

# Unsupervised Learning of Probabilistic Context-Free Grammar Using Iterative Biclustering

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**Abstract.** This paper presents PCFG-BCL, an unsupervised algorithm that learns a probabilistic context-free grammar (PCFG) from positive samples. The algorithm acquires rules of an unknown PCFG through iterative biclustering of bigrams in the training corpus. Our analysis shows that this procedure uses a greedy approach to adding rules such that each set of rules that is added to the grammar results in the largest increase in the posterior of the grammar given the training corpus. Results of our experiments on several benchmark datasets show that PCFG-BCL is competitive with existing methods for unsupervised CFG learning.

## 1 Introduction

Context-free grammars (CFG) constitute an important class of grammars, with a broad range of applications including programming languages, natural language processing, and bioinformatics, among others. A probabilistic context-free grammar (PCFG) is a CFG with probabilities assigned to grammar rules, which can better accommodate the ambiguity and the need for robustness in real-world applications. Hence, the problem of learning a PCFG from data (typically, positive samples generated by the target grammar) is an important problem in grammar induction and machine learning. Several methods for learning (P)CFG from positive data have been proposed. Some rely on different heuristics to iteratively construct an approximation of the unknown CFG [1,2,3,4,5]; others search for a PCFG that has the largest posterior given the training corpus [6,7,8,9].

In this paper we propose PCFG-BCL, a new unsupervised algorithm that learns a PCFG from a positive corpus. The proposed algorithm uses (distributional) biclustering to group symbols into non-terminals. This is a more natural and robust alternative to the more widely used substitutability heuristic or distributional clustering, especially in the presence of ambiguity, e.g., when a symbol can be reduced to different nonterminals in different contexts, or when a context can contain symbols of different nonterminals, as illustrated in [1]. PCFG-BCL can be understood within a Bayesian structure search framework. Specifically, it uses a greedy approach to adding rules to a partially constructed grammar, choosing at each step a set of rules that yields the largest possible increase in

the posterior of the grammar given the training corpus. The Bayesian framework also supports an ensemble approach to PCFG learning by effectively *combining* multiple candidate grammars. Results of our experiments on several benchmark datasets show that the proposed algorithm is competitive with other methods for learning CFG from positive samples.

The rest of the paper is organized as follows. Section 2 introduces the representation of PCFG used in PCFG-BCL. Section 3 describes the key ideas behind PCFG-BCL. Section 4 presents the complete algorithm and some implementation details. Section 5 presents the results of experiments. Section 6 concludes with a summary and a brief discussion of related work.

## 2 Grammar Representation

It is well-known that any CFG can be transformed into the Chomsky normal form (CNF), which only has two types of rules:  $A \rightarrow BC$  or  $A \rightarrow a$ . Because a PCFG is simply a CFG with a probability associated with each rule, it is easy to transform a PCFG into a probabilistic version of CNF.

To simplify the explanation of our algorithm, we make use of the fact that a CNF grammar can be represented in an AND-OR form containing three types of symbols, i.e., AND, OR, and terminals. An AND symbol appears on the left-hand side of exactly one grammar rule, and on the right-hand side of that rule there are exactly two OR symbols. An OR symbol appears on the left-hand side of one or more rules, each of which has only one symbol on the right-hand side, either an AND symbol or a terminal. A multinomial distribution can be assigned to the set of rules of an OR symbol, defining the probability of each rule being chosen. An example is shown below (with rules probabilities in the parentheses).

<b>CNF</b>	<b>The AND-OR Form</b>
$S \rightarrow a$ (0.4)   $AB$ (0.6)	$OR_S \rightarrow a$ (0.4)   $AND_{AB}$ (0.6)
$A \rightarrow a$ (1.0)	$AND_{AB} \rightarrow OR_A OR_B$
$B \rightarrow b_1$ (0.2)   $b_2$ (0.5)   $b_3$ (0.3)	$OR_A \rightarrow a$ (1.0)
	$OR_B \rightarrow b_1$ (0.2)   $b_2$ (0.5)   $b_3$ (0.3)

It is easy to show that a CNF grammar in the AND-OR form can be divided into a set of *AND-OR groups* plus the start rules (rules with the start symbol on the left-hand side). Each AND-OR group contains an AND symbol  $N$ , two OR symbols  $A$  and  $B$  such that  $N \rightarrow AB$ , and all the grammar rules that have one of these three symbols on the left-hand side. In the above example, there is one such AND-OR group, i.e.,  $AND_{AB}$ ,  $OR_A$ ,  $OR_B$  and the corresponding rules (the last three lines). Note that there is a bijection between the AND symbols and the groups; but an OR symbol may appear in multiple groups. We may simply make identical copies of such OR symbols to eliminate overlap between groups.

## 3 Main Ideas

PCFG-BCL is designed to learn a PCFG using its CNF representation in the AND-OR form. Sentences in the training corpus are assumed to be sampled from

an unknown PCFG under the i.i.d. (independent and identically distributed) assumption.

