Machine Learning Guidance and Proof Certification for Connection Tableaux

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Abstract
Connection calculi allow for very compact implementations of goal-directed proof search. We give an overview of our work related to connection tableaux calculi: First, we show optimised functional implementations of clausal and nonclausal proof search, including a consistent Skolemisation procedure for machine learning. Then, we show two guidance methods based on machine learning, namely reordering of proof steps with Naive Bayesian probabilities, and expansion of a proof search tree with Monte Carlo Tree Search. Finally, we give a translation of connection proofs to LK, enabling proof certification and automatic proof search in interactive theorem provers.

1 Introduction
Connection calculi have enabled proof search in a variety of logics: First-order automated theorem provers (ATPs) based on connection calculi have been implemented for classical (leanCoP [Otten 2008]), intuitionistic (iLeanCoP [Otten 2005]), and modal logic (MLeanCoP [Otten 2014]). A variant of leanCoP with interpreted linear arithmetic (leanCoP-Ω) won the TFA division of CASC-J5 [Sutcliffe 2011]. Furthermore, nanoCoP [Otten 2016] is a version of leanCoP able to perform proof search without clausification.

The size of these provers is only in the range of hundreds of bytes. This makes these provers suitable as a basis for experiments and adaptions, such as machine learning and proof certification. For these applications, we implemented connection

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1 The prover at http://www.leancoq.de/programs/veryleancoq.pl is as small as 199 bytes.
provers in functional instead of logic programming languages. There are several reasons: First, a large number of interactive theorem provers (ITPs), such as HOL Light (Harrison 2009), HOL4 (Slind and Norrish 2008), Isabelle (Wenzel et al. 2008), Coq (Bertot 2008), and Agda (Bove et al. 2009) are written in functional programming languages, lending themselves well to integration of functional proof search tactics. Second, several machine learning algorithms have been recently implemented efficiently for these ITPs in the functional languages. Third, we achieve better performance with functional-style implementations, which is important to compensate for the performance penalty incurred by machine learning.

The machine learning connection provers MaLeCoP (Urban et al. 2011) and FEMaLeCoP (Kaliszyk and Urban 2015a) integrate Naive Bayesian clause ordering into leanCoP’s proof search. The monteCoP (Färber et al. 2017) system implements Monte Carlo Tree Search in leanCoP. The resulting connection proofs can be certified in interactive theorem provers (Kaliszyk et al. 2015a), giving at the same time rise to proof search tactics similar to Metis (Hurd 2003) or MESON (Harrison 1996).

In this paper we develop an integration of internal guidance based on machine learning and Monte Carlo methods in connection-style proof search, as well as how to certify the resulting connection calculus proofs. The contributions described in this paper are:

- Efficient implementations of proof search for the clausal and nonclausal connection calculi in functional programming languages, see section 3.
- Integration of machine learning based internal guidance, see section 5. We integrate a multi-layer indexing based on previous proofs suitable for a Naive Bayes classifier of extension steps. These rely on consistent symbol names (section 4). We further provide various strategies to improve the proof search based on the learned information.
- Integration of Monte Carlo Tree Search, see section 6. This includes a number of proof state evaluation heuristics, some learned on previous proofs.
- A unified formulation of clausal and nonclausal connection calculi adapted for proof translation, and proof certification integrated into HOL Light, see section 7.

The paper combines and extends our works presented at CPP 2015 (Kaliszyk et al. 2015a), LPAR 2015 (Kaliszyk and Urban 2015a), and CADE 2017 (Färber et al. 2017). The techniques added over the conference versions include: the higher-order logic reconstruction of nonclausal proofs; consistent Skolemisation applicable also for nonclausal proof search; and efficient functional-style implementation of proof search in clausal and nonclausal connection calculi.

2 Connection Tableaux Calculi

Connection calculi provide a goal-oriented way to search for proofs in classical and nonclassical logics (Otten 2008). Common to these calculi is the concept of connections \{P, \neg P\} between literals \(P\) and \(\neg P\), which correspond to closing a branch in the tableaux calculus (Hähnle 2001).
Axiom \{\}, M, Path

\[
\begin{array}{c}
\text{Start} \\
\epsilon, M, \epsilon
\end{array}
\]

where \( C_2 \) is copy of \( C_1 \in M \)

Reduction \( C \cup \{L\}, M, Path \cup \{L'\} \)

\[
\begin{array}{c}
\text{where } \sigma(L) = \sigma(L')
\end{array}
\]

Extension \( C \cup \{L\}, M, Path \)

\[
\begin{array}{c}
\text{where } C_2 \text{ is copy of } C_1 \in M \\
\text{and } L' \in C_2 \text{ with } \sigma(L) = \\
\sigma(L')
\end{array}
\]

Fig. 1: Clausal connection calculus rules.

Connection tableaux calculi, such as (Bibel 1983), are members of the family of connection calculi. As the calculi considered in this paper have a very small set of rules, they lend themselves very well to proof translation and machine learning.

In this section, we introduce the clausal and the nonclausal connection calculus that we will use throughout the paper.

