labeled by \( x_{s_i} \), for \( i \in [k] \) and some \( \sigma \in \Sigma \), by the tree \( s_i \). Similarly, for \( s \in U_{\Sigma}(A) \) and \( t \in U_{\Sigma}(Z) \), let \( t[y/s] \) denote the tree obtained from \( t \) by replacing every node that is labelled with \( z \) by \( s \).

For every alphabet \( \Sigma \) and \( k \in \mathbb{N} \), second-order substitution of the trees \( s_1, \ldots, s_k \in U_{\Sigma}(Z) \) into the tree \( t \in U_{\Sigma,\Delta_Y}(X_k) \) will be denoted by \( t[\llbracket y_{1/k} \rrbracket/s_1, \ldots, \llbracket y_k/s_k \rrbracket] \in U_{\Sigma} \), or shorter, by \( t[\llbracket y/s \rrbracket] \). For every symbol \( \sigma \in \Sigma \) and variable \( y_i \in Y_k \), we define \( \sigma_{y_i}(t_1, \ldots, t_n)[y/s] = \sigma_{y_i}([z/\sigma(t_1)[y/s], \ldots, t_n[y/s]]) \), and we define \( \sigma(t_1, \ldots, t_n)[y/s] = \sigma(t_1[y/s], \ldots, t_n[y/s]) \) for \( \sigma \in \Sigma \).

### 2.2 Hypergraphs

A hypergraph is a tuple \((V, E, \mu, g)\) where the set \( V \) contains the graph’s vertices and \( E \) the hyperedges (or just edges). Edge connectivity is denoted by the function \( \mu : E \to V^+ \) and \( g \in V \) is the graph’s goal vertex. For a hyperedge \( e \) with \( \mu(e) = a_0 a_1 \cdots a_n \), we define its head as \( \text{hd}(e) = a_0 \), its tail as \( \text{tl}(e) = a_1 \cdots a_n \) and its arity as \( \text{ar}(e) = n \). The set of \( a \)-hyperpaths \( H_a^G \) of a hypergraph \( G = (V, E, \mu, g) \), \( a \in V \), is the largest set of trees \( H \subseteq U_{E} \) such that for every \( d \in H, w \in \text{pos}(d) \), we have \( \text{hd}(d(e)) = a, \) \( \llbracket v \in \text{pos}(d) \mid v = wi, i \in \mathbb{N} \rrbracket = \| \text{tl}(e) \|, \) and \( \text{tl}(d(w)) = \text{hd}(d(w1)) \cdots \text{hd}(d(wn)) \), where
A tuple \((V, E, \mu, g, p)\) is called a probabilistic hypergraph (phg) if \((V, E, \mu, g)\) is a hypergraph and \(p: E \rightarrow [0, 1]\) assigns a probability to every hyperedge. We will denote the class of all probabilistic hypergraphs by \(\mathcal{H}\) and assume definitions for unweighted hypergraphs to carry over to the probabilistic case. The probability of a derivation \(d \in G\) is defined to be
\[
P(d \mid G) = \prod_{w \in \text{pos}(d)} p(d(w)).
\]

In the following, we will fix the phg \((\Sigma, S, A, P, Q)\) to be of the form \((V, E, \mu, g, p)\) (resp. \((V', E', \mu', g', p')\), etc.).

### 2.3 Tree-Adjoining Grammars

In our definition of tree-adjoining grammars, the variable \(x_i\) (resp. \(y_j\)) in a symbol \(\sigma_{x_i}\) (resp. \(\sigma_{y_j}\)) will be used to tag \(\sigma\) with the information that it labels the \(i\)th substitution (resp. \(j\)th adjoining) site of the respective tree. The variable \(z\) in an auxiliary tree denotes the tree’s foot node. This formalization allows us, among others, to give a straightforward definition of derived trees.