Starting from only terminals, PCFG-BCL iteratively adds new symbols and rules to the grammar. At each iteration, it first learns a new AND-OR group by biclustering, as explained in Section 3.1. Once a group is learned, it tries to find rules that attach the newly learned AND symbol to existing OR symbols, as discussed in Section 3.2. This second step is needed because the first step alone is not sufficient for learning such rules. In both steps, once a new set of rules are learned, the corpus is *reduced* using the new rules, so that subsequent learning can be carried out on top of the existing learning result. These two steps are repeated until no further rule can be learned. Then start rules are added to the learned grammar in a postprocessing step (Section 3.3). Since any CNF grammar can be represented in the form of a set of AND-OR groups and a set of start rules, these three steps are capable, in principle, of constructing any CNF grammar.

We will show later that the first two steps of PCFG-BCL outlined above attempt to find rules that yield the greatest increase in the posterior probability of the grammar given the training corpus. Thus, PCFG-BCL performs a local search over the space of grammars using the posterior as the objective function.

### 3.1 Learning a New AND-OR Group by Biclustering

**Intuition.** In order to show what it means to learn a new AND-OR group, it is helpful to construct a table  $T$ , where each row or column represents a symbol appearing in the corpus, and the cell at row  $x$  and column  $y$  records the number of times the pair  $xy$  appears in the corpus. Because the corpus might have been partially reduced in previous iterations, a row or column in  $T$  may represent either a terminal or a nonterminal.

Since we assume the corpus is generated by a CNF grammar, there must be some symbol pairs in the corpus that are generated from AND symbols of the target grammar. Let  $N$  be such an AND symbol, and let  $A, B$  be the two OR symbols such that  $N \rightarrow AB$ . The set  $\{x|A \rightarrow x\}$  corresponds to a set of rows in the table  $T$ , and the set  $\{y|B \rightarrow y\}$  corresponds to a set of columns in  $T$ . Therefore, the AND-OR group that contains  $N, A$  and  $B$  is represented by a *bicluster*[10] (i.e., a submatrix) in  $T$ , and each pair  $xy$  in this bicluster can be reduced to  $N$ . See Fig.1 (a), (b) for an example, where the AND-OR group shown in Fig.1(a) corresponds to the bicluster shown in Fig.1(b).

Further, since we assume the target grammar is a PCFG, we have two multinomial distributions defined on  $A$  and  $B$  respectively that independently determine the symbols generated from  $A$  and  $B$ . Because the corpus is assumed to be generated by this PCFG, it is easy to prove that the resulting bicluster must be *multiplicatively coherent*[10], i.e., it satisfies the following condition:

$$\frac{a_{ik}}{a_{jk}} = \frac{a_{il}}{a_{jl}} \quad \text{for any two rows } i, j \text{ and two columns } k, l \quad (1)$$

where  $a_{xy}$  is the cell value at row  $x$  ( $x = i, j$ ) and column  $y$  ( $y = k, l$ ).

$AND_{NP} \rightarrow OR_{Det} OR_N$ $OR_{Det} \rightarrow the(0.67) \mid a(0.33)$ $OR_N \rightarrow circle(0.2)$ $\mid triangle(0.3) \mid square(0.5)$	below above <b>the</b> <b>a</b> circle triangle ⋮	<table style="border-collapse: collapse; text-align: center;"> <tr> <td style="padding: 2px 10px;">is</td> <td style="padding: 2px 10px;"><b>circle</b></td> <td style="padding: 2px 10px;"><b>triangle</b></td> <td style="padding: 2px 10px;"><b>square</b></td> <td style="padding: 2px 10px;">the</td> <td style="padding: 2px 10px;">⋯</td> </tr> <tr> <td style="padding: 2px 10px;">8</td> <td colspan="3" style="border: 2px solid black; padding: 5px;"> <table style="border-collapse: collapse; text-align: center;"> <tr> <td style="padding: 2px 10px;">24</td> <td style="padding: 2px 10px;">36</td> <td style="padding: 2px 10px;">60</td> </tr> <tr> <td style="padding: 2px 10px;">12</td> <td style="padding: 2px 10px;">18</td> <td style="padding: 2px 10px;">30</td> </tr> </table> </td> <td style="padding: 2px 10px;">10</td> <td></td> </tr> </table>	is	<b>circle</b>	<b>triangle</b>	<b>square</b>	the	⋯	8	<table style="border-collapse: collapse; text-align: center;"> <tr> <td style="padding: 2px 10px;">24</td> <td style="padding: 2px 10px;">36</td> <td style="padding: 2px 10px;">60</td> </tr> <tr> <td style="padding: 2px 10px;">12</td> <td style="padding: 2px 10px;">18</td> <td style="padding: 2px 10px;">30</td> </tr> </table>			24	36	60	12	18	30	10	
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(a) An AND-OR group (with rule probabilities in the parentheses)

(b) A part of the table  $T$  and the bicluster that represents the AND-OR group. Zero cells are left blank.

⋯ covers (.)	⋯ touches (.)	⋯ is above (.)	⋯ is below (.)	(.) rolls.	(.) bounces.	⋯
(a, circle)	1	2	1	1	0	0
(a, triangle)	1	2	1	3	2	1
(a, square)	3	4	2	4	4	1
(the, circle)	2	3	1	3	2	1
(the, triangle)	3	5	2	5	4	2
(the, square)	5	8	4	8	7	3

(c) A part of the expression-context matrix of the bicluster

**Fig. 1.** Example: a bicluster and its expression-context matrix

Given a bicluster in  $T$ , we can construct an *expression-context matrix*, in which the rows represent the set of symbol pairs (expressions) in the bicluster, the columns represent all the contexts in which these symbol pairs appear, and the value in each cell denotes the number of times the corresponding expression-context combination appears in the corpus (see Fig.1(c) for an example). Because the target grammar is context-free, if a bicluster represents an AND-OR group of the target grammar, then the choice of the symbol pair is independent of its context and thus the resulting expression-context matrix should also be multiplicatively coherent, i.e., it must satisfy Eq.1.

The preceding discussion suggests an intuitive approach to learning a new AND-OR group: first find a bicluster of  $T$  that is multiplicatively coherent and has a multiplicatively coherent expression-context matrix, and then construct an AND-OR group from it. The probabilities associated with the grammar rules can be estimated from the statistics of the bicluster. For example, if we find that the bicluster shown in Fig.1(b) and its expression-context matrix shown in Fig.1(c) are both multiplicatively coherent, we can learn an AND-OR group as shown in Fig.1(a).

**Probabilistic Analysis.** We now present an analysis of the intuitive idea outlined above within a probabilistic framework. Consider a trivial initial grammar where the start symbol directly generates each sentence of the corpus with equal probability. We can calculate how the likelihood of the corpus given the grammar

is changed by extracting a bicluster and learning a new AND-OR group as described above.

Suppose we extract a bicluster  $BC$  and add to the grammar an AND-OR group with an AND symbol  $N$  and two OR symbols  $A$  and  $B$ . Suppose there is a sentence  $d$  containing a symbol pair  $xy$  that is in  $BC$ . First, since  $xy$  is reduced to  $N$  after this learning process, the likelihood of  $d$  is reduced by a factor of  $P(N \rightarrow xy|N) = P(A \rightarrow x|A) \times P(B \rightarrow y|B)$ . Second, the reduction may make some other sentences in the corpus become identical to  $d$ , resulting in a corresponding increase in the likelihood. Suppose the sentence  $d$  is represented by row  $p$  and column  $q$  in the expression-context matrix of  $BC$ , then this second factor is exactly the ratio of the sum of column  $q$  to the value of cell  $pq$ , because before the reduction only those sentences represented by cell  $pq$  are equivalent to  $d$ , and after the reduction the sentences in the entire column become equivalent (the same context plus the same expression  $N$ ).

Let  $LG(BC)$  be the likelihood gain resulting from extraction of  $BC$ ; let  $G_k$  and  $G_{k+1}$  be the grammars before and after extraction of  $BC$ ,  $D$  be the training corpus; in the bicluster  $BC$ , let  $A$  denote the set of rows,  $B$  the set of columns,  $r_x$  the sum of entries in row  $x$ ,  $c_y$  the sum of entries in column  $y$ ,  $s$  the sum over all the entries in  $BC$ , and  $a_{xy}$  the value of cell  $xy$ ; in the expression-context matrix of  $BC$ , let EC-row denote the set of rows, EC-col the set of columns,  $r'_p$  the sum of entries in row  $p$ ,  $c'_q$  the sum of entries in column  $q$ ,  $s'$  the sum of all the entries in the matrix, and  $EC(p, q)$  or  $a'_{pq}$  the value of cell  $pq$ . With a little abuse of notation we denote the context of a symbol pair  $xy$  in a sentence  $d$  by  $d - \text{“xy”}$ . We can now calculate the likelihood gain as follows:

$$\begin{aligned}
 LG(BC) &= \frac{P(D|G_{k+1})}{P(D|G_k)} = \prod_{d \in D} \frac{P(d|G_{k+1})}{P(d|G_k)} \\
 &= \prod_{x \in A, y \in B, xy \text{ appears in } d \in D} P(x|A)P(y|B) \frac{\sum_{p \in \text{EC-row}} EC(p, d - \text{“xy”})}{EC(\text{“xy”}, d - \text{“xy”})} \\
 &= \prod_{x \in A} P(x|A)^{r_x} \prod_{y \in B} P(y|B)^{c_y} \frac{\prod_{q \in \text{EC-col}} c'_q}{\prod_{\substack{p \in \text{EC-row} \\ q \in \text{EC-col}}} a'_{pq}}
 \end{aligned}$$