A tree-adjoining grammar (TAG) is a tuple \(G = (\Sigma, S, S, A)\) where \(\Sigma\) is an alphabet, \(S \in \Sigma\) is the start symbol, \(S \subseteq U_1(\Delta)\) the set of initial trees, and \(A \subseteq U_1(\Delta \cup Z)\) the set of auxiliary trees, with \(\Gamma = \Sigma \cup \Sigma_Y\) and \(\Delta = \Sigma_X\). We demand for every \(t \in S \cup A\) that \(t(\varepsilon) \in \Sigma\), and that there are \(n, m \in \mathbb{N}\) such that \(t\) is proper in \(X_n\) and in \(Y_m\). In the following, we will denote these unique \(n\) and \(m\) by \(rk_1(t)\), resp. \(rk_2(t)\). Moreover, we require that for every \(t \in A\), \(z\) appears exactly once in \(t\).

A probabilistic tree-adjoining grammar (PTAG) is then a tuple \(G' = (\Sigma, S, S, A, P, Q)\) such that \((\Sigma, S, S, A)\) is a TAG, \(P: S \cup A \rightarrow [0, 1]\) maps trees to their probabilities and \(Q = (Q_t: Y_{rk_2(t)} \rightarrow [0, 1])_{t \in S \cup A}\) assigns to adjoining sites the probability of their activation. We will denote the class of all PTAG by \(\mathcal{T}\).

Let us examine an example PTAG \(G\), with \(\Sigma = \{A, B, C, c, b\}\), \(S = A\), initial trees \(S = \{\alpha_1, \alpha_2\}\), and an auxiliary tree \(A = \{\beta\}\). Refer to Fig. 1, which depicts the tree \(\alpha_1\) with two substitution sites labeled, resp., with symbols \(A\) and \(C\), as well as one adjoining site, labeled with \(B\). To the right are the initial tree \(\alpha_2\) and the auxiliary tree \(\beta\), both with no substitution or adjoining sites. The foot node of \(\beta\) is indicated by \(z\).

We denote the conditional probability that an elementary tree \(t\) with root symbol \(A\) is used to rewrite substitution or adjoining sites that are labeled with \(A\) by \(P(t)\). For \(G\), e.g., let \(P(\alpha_1) = 0.9\), \(P(\alpha_2) = 0.5\), and \(P(\beta) = 0.6\). The probability that the adjoining site in \(\alpha_1\), tagged with \(y_1\), is activated during a derivation, is denoted by \(Q_{\alpha_1}(y_1)\). In the case of this running example, let \(Q_{\alpha_1}(y_1) = 0.7\).

### 3 Hypergraph Representations

For every PTAG \(G\), we can construct a hypergraph \(G = \text{hg}(\mathcal{G})\), whose hyperpaths stand in a one-to-one correspondence to the grammar’s derivations. Hence, we will call \(G\) a hypergraph representation of \(\mathcal{G}\).

In our following definition, such a hypergraph \(\text{hg}(\mathcal{G})\) can contain three different types of vertices. The vertices of the first type model the derivation of initial trees. These vertices are just copies of the symbols of \(\mathcal{G}\): for every symbol \(A \in \Sigma\), a vertex \(A\) is introduced. Refer to Fig. 2, which depicts the hypergraph \(\text{hg}(\mathcal{G})\) that represents the derivational structure of the PTAG \(G\) from our running example. Its A- and C-hyperpaths model derivation of initial
trees with respective root symbols. Other, irrelevant, vertices of this form are omitted from the figure.

The second vertex type helps in the derivation of auxiliary trees. For each \( A \in \Sigma\), the hypergraph contains a corresponding vertex \( A^*\). In Fig. 2, the only relevant vertex of this form is \( B^*\), whose hyperpaths represent derivations of auxiliary trees with root symbol \( B\).

Lastly, for every adjoining site that appears in an elementary tree \( t\) and is tagged with \( y_i\), we include a vertex \( S(t,y_i)\). This vertex is used to explicitly model the decision to activate or not to activate the corresponding adjoining site. In the figure, there is only one such vertex, \( S(\alpha_1, y_1)\).

The hyperedges of \( hsg(G)\) can also be classified by their intended meaning: a hyperedge of the form \( s(\alpha)\) signifies the substitution of the initial tree \( \alpha\) during a derivation. Its head vertex is its root symbol. Its tail vertices are, in order, the labels of \( \alpha\)'s substitution sites (indicating that the derivation must continue with derivations of trees with the respective symbols at their root) and the vertices \( S(\alpha, y_i)\) modelling its adjoining sites (these indicate the necessary decision on activating the sites).

In Fig. 2, we see, among others, \( s(\alpha_1)\), whose head vertex \( A\) corresponds to \( \alpha_1\)'s root symbol, while its two tail vertices \( C\) stand for its respective substitution sites, and \( S(\alpha_1, y_1)\) for its adjoining site.

Hyperedges of the form \( a(\beta)\), with \( \beta\) an elementary auxiliary tree, possess essentially the same structure as the former, but signify derivation of auxiliary trees. In the figure, the only edge of this form is \( a(\beta)\). Its head vertex is \( B^*\) because \( \beta\)'s root symbol is \( B\), and it has no tail vertices, since there are no sites in \( \beta\).

Finally, the hyperedge \( y(t, y_i)\) (resp. \( n(t, y_i)\)) encodes the information that an adjoining site in \( t\) was activated (deactivated). Both have \( S(t, y_i)\) as head, and while \( n(t, y_i)\) has no tail, the tail of \( y(t, y_i)\) signifies that the derivation should continue with the adjoining of an auxiliary tree. In Fig. 2, e.g., \( y(\alpha_1, y_1)\) models the activation of the site that corresponds to its head vertex \( S(\alpha_1, y_1)\), and has the tail vertex \( B^*\), because that site is labeled with \( B\).

The probabilities of these hyperedges are taken over from \( P\) and \( Q\) in the obvious way. Formally, we define \( hsg(G) = G\) with

\[
V = \{ A, A^* \mid A \in \Sigma \} \\
\cup \{ S(t, y_i) \mid t \in S \cup A, i \in [\text{rk}_2(t)] \},
\]

\[
E = \{ s(t) \mid t \in S \} \cup \{ a(t) \mid t \in A \} \\
\cup \{ y(t, y_i), n(t, y_i) \mid t \in S \cup A, i \in [\text{rk}_2(t)] \},
\]

goal vertex \( g = S\), and

\[
\mu(s(t)) = A B_1 \ldots B_n S(t, y_1) \ldots S(t, y_m),
\]

\[
\mu(a(t)) = A^* B_1 \ldots B_n S(t, y_1) \ldots S(t, y_m),
\]

\[
\mu(y(t, y_j)) = S(t, y_j) C_j',
\]

\[
\mu(n(t, y_j)) = S(t, y_j),
\]

where \( n = \text{rk}_1(t), m = \text{rk}_2(t), A = t(\varepsilon), B_i = \text{lb}_t(x_i)\) for \( i \in [n]\), and \( C_j = \text{lb}_t(y_j)\) for \( j \in [m]\), while

\[
p(s(t)) = P(t), \quad p(y(t, y_j)) = Q_t(y_j),
\]

\[
p(a(t)) = P(t), \quad p(n(t, y_j)) = 1 - Q_t(y_j).
\]

Note that for our simple running example from Fig. 1, there are only two possible derivations of trees with root symbol \( A\): in the first one, we substitute two instances of \( \alpha_2\) into \( \alpha_1\), and, after activation of the adjoining site in \( \alpha_1\), adjoining it into this site. The corresponding \( A\)-hyperpath in Fig. 2 is \( d_1 = s(\alpha_1)(s(\alpha_2), s(\alpha_2), y(\alpha_1, y_1)(a(\beta)))\).

Alternatively, we can ignore the adjoining site, and arrive at the corresponding derivation \( d_2 = s(\alpha_1)(s(\alpha_2), s(\alpha_2), n(\alpha_1, y_1))\).

Given such a hyperpath that represents a PTAG derivation, we can compute the derivation’s derived tree in a bottom-up manner with the function \( yd: hsg(G) \rightarrow U_\Sigma(X \cup Z)\) defined by

\[
yd(s(t)(d_1, \ldots, d_n, d'_1, \ldots, d'_m))
= t[x/\ yd(d)][y/\ yd(d')]
\]

\[
yd(a(t)(d_1, \ldots, d_n, d'_1, \ldots, d'_m))
= t[x/\ yd(d)][y/\ yd(d')]
\]

\[
yd(y(t, y_j)(d)) = yd(d)
\]

\[
yd(n(t, y_j)) = z,
\]

where again \( n = \text{rk}_1(t), m = \text{rk}_2(t), \) and \( yd(d)\) denotes the element-wise application of \( yd\) to all \( d_1, \ldots, d_n\), analogously for \( yd(d')\).