It can be shown that, the likelihood gain is maximized by setting:

$$P(x|A) = \frac{r_x}{s} \qquad P(y|B) = \frac{c_y}{s}$$

Substituting this into the likelihood gain formula, we get

$$\begin{aligned}
 \max_{P_r} LG(BC) &= \prod_{x \in A} \left(\frac{r_x}{s}\right)^{r_x} \prod_{y \in B} \left(\frac{c_y}{s}\right)^{c_y} \frac{\prod_{q \in \text{EC-col}} c'_q}{\prod_{\substack{p \in \text{EC-row} \\ q \in \text{EC-col}}} a'_{pq}} \\
 &= \frac{\prod_{x \in A} r_x^{r_x} \prod_{y \in B} c_y^{c_y}}{s^{2s}} \times \frac{\prod_{q \in \text{EC-col}} c'_q}{\prod_{\substack{p \in \text{EC-row} \\ q \in \text{EC-col}}} a'_{pq}}
 \end{aligned}$$

where  $P_r$  represents the set of grammar rule probabilities. Notice that  $s = s'$  and  $a_{xy} = r'_p$  (where row  $p$  of the expression-context matrix represents the symbol pair  $xy$ ). Thus we have

$$\max_{P_r} LG(BC) = \frac{\prod_{x \in A} r_x^{r_x} \prod_{y \in B} c_y^{c_y}}{s^s \prod_{\substack{x \in A \\ y \in B}} a_{xy}^{a_{xy}}} \times \frac{\prod_{p \in \text{EC-row}} r'_p{}^{r'_p} \prod_{q \in \text{EC-col}} c'_q{}^{c'_q}}{s'^{s'} \prod_{\substack{p \in \text{EC-row} \\ q \in \text{EC-col}}} a'_{pq}{}^{a'_{pq}}}$$

The two factors in the righthand side are of the same form, one for the bicluster and one for the expression-context matrix. This form of formula actually measures the multiplicative coherence of the underlying matrix (in a slightly different way from Eq.18 of [10]), which is maximized when the matrix is perfectly coherent. Therefore, we see that when extracting a bicluster (with the new grammar rule probabilities set to the optimal values), the likelihood gain is the product of the multiplicative coherence of the bicluster and its expression-context matrix, and that the maximal gain in likelihood is obtained when both the bicluster and its expression-context matrix are perfectly multiplicatively coherent. This validates the intuitive approach in the previous subsection. More derivation details can be found in the appendix in [11].

It must be noted however, in learning from data, simply maximizing the likelihood can result in a learned model that overfits the training data and hence generalizes poorly on data unseen during training. In our setting, maximizing the likelihood is equivalent to finding the most coherent biclusters. This can result in a proliferation of small biclusters and hence grammar rules that encode highly specific patterns appearing in the training corpus. Hence learning algorithms typically have to trade off the complexity of the model against the quality of fit on the training data. We achieve this by choosing the prior  $P(G) = 2^{-DL(G)}$  over the set of candidate grammars, where  $DL(G)$  is the description length of the grammar  $G$ . This prior penalizes more complex grammars, as complex grammars are more likely to overfit the training corpus.

Formally, the logarithm of the gain in posterior as a result of extracting an AND-OR group from a bicluster and updating the grammar from  $G_k$  to  $G_{k+1}$  (assuming the probabilities associated with the grammar rules are set to their optimal values) is given by:

$$\begin{aligned} \max_{P_r} LPG(BC) &= \max_{P_r} \log \frac{P(G_{k+1}|D)}{P(G_k|D)} \\ &= \left( \sum_{x \in A} r_x \log r_x + \sum_{y \in B} c_y \log c_y - s \log s - \sum_{x \in A, y \in B} a_{xy} \log a_{xy} \right) \\ &\quad + \left( \sum_{p \in \text{EC-row}} r'_p \log r'_p + \sum_{q \in \text{EC-col}} c'_q \log c'_q - s' \log s' - \sum_{\substack{p \in \text{EC-row} \\ q \in \text{EC-col}}} a'_{pq} \log a'_{pq} \right) \\ &\quad + \alpha \left( 4 \sum_{x \in A, y \in B} a_{xy} - 2|A| - 2|B| - 8 \right) \end{aligned} \quad (2)$$

where  $LPG(BC)$  denotes the logarithmic posterior gain resulting from extraction of the bicluster  $BC$ ;  $\alpha$  is a parameter in the prior that specifies how much the prior favors compact grammars, and hence it controls the tradeoff between the complexity of the learned grammar and the quality of fit on the training corpus. Note that the first two terms in this formula correspond to the gain in log likelihood (as shown earlier). The third term is the logarithmic prior gain, biasing the algorithm to favor large biclusters and hence compact grammars (see the appendix in [11] for details).

### 3.2 Attaching a New AND Symbol under Existing OR Symbols

**Intuition.** For a new AND symbol  $N$  learned in the first step, there may exist one or more OR symbols in the current partially learned grammar, such that for each of them (denoted by  $O$ ), there is a rule  $O \rightarrow N$  in the target grammar. Such rules cannot be acquired by extracting biclusters as described above: When  $O$  is introduced into the grammar,  $N$  simply does not exist in the table  $T$ , and when  $N$  is introduced, it only appears in a rule of the form  $N \rightarrow AB$ . Hence, we need a strategy for discovering such OR symbols and adding the corresponding rules to the grammar. Note that, if there are recursive rules in the grammar, they are learned in this step. This is because the first step establishes a partial order among the symbols, and only by this step can we connect nonterminals to form cycles and thus introduce recursions into the grammar.

Consider an OR symbol  $O$  that was introduced into the grammar as part of an AND-OR group obtained by extracting a bicluster  $BC$ . Let  $M$  be the AND symbol and  $P$  the other OR symbol in the group, such that  $M \rightarrow OP$ . So  $O$  corresponds to the set of rows and  $P$  corresponds to the set of columns of  $BC$ .

If  $O \rightarrow N$ , and if we add to  $BC$  a new row for  $N$ , where each cell records the number of appearances of  $Nx$  (for all  $x$  s.t.  $P \rightarrow x$ ) in the corpus, then the expanded bicluster should be multiplicatively coherent, for the same reason that  $BC$  was multiplicatively coherent. The new row  $N$  in  $BC$  results in a set of new rows in the expression-context matrix. This expanded expression-context matrix should be multiplicatively coherent for the same reason that the expression-context matrix of  $BC$  was multiplicatively coherent. The situation is similar when we have  $M \rightarrow PO$  instead of  $M \rightarrow OP$  (thus a new *column* is added to  $BC$  when adding the rule  $O \rightarrow N$ ). An example is shown in Fig.2.

Thus, if we can find an OR symbol  $O$  such that the expanded bicluster and the corresponding expanded expression-context matrix are both multiplicatively coherent, we should add the rule  $O \rightarrow N$  to the grammar.

**Probabilistic Analysis.** The effect of attaching a new AND symbol under existing OR symbols can be understood within a probabilistic framework. Let  $\overline{BC}$  be a *derived* bicluster, which has the same rows and columns as  $BC$ , but the values in its cells correspond to the expected numbers of appearances of the symbol pairs when applying the current grammar to expand the current partially reduced corpus.  $\overline{BC}$  can be constructed by traversing all the AND symbols that  $M$  can be directly or indirectly reduced to in the current grammar.  $\overline{BC}$  is close to

AND  $\rightarrow$  OR<sub>1</sub>OR<sub>2</sub>

OR<sub>1</sub>  $\rightarrow$  big (0.6) | old (0.4)

OR<sub>2</sub>  $\rightarrow$  dog (0.6) | cat (0.4)

	dog	cat	AND
big	27	18	15
old	18	12	10

**New rule:** OR<sub>2</sub>  $\rightarrow$  AND

(a) An existing AND-OR group and a proposed new rule

(b) The bicluster and its expansion (a new column)

	the (.) slept.	the big (.) slept.	the old (.) slept.	the old big (.) slept.	... heard the (.)	... heard the old (.)	...
(old, dog)	6	1	1	0	3	1	
(big, dog)	9	2	1	1	4	1	
(old, cat)	4	1	0	0	2	1	...
(big, cat)	6	1	1	0	4	1	
(old, AND)	3	1	0	0	2	1	
(big, AND)	5	1	1	0	2	1	...

(c) The expression-context matrix and its expansion

**Fig. 2.** An example of adding a new rule that attaches a new AND under an existing OR. Here the new AND is attached under one of its own OR symbols, forming a self-recursion.

$BC$  if for all the AND symbols involved in the construction, their corresponding biclusters and expression-context matrices are approximately multiplicatively coherent, a condition that is ensured in our algorithm. Let  $\widetilde{BC}'$  be the expanded derived bicluster that contains both  $\widetilde{BC}$  and the new row or column for  $N$ . It can be shown that the likelihood gain of adding  $O \rightarrow N$  is approximately the likelihood gain of extracting  $\widetilde{BC}'$ , which, as shown in Section 3.1, is equal to the product of the multiplicative coherence of  $\widetilde{BC}'$  and its expression-context matrix (when the optimal new rule probabilities are assigned that maximize the likelihood gain). Thus it validates the intuitive approach in the previous subsection. See the appendix in [11] for details.