For example, for \( d_1\) from above, we can compute its derived tree as

\[
yd(d_1) = \alpha_1[x_1/\alpha_2, x_2/\alpha_2][y_1/\beta]
= A(C(c), B_{y_1}(c, C(c)))[y_1/\beta]
= A(C(c), \beta[z/B(c, C(c))])
= A(C(c), B(b, B(c, C(c)))).
\]

4 State-Split Hypergraphs

In this section, we will detail how to generalize the state-split method presented by Petrov et al. to hypergraphs that represent PTAGs.
As explained in the introduction, the state-split algorithm proceeds in three distinct phases: first of all, it splits every vertex into two, and then it trains the probabilities of the resulting hyperedges on a given treebank corpus, using the EM algorithm. In a third step, vertices which do not increase likelihood are merged back together. However, due to the nature of adjunction in tree-adjoining grammar, the splits and merges cannot be quite as liberal as in the case of context-free grammars.

The reason for this will be shown immediately, but first and foremost, let us define how to represent split vertices. Given a hypergraph $G$, for any $a \in V$, and $b \in \{0, 1, 2\}$, define
\[
a^b = \begin{cases} (a, b) & \text{if } b \in \{1, 2\} \\ a & \text{if } b = 0. \end{cases}
\]
For a vertex $a$, the so-defined $a^1$ and $a^2$ will denote the two vertices which result from splitting $a$, while $a^0$ is just a notation for the merged-back-together vertex $a$. We will also have to annotate split hyperedges in this way: for a hyperedge $e \in E$ with $\text{ar}(e) = n$, as well as a tuple $b \in \{0, 1, 2\}^{n+1}$, we introduce the syntax $e^b$, which stands for $(e, b)$.

Given this notation, we can examine the mentioned complication of the state-split procedure, which arises when splitting hyperedges of the form $y(t, y_j)$. Let us assume that the vertices $S(\alpha_1, y_1)$, $B^*$, as well as the hyperedge $y(\alpha_1, y_1)$ from Fig. 2 are to undergo subcategorization.

If we split the vertices and hyperedges indiscriminately, we arrive at the situation displayed in Fig. 3: each of the vertices has been split into two copies, and four new $y$-hyperedges were introduced. What is the meaning of these hyperedges? In a hyperpath representing a PTAG derivation, the appearance of the hyperedge $y(\alpha_1, y_1)^{11}$ signifies that the adjoining site in $\alpha_1$, labeled with the split symbol $B(1)$, is activated, and next, an auxiliary tree with equal root symbol must be adjoining into it.

However, there is a problem with the hyperedge $y(\alpha_1, y_1)^{21}$ which crosses the shaded ellipses in the figure (and, analogously, with $y(\alpha_1, y_1)^{12}$). This hyperedge can be interpreted as activation of the mentioned adjoining site, labeled with $B(1)$, and preparation of adjoining an auxiliary tree with root symbol $B(2)$. This stands in conflict to the concept of adjoining, where the label of the node to be replaced must be identical to the symbol at the root of the auxiliary tree.

There are several distinct possibilities to handle this complication. First of all, one could just do away with the above condition regarding adjoining. Actually, such a relaxation of the formalism was already proposed by Rogers (2003), resulting in non-strict tree-adjoining grammars.

As a second option, the formalism of TAG could be extended by introducing states (cf. Büchse et al., 2011) for synchronous TAG). In this modification, the derivational structure of the grammar is no longer dependent on the labels of adjoining and substitution sites, this information is instead encoded into the states, which only appear as intermediate symbols in a derivation. Performing the splits and merges on such states, instead of symbols, could also remedy the problem.

However, for this work, we chose to stick to a conceptually simpler solution, thus staying close to the established notion of tree-adjoining grammar: we just disallow the creation of such crossing hyperedges during the split-merge cycle; or, to put it differently, we only introduce a hyperedge $y(t, y)^{(i)}$ into the split hypergraph if $i = j$. Hence, in Fig. 3, only the two hyperedges $y(\alpha_1, y_1)^{11}$ and $y(\alpha_1, y_1)^{22}$, which are both “within” the two shaded ellipses, would be generated.