As before, we need to incorporate the effect of the prior into the above analysis. So we search for existing OR symbols that result in maximal posterior gains exceeding a user-specified threshold. The maximal posterior gain is approximated by the following formula.

$$\max_{P_r} \log \frac{P(G_{k+1}|D)}{P(G_k|D)} \approx \max_{P_r} LPG(\widetilde{BC}') - \max_{P_r} LPG(\widetilde{BC}) \quad (3)$$

where  $P_r$  is the set of new grammar rule probabilities,  $G_k$  and  $G_{k+1}$  is the grammar before and after adding the new rule,  $D$  is the training corpus,  $LPG()$  is defined in Eq.2. Please see the appendix in [11] for the details.



### 3.3 Postprocessing

The two steps described above are repeated until no further rule can be learned. Since we reduce the corpus after each step, in an ideal scenario, upon termination of this process the corpus is fully reduced, i.e., each sentence is represented by a single symbol, either an AND symbol or a terminal. However, in practice there may still exist sentences in the corpus containing more than one symbol, either because we have applied the wrong grammar rules to reduce them, or because we have failed to learn the correct rules that are needed to reduce them.

At this stage, the learned grammar is almost complete, and we only need to add the start symbol  $S$  (which is an OR symbol) and start rules. We traverse the whole corpus: In the case of a fully reduced sentence that is reduced to a symbol  $x$ , we add  $S \rightarrow x$  to the grammar if such a rule is not already in the grammar (the probability associated with the rule can be estimated by the fraction of sentences in the corpus that are reduced to  $x$ ). In the case of a sentence that is not fully reduced, we can re-parse it using the learned grammar and attempt to fully reduce it, or we can simply discard it as if it was the result of noise in the training corpus.

## 4 Algorithm and Implementation

The complete algorithm is presented in Algorithm 1, and the three steps are shown in Algorithm 2 to 4 respectively. Algorithm 2 describes the “learning by biclustering” step (Section 3.1). Algorithm 3 describes the “attaching” step (Section 3.2), where we use a greedy solution, i.e., whenever we find a good enough OR symbol, we learn the corresponding new rule. In both Algorithm 2 and 3, a *valid* bicluster refers to a bicluster where the multiplicative coherence of the bicluster and that of its expression-context matrix both exceed a threshold  $\delta$ . This corresponds to the heuristic discussed in the “intuition” subsections in Section 3, and it is used here as an additional constraint in the posterior-guided search. Algorithm 4 describes the postprocessing step (Section 3.3), wherein to keep things simple, sentences not fully reduced are discarded.

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#### Algorithm 1. PCFG-BCL: PCFG Learning by Iterative Biclustering

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**Input:** a corpus  $C$

**Output:** a CNF grammar in the AND-OR form

1. create an empty grammar  $G$
  2. create a table  $T$  of the number of appearances of each symbol pair in  $C$
  3. **repeat**
  4.    $G, C, T, N \leftarrow \text{LearningByBiclustering}(G, C, T)$
  5.    $G, C, T \leftarrow \text{Attaching}(N, G, C, T)$
  6. **until** no further rule can be learned
  7.  $G \leftarrow \text{Postprocessing}(G, C)$
  8. **return**  $G$
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**Algorithm 2.** LearningByBiclustering( $G, C, T$ )

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**Input:** the grammar  $G$ , the corpus  $C$ , the table  $T$ **Output:** the updated  $G, C, T$ ; the new AND symbol  $N$ 

1. find the valid bicluster  $Bc$  in  $T$  that leads to the maximal posterior gain (Eq.2)
  2. create an AND symbol  $N$  and two OR symbols  $A, B$
  3. **for all** row  $x$  of  $Bc$  **do**
  4.   add  $A \rightarrow x$  to  $G$ , with the row sum as the rule weight
  5. **for all** column  $y$  of  $Bc$  **do**
  6.   add  $B \rightarrow y$  to  $G$ , with the column sum as the rule weight
  7. add  $N \rightarrow AB$  to  $G$
  8. in  $C$ , reduce all the appearances of all the symbol pairs in  $Bc$  to  $N$
  9. update  $T$  according to the reduction
  10. **return**  $G, C, T, N$
- 

---

**Algorithm 3.** Attaching( $N, G, C, T$ )

---

**Input:** an AND symbol  $N$ , the grammar  $G$ , the corpus  $C$ , the table  $T$ **Output:** the updated  $G, C, T$ 

1. **for each** OR symbol  $O$  in  $G$  **do**
  2.   **if**  $O$  leads to a valid expanded bicluster as well as a posterior gain (Eq.3) larger than a threshold **then**
  3.     add  $O \rightarrow N$  to  $G$
  4.     maximally reduce all the related sentences in  $C$
  5.     update  $T$  according to the reduction
  6. **return**  $G, C, T$
- 

#### 4.1 Implementation Issues

In the “learning by biclustering” step we need to find the bicluster in  $T$  that leads to the maximal posterior gain. However, finding the optimal bicluster is computationally intractable [10]. In our current implementation, we use stochastic hill-climbing to find only a fixed number of biclusters, from which the one with the highest posterior gain is chosen. This method is not guaranteed to find the optimal bicluster when there are more biclusters in the table than the fixed number of biclusters considered. In practice, however, we find that if there are many biclusters, often it is the case that several of them are more or less equally optimal and our implementation is very likely to find one of them.

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**Algorithm 4.** Postprocessing( $G, C$ )

---

**Input:** the grammar  $G$ , the corpus  $C$ **Output:** the updated  $G$ 

1. create an OR symbol  $S$
  2. **for each** sentence  $s$  in  $C$  **do**
  3.   **if**  $s$  is fully reduced to a single symbol  $x$  **then**
  4.     add  $S \rightarrow x$  to  $G$ , or if the rule already exists, increase its weight by 1
  5. **return**  $G$
-

Constructing the expression-context matrix becomes time-consuming when the average context length is long. Moreover, when the training corpus is not large enough, long contexts often result in rather sparse expression-context matrices. Hence, in our implementation we only check context of a fixed size (by default, only the immediate left and immediate right neighbors). It can be shown that this choice leads to a matrix whose coherence is no lower than that of the true expression-context matrix, and hence may overestimate the posterior gain.

## 4.2 Grammar Selection and Averaging

Because we use stochastic hill-climbing with random start points to do biclustering, our current implementation can produce different grammars in different runs. Since we calculate the posterior gain in each step of the algorithm, for each learned grammar an overall posterior gain can be obtained, which is proportional to the actual posterior. We can use the posterior gain to evaluate different grammars and perform model selection or model averaging, which usually leads to better performance than using a single grammar.

To perform model selection, we run the algorithm multiple times and return the grammar that has the largest posterior gain. To perform model averaging, we run the algorithm multiple times and obtain a set of learned grammars. Given a sentence to be parsed, in the spirit of Bayesian model averaging, we parse the sentence using each of the grammars and use a weighted vote to accept or reject it, where the weight of each grammar is its posterior gain. To generate a new sentence, we select a grammar in the set with the probability proportional to its weight, and generate a sentence using that grammar; then we parse the sentence as described above, and output it if it's accepted, or start over if it is rejected.

## 5 Experiments

A set of PCFGs obtained from available artificial, English-like CFGs were used in our evaluation, as listed in the table below. The CFGs were converted into CNF with uniform probabilities assigned to the grammar rules. Training corpora were then generated from the resulting grammars. We compared PCFG-BCL with EMILE [1] and ADIOS [5]. Both EMILE and ADIOS produce a CFG from a training corpus, so we again assigned uniform distributions to the rules of the learned CFG in order to evaluate them.

Grammar Name	Size (in CNF)	Recursion	Source
Num-agr	19 Terminals, 15 Nonterminals, 30 Rules	No	Boogie[12]
Langley1	9 Terminals, 9 Nonterminals, 18 Rules	Yes	Boogie[12]
Langley2	8 Terminals, 9 Nonterminals, 14 Rules	Yes	Boogie[12]
Emile2k	29 Terminals, 15 Nonterminals, 42 Rules	Yes	EMILE[1]
TA1	47 Terminals, 66 Nonterminals, 113 Rules	Yes	ADIOS[5]

We evaluated our algorithm by comparing the learned grammar with the target grammar on the basis of *weak generative capacity*. That is, we compare

the language of the learned grammar with that of the target grammar in terms of *precision* (the percentage of sentences generated by the learned grammar that are accepted by the target grammar), *recall* (the percentage of sentences generated by the target grammar that are accepted by the learned grammar), and *F-score* (the harmonic mean of precision and recall). To estimate precision and recall, 200 sentences were generated using either the learned grammar or the target grammar (as the case may be), and then parsed by the other grammar.

To ensure a fair comparison, we tuned the parameters of PCFG-BCL, EMILE and ADIOS on a separate dataset before running the evaluation experiments. Table 1 shows the experimental results. Each table cell shows the mean and standard deviation of performance estimates from 50 independent runs. In each run, each algorithm produced a single grammar as the output.

The results summarized in Table 1 show that PCFG-BCL outperformed both EMILE and ADIOS, on each of the test grammars, and by substantial margins on several of them. Moreover, in a majority of the tests, the standard deviations of the performance estimates of PCFG-BCL were lower than those of EMILE and ADIOS, suggesting that PCFG-BCL is more stable than the other two methods. It should be noted however, that neither EMILE nor ADIOS assume the training corpus to be generated from a PCFG, and thus they do not make full use of the distributional information in the training corpus. This might explain in part the superior performance of PCFG-BCL relative to EMILE and ADIOS.