To formalize this idea, we augment the state-split method with what we call split relations. Given a hypergraph $G$ which is to undergo a split-merge cycle, a split relation on $G$ is a symmetric relation $R \subseteq V \times V$ on the graph’s vertices. If a hyperedge $e$ from $G$ connects, among others, two vertices $a_1$ and $a_2$ such that $a_1 Ra_2$, then the idea is to split $e$ only into such hyperedges which connect either only $a_1^1$ and $a_2^1$, or only $a_1^2$ and $a_2^2$, but not, e.g., $a_1^1$ and $a_2^2$.

This invariant must also be heeded when we merge back together parts of the hypergraph: for example, if $a_1 Ra_2$, we cannot merge back together
a_1(1) and a_1(2) but leave a_2(1) and a_2(2) split at the same time. Hence, what we must consider is merging all elements which are (in-)directly related by \( R \) simultaneously together. More succinctly, the objects considered to be merged must be the equivalence classes of the reflexive-transitive closure \( R^* \) of \( R \), which we also call split classes.

### 4.1 Splitting

When we split the vertices of a hypergraph, we must take care that the created hyperedges respect the supplied split relation \( R \), as explained above.

This is achieved by the following function \( \text{split}_R \), which splits every node and introduces new hyperedges respecting \( R \). Given a hypergraph \( G \) and split relation \( R \subseteq V \times V \), we let \( \text{split}_R(G) = G' \) with

- \( V' = \{ a(b) \mid a \in V, b \in \{1, 2\} \} \),
- \( E' = \{ e(b_0, \ldots, b_k) \mid e \in E, \mu(e) = a_0 \cdots a_k, b_0, \ldots, b_k \in \{1, 2\} \}, \)
- \( \mu'(e(b_0, \ldots, b_k)) = a_0(b_0) \cdots a_k(b_k) \),
- \( g' = g(1) \), and
- \( p'(e(b_0, \ldots, b_k)) = \frac{p(e)}{2^c} \),

where \( c = |\{ e(b') \in E' \mid b' = b_0 \cdots b_k \}| \).

Note that the probabilities of hyperedges are distributed uniformly to their split copies in \( G' \). In an implementation, these should be slightly randomized to give starting values for the EM algorithm, as mentioned by Petrov et al. (2006).

The split hypergraph’s number of hyperedges is exponential in their arity. We can try to mitigate the problem of this exponential blowup by binarizing the trees of the TAG which was initially extracted from a corpus, following the description of Lang (1994).

### 4.2 Merging

As explained above, we have to merge all elements of a split class back together simultaneously. This will be denoted with the following function. Let \( G' = \text{split}_R(G) \) be a hypergraph resulting from a split, \( R \subseteq V \times V \) a split relation, and \( C \in V \times R^* \) one of its split classes. The hypergraph which results from merging \( C \) back together is denoted by \( G'' = \text{merge}_R(G') \) with

- \( V'' = V' \setminus \{ a(b) \mid a \in C, b \in \{1, 2\} \} \cup C \),
- \( E'' = \{ e(b_0', \ldots, b'_k) \mid e(b_0, \ldots, b_k) \in E' \}, \)
- \( \mu(e) = a_0 \cdots a_k \),
- \( a_i \in C \text{ implies } b'_i = 0 \),
- \( a_i \not\in C \text{ implies } b'_i = b_i \),

where we write \( \alpha(e(b_0', \ldots, b'_k)) = e(b_0, \ldots, b_k) \) for the relation of \( e(b_0', \ldots, b'_k) \) to \( e(b_0, \ldots, b_k) \),

\[
\mu''(e(b_0', \ldots, b'_k)) = \alpha(e(b_0(b_0) \cdots a_k(b_k)),
\]

where \( \mu(e) = a_0 \cdots a_k \),

\[
g'' = \begin{cases} g & \text{if } g \in C \\ g' & \text{otherwise, and} \end{cases}
\]

\[
p''(e'') = \begin{cases} \frac{\sum_{e' \in \alpha^{-1}(e'')} p'(e')}{2} & \text{if } \text{hd}(e) \in C \\ \sum_{e' \in \alpha^{-1}(e'')} p'(e') & \text{otherwise} \end{cases}
\]

Note that the probabilities of hyperedges which are merged back together are summed up. In the case that a hyperedge’s head vertex is merged, we have to normalize the resulting probability.

### 4.3 Treebank Corpora and Likelihood

During the split-merge procedure, we want to train the split hypergraph representations on a supplied treebank. Following the presentation of Prescher (2005), we will abstract away from the concrete data structures which might be used to represent a collection of trees, and just define a treebank corpus as a function \( K : U_\Sigma \rightarrow \mathbb{R}_{\geq 0} \), assigning to every tree over an alphabet \( \Sigma \) a certain frequency, such that the set of trees with non-zero frequency is finite.

Let us assume that \( G_0 = \text{hg}(G) \) is the hypergraph representation of a PTAG \( G \) and \( G_n \) is the result of \( n \) split-merge cycles on \( G_0 \). Then we can define the likelihood of a corpus \( K : U_\Sigma \rightarrow \mathbb{R}_{\geq 0} \) on \( G_n \) as

\[
L(K \mid G_n) = \prod_{t \in U_\Sigma} \left( \sum_{d \in H_{G_n}} P(d \mid G_n) \right)^{K(t)}
\]

\[
= \prod_{t \in U_\Sigma} \left( \sum_{d' \in H_{G_0}} \left( \sum_{d \in H_{G_n}} P(d \mid G_n) \right) \right)^{K(t)}.
\]

Hereby, the function \( u_n \) removes \( n \) levels of annotation from an annotated derivation, for every \( n \in \mathbb{N} \). It is defined as the homomorphic extension of the function \( \bar{u}_n \) on hyperedges to unranked trees, where \( \bar{u} \) is defined for every hyperedge \( e \) by \( \bar{u}_0(e) = e \), and for \( n > 1 \), \( \bar{u}_n(e(b)) = \bar{u}_{n-1}(e) \).
Algorithm 1 The state-split algorithm

Require: phg $G$, $n \in \mathbb{N}$, corpus $K : U_\Sigma \rightarrow \mathbb{R}_{\geq 0}$
1: function STATE_SPLIT($G, n, K$)
2: $G_0 \leftarrow G$
3: compute split relation $R_0$
4: for all $i \in [n]$ do
5: \quad $G_i \leftarrow \text{SPLIT_MERGE}(G_{i-1}, R_{i-1}, K)$
6: \quad update split relation $R_{i-1}$ to $R_i$
7: end for
8: return $G_n$
9: end function

Note that in (1), for every $t \in U_\Sigma$ with non-zero frequency, there are only finitely many derivations $d' \in H_{G_0}$, which can be determined by employing a TAG parser at the beginning of the state-split process. For each of these $d'$ we can compute the value of the innermost sum in a bottom-up manner, similarly to the computation of inside probabilities as described by Petrov et al. (2006).

In the following, given a hypergraph $G_n$, $n > 0$, we will identify $yd(d)$ with $yd(u_n(d))$, for every $d \in H_{G_n}$.

4.4 Overview of the Algorithm

Now we can denote the state-split algorithm for hypergraphs in pseudocode, cf. Alg. 1. After computing the initial split relation, the algorithm’s outer loop (ll. 4–7) executes $n$ split-merge cycles on $G$ using the treebank corpus $K$ for training. Additionally, in each step it updates the split relation to the newly generated hypergraph.

Note that the concrete computation of split classes depends strongly on the grammar formalism represented by the hypergraph, hence we leave it abstract in the general formulation of the algorithm. In our case, where we use tree-adjointing grammars as underlying formalism, we can instantiate it as follows: $R_0$ is defined as the finest symmetric relation $R$ such that, for every vertex of the form $S(t, y_i)$ in $G_0$, we have $(S(t, y_i), lb_t(y_i)^*) \in R$. Similarly, given a split relation $R_{i-1}$, the updated split relation $R_i$ is the finest symmetric relation $R$ such that, for every $b \in \{0, 1, 2\}$ and pair $a_1(b)$, $a_2(b)$, if $a_1(b)$ and $a_2(b)$ are vertices in $G_i$ such that $a_1 R_{i-1} a_2$, then $a_1(b) R a_2(b)$.