We also examined the effect of grammar selection and grammar averaging (see Section 4.2), on the four datasets where PCFG-BCL did not achieve a perfect F-score on its own. In each case, we ran the algorithm for 10 times and then used the resulting grammars to perform grammar selection or grammar averaging as described in Section 4.2. The results (data not shown) show that grammar selection improved the F-score by 1.5% on average, and the largest increase of 4.4% was obtained on the TA1-200 data; grammar averaging improved the F-score by 3.2% on average, and the largest increase of 9.3% was obtained also on the TA1-200 data. In addition, both grammar selection and averaging reduced the standard deviations of the performance estimates.

**Table 1.** Experimental results. The training corpus sizes are indicated in the parentheses after the grammar names. P=Precision, R=Recall, F=F-score. The numbers in the table denote the performance estimates averaged over 50 trials, with the standard deviations in parentheses.

Grammar Name	PCFG-BCL			EMILE			ADIOS		
	P	R	F	P	R	F	P	R	F
Num-agr (100)	100 (0)	100 (0)	100 (0)	50 (4)	100 (0)	67 (3)	100 (0)	92 (6)	96 (3)
Langley1 (100)	100 (0)	100 (0)	100 (0)	100 (0)	99 (1)	99 (1)	99 (3)	94 (4)	96 (2)
Langley2 (100)	98 (2)	100 (0)	99 (1)	96 (3)	39 (7)	55 (7)	76 (21)	78 (14)	75 (14)
Emile2k (200)	85 (3)	90 (2)	87 (2)	75 (12)	68 (4)	71 (6)	80 (0)	65 (4)	71 (3)
Emile2k (1000)	100 (0)	100 (0)	100 (0)	76 (7)	85 (8)	80 (6)	75 (3)	98 (3)	85 (3)
TA1 (200)	82 (7)	73 (5)	77 (5)	77 (3)	14 (3)	23 (4)	77 (24)	55 (12)	62 (14)
TA1 (2000)	95 (6)	100 (1)	97 (3)	98 (5)	48 (4)	64 (4)	50 (22)	92 (4)	62 (17)

## 6 Summary and Discussion

### 6.1 Related Work

Several algorithms for unsupervised learning of CFG from only positive samples are available in the literature. EMILE [1] uses a simpler form of biclustering to create new nonterminals. It performs biclustering on an initial table constructed from the unreduced corpus, finding rules with only terminals on the right-hand side; and then it turns to the substitutability heuristic to find high-level rules. In contrast, PCFG-BCL performs iterative biclustering that finds both kinds of rules. ABL [2] employs the substitutability heuristic to group possible constituents to nonterminals. Clark’s algorithm [4] uses the “substitution-graph” heuristic or distributional clustering [3] to induce new nonterminals and rules. These techniques could be less robust than the biclustering method, especially in the presence of ambiguity as discussed in Section 1 and also in [1]. Both ABL and Clark’s method rely on some heuristic criterion to filter non-constituents, whereas PCFG-BCL automatically identifies constituents as a byproduct of learning new rules from biclusters that maximize the posterior gain. ADIOS [5] uses a probabilistic criterion to learn “patterns” (AND symbols) and the substitutability heuristic to learn “equivalence classes” (OR symbols). In comparison, our algorithm learns the two kinds of symbols simultaneously in a more unified manner.

The inside-outside algorithm [13,14], one of the earliest algorithms for learning PCFG, assumes a fixed, usually fully connected grammar structure and tries to maximize the likelihood, making it very likely to overfit the training corpus. Subsequent work has adopted the Bayesian framework to maximize the posterior of the learned grammar given the corpus [6,7], and has incorporated grammar structure search [6,8]. Our choice of prior over the set of candidate grammars is inspired by [6]. However, compared with the approach used in [6], PCFG-BCL adds more grammar rules at each step without sacrificing completeness (the ability to find any CFG); and the posterior re-estimation in PCFG-BCL is more straightforward and efficient (by using Eq.2 and 3). An interesting recent proposal within the Bayesian framework [9] involves maximizing the posterior using a non-parametric model. Although there is no structure search, the prior used tends to concentrate the probability mass on a small number of rules, thereby biasing the learning in favor of compact grammars.

Some unsupervised methods [15,16] for learning grammatical structures other than CFG with the goal of parsing natural language sentences also employ some techniques similar to those used in CFG learning.

### 6.2 Summary and Future Work

We have presented PCFG-BCL, an unsupervised algorithm that learns a probabilistic context-free grammar (PCFG) from positive samples. The algorithm acquires rules of an unknown PCFG through iterative biclustering of bigrams in the training corpus. Results of our experiments on several benchmark datasets

show that PCFG-BCL is competitive with the state of the art methods for learning CFG from positive samples. Work in progress is aimed at improving PCFG-BCL e.g., by exploring alternative strategies for optimizing the objective function, and more systematic empirical evaluation of PCFG-BCL on real-world applications (e.g., induction of grammars from natural language corpora) with respect to both weak and strong generative capacity.

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