The split-merge cycle (cf. Alg. 2) can be considered as the core of the state-split algorithm. Supplied with a phg $G$, split relation $R$ on $G$, and treebank corpus $K$, SPLIT_MERGE first of all splits the nodes of $G$, as defined in section 4.1. Then it uses the EM algorithm for maximum likelihood estimation on incomplete data to train the newly-split phg on the treebank $K$. Finally, in ll. 4–9, each split class is tentatively merged back together, and if the concomitant loss in likelihood does not fall below a certain factor $\lambda \in [0, 1]$, this merge is taken over permanently. As noted by Petrov et al., this combats the exponential blow-up of the hypergraph, as well as the phenomenon of overfitting.

For the sake of completeness, let us give a rough sketch of the EM algorithm for training state-split hypergraphs on treebank corpora, following the exposition of Prescher (2005). Given a phg $G$ and a treebank corpus $K$, the EM algorithm alternatingly repeats two computations, called the Expectation step (E-step) and the Maximization step (M-step), until the increase in likelihood of the newly-computed hypergraph on the corpus $K$ falls beneath a certain threshold $\delta \in \mathbb{R}$.

Note that the EM algorithm is not guaranteed to find the actual global maximum of the likelihood, however, as already shown by Dempster et al. (1977), the likelihoods of the respective grammars are monotonically non-decreasing, and so at least a local maximum can be approximated.

In the algorithm’s E-step, a complete-data corpus $C : H_G \rightarrow \mathbb{R}_{\geq 0}$ on the hyperpaths of $G$ is generated by distributing the frequencies of every derived tree $t \in U_\Sigma$ in the corpus $K$ to the hyperpaths representing derivations of $t$, weighted by their conditional probability given $t$. The M-step then uses this complete-data corpus to compute hyperedge probabilities by relative frequency estimation. Thereby, $ct_e(d)$ denotes the number of appearances of the hyperedge $e$ in the derivation $d$,
Algorithm 3 EM for (state-split) hypergraphs

Require: phg $G$, corpus $K: U\Sigma \rightarrow \mathbb{R}_{\geq 0}$

1: function EMTRAIN($G, K$)
2: repeat
3: ... nodes or hyperedges
4: E-Step: define $C: H_G \rightarrow \mathbb{R}$ by:
5: $C(d) = K(yd(d)) \cdot P(d \mid yd(d), G)$
6: M-step: set new probabilities:
7: for all $e \in E$ do
8: $p(e) \leftarrow \sum_{d \in H_G} C(d) \cdot ct_e(d)$
9: end for
10: until $L(G | K) - L(G' | K) < \delta$
11: return $G$
12: end function

and $ct_{\text{rd}(e)}(d)$ the number of appearing hyperedges with the same head vertex as $e$.

One might remark that this concise, but formulaic presentation of EM is not immediately suitable for implementation, but, using the derivation employed by Gupta and Chen (2011), it is straightforward to bring it into the form of the well-known Inside-Outside algorithm, which has been adapted to PTAG by Schabes (1992).

5 State-Split preserves Hypergraph Representations

After all these definitions, we might ask ourselves the following question: given a hypergraph representation $G'$ of some PTAG $G$, does the hypergraph which results from an application of the split-merge cycle to $G'$ still represent a PTAG? This question indeed arises quite naturally, after all it is an important requirement for the correctness of the state-split procedure for PTAGs with hypergraphs.

If we denote the result of a split-merge cycle on a phg $G$ by $\text{sm}(G)$, and the class of all hypergraph representations of probabilistic tree-adjoining grammars by $\mathcal{H}_T$, then this question can essentially be answered by proving the inclusion

$$\text{sm}(\mathcal{H}_T) \subseteq \mathcal{H}_T. \quad (2)$$

But the validity of this inclusion does certainly depend on the formal definition of $\mathcal{H}_T$. Indeed, for the definition which comes to mind first, in which we just fix $\mathcal{H}_T$ to be the set $\{hg(G) \mid G \in T\}$, i.e. the image of the class of all PTAGs under hg, the inclusion is not valid! This is due to the annotation of vertices and hyperedges in a split-merge cycle: hypergraphs that contain, for example, a vertex $A(2), which was generated by splitting a vertex $A$, are arguably not in the image of hg!

However, one can show that the structure of a split-and-merged hypergraph still corresponds to the image of a PTAG $G$ under hg. We will capture this structural identity by means of hypergraph isomorphisms.

A hypergraph isomorphism $\Phi: G \xrightarrow{\sim} G'$ is a tuple $(\Phi_1, \Phi_2)$, where $\Phi_1: V \rightarrow V'$ and $\Phi_2: E \rightarrow E'$ are bijections such that $\Phi_1(g) = g'$ and $\mu(\Phi_2(e)) = \Phi_1(a_0) \cdots \Phi_1(a_n)$ if $\mu(e) = a_0 \cdots a_n$. We write $G \cong G'$ if there is an isomorphism $\Phi: G \xrightarrow{\sim} G'$.

We define the set of all possible hypergraph representations of PTAG as

$$\mathcal{H}_T = \{G \in \mathcal{H} \mid \exists G' \in T. \ hg(G) \cong G\}.$$  

Obviously, for every PTAG $G$, $\ hg(G) \in \mathcal{H}_T$, i.e., it is indeed a hypergraph representation according to this definition. As visualized in Fig. 4, the core of the proof of (2) is then as follows: Given $G \in T, G \in \mathcal{H}$, and $G' = \text{sm}(G)$, we have to construct a PTAG $G''$ and hypergraph isomorphism $\Phi: \ hg(G'') \xrightarrow{\sim} G''$.

We construct $G''$ so that the trees of $G'$ are relabelings of those in $G$, generated by incorporating the annotations to the hyperedges in $G$ to substitution and adjoining sites:

$$S' = \{t(b) \mid s(t)(b) \in E'\},$$

$$A' = \{t(b) \mid a(t)(b) \in E'\},$$

where $t(a b_1 \cdots b_i k_j(t) c_1 \cdots c k_j(t))$ is the result of replacing the root symbol $A$ of $t$ by $A(a)$, every substitution site $A_{x_i}$ in $t$ by $A(b_i x_i)$, and every adjoining site $A_{y_j}$ by $A(c_j y_j)$, for $i \in [rk_1(t)]$ and $j \in [rk_2(t)]$. The probabilities $P(t)$ of elementary trees $t$, as well as the activation probabilities $Q(t, y_j)$ are just read off from $p(s(t)), p(a(t))$, resp. $p(y(t, y_j))$.

The hypergraph isomorphism $\Phi$ then just reverses this relabeling. Given nodes or hyperedges from $\ hg(G'')$ with annotations in them, it removes them from the contained symbols resp. elementary
trees and moves them “to the back”, i.e.,
$$\Phi_1(A\langle b \rangle) = A\langle b \rangle, \quad \Phi_1((A\langle b \rangle)^*) = A^*\langle b \rangle,$$
$$\Phi_1(S(t\langle b \rangle, y_i)) = \ldots$$
and
$$\Phi_2(s(t\langle b \rangle)) = s(t)\langle b \rangle, \quad \Phi_2(s(t\langle b \rangle)) = s(t)\langle b \rangle,$$
$$\Phi_2(y(t\langle b \rangle, y_i)) = y(t, y_i)\langle b^{(i)} \rangle, \quad \Phi_2(n(t\langle b \rangle, y_i)) = n(t, y_i)\langle b^{(i)} \rangle,$$
where, in all three cases, $b^{(i)} = b(\text{rk}_1(t) + i)$.

Now, $\Phi$ can indeed be proven to be a hypergraph isomorphism between $G'$ and $sm(G)$, but for reasons of space, we will omit these details from this work. Note that the construction of $G'$ and $\Phi$ can alternatively be interpreted as the definition of a read-off procedure, which allows our system Vanda to convert back its internal state-split hypergraph representation into a probabilistic tree-adjoining grammar, e.g. to display the resulting grammars for means of debugging. Thus, it also has a hands-on relevance for implementation.

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