2.1 Connection Calculi

The connection calculi in this paper operate on matrices, where a matrix is a set of clauses. In the nonclausal calculus, clauses do not only contain literals, but also matrices, giving rise to a nested structure. \( M \) stands for a matrix, \( C \) for a clause, \( L \) for a literal, \( x \) for a variable, and \( x \) for a sequence of variables, as in \( \forall x.P(x) \). A substitution \( \sigma \) is a mapping from variables to terms. The complement \( L \) is \( A \) if \( L \) has the shape \( \neg A \), otherwise \( L \) is \( \neg A \). A \( \sigma \)-complementary connection \( \{L, L'\} \) exists if \( \sigma L = \sigma L' \). Given a relation \( R \), its transitive closure is denoted by \( R^+ \) and its transitive reflexive closure by \( R^* \).

We will focus on two variants of the calculus: clausal and nonclausal. As the two alternatives will differ only in the clauses and rules, we first give a definition of the common parts of the clausal and nonclausal connection calculi, omitting the calculus rules.

Definition 1 (Connection Calculus) A connection calculus is a calculus satisfying the following conditions. The words of the calculus are tuples \( \langle C, M, Path \rangle \), where \( C \) is a clause, \( M \) is a matrix, and \( Path \) is a set of literals called the active path. \( C \) and \( Path \) can also be empty, denoted \( \epsilon \). In the rules of the calculus, \( \sigma \) is a term substitution, and \( \{L, L'\} \) is a \( \sigma \)-complementary connection. The substitution \( \sigma \) is global (or rigid), i.e. it is applied to the whole derivation.

To complete the definitions of the variants of the connection calculus, we need to specify the types of clauses and the rules. In the clausal connection calculus, a clause is a set of literals. The calculus rules are presented in Figure 1.

In the nonclausal connection calculus, a clause is a set of literals and matrices. The following definitions of the concepts used in the extension rule follow Otten (Otten 2011, 2016).

Definition 2 (Clause Predicates) A clause \( C \) contains \( L \) iff \( L \in^+ C \). A clause \( C \in^+ M \) is \( \alpha \)-related to a literal \( L \) iff \( M' \in^+ M \) with \( \{C_L, C_C\} \subseteq M' \) such that
Example 1 Consider the following formula $F$ and its conjunctive normal form $F'$.
We will attempt to show that they imply $\bot$:

\[
F = Q \land P(a) \land \forall x. (\neg P(x) \lor (\neg P(s^2x) \land (P(sx) \lor \neg Q))),
\]

\[
F' = \forall x. (Q \land P(a) \land (\neg P(s^2x)) \land (\neg P(x) \lor P(sx) \lor \neg Q)).
\]

For brevity, we write $sx$ for $s(x)$ and $s^2x$ for $s(s(x))$. The nonclausal matrix $M$ corresponds to $F$ and the clausal matrix $M'$ to $F'$:

\[
M = \begin{bmatrix} Q \mid P(a) \mid \neg P(x) \\ \neg P(s^2x) \mid P(sx) \mid \neg Q \end{bmatrix}, \quad M' = \begin{bmatrix} Q \mid P(a) \mid \neg P(x) \\ \neg P(s^2x) \mid P(sx) \mid \neg Q \end{bmatrix}.
\]

Graphical proofs for the problem are given in Figure 3 respectively Figure 4:

There, lines represent connections, and the substitution used is $\sigma = \{x' \mapsto a, x \mapsto sx', \bar{x} \mapsto x'\}$. A formal proof for $M'$ in the clausal connection calculus is given in Figure 5:

A shorter proof for $M'$ as well as a formal proof for $M$ will be given using slightly modified versions of the calculi in subsection 7.2.

Soundness and completeness have been proved both for the clausal (Letz and Stenz 2001) and for the nonclausal calculus (Otten 2011). We will discuss practical functional-style implementations of proof search for the presented calculi in section 8.
3 Functional-style Connection Prover

In this section, we develop an efficient implementation of a connection prover for classical first-order logic in a functional programming language. The resulting implementation will be the basis for all experiments in the remainder of the paper.

The connection prover performs the following tasks. Given a classical first-order logic problem, it creates a matrix for the problem. The matrix is then used to build an index (usually in the form of a literal database) which will be used to provide an efficient way to find connections during proof search. Finally, proof search with iterative deepening is performed. We detail these steps in the next sections.

3.1 Problem Preprocessing

We focus on first-order logic problems represented as a set of axioms \( \{A_1, \ldots, A_n\} \) together with a conjecture \( C \), where all axioms and the conjecture are closed formulas. The goal is to show that the axioms imply the conjecture. For convenience, in the actual implementation we use the TPTP format (Sutcliffe 2009b) as input. Each parsed input problem is transformed according to the following procedure. Only the steps 2 and 6 differ in comparison with the original Prolog implementations of leanCoP and nanoCoP (Otten 2008, 2016).

1. The conjecture \( C \) is combined with the axioms \( \{A_1, \ldots, A_n\} \) to form the new problem \( (A_1 \land \cdots \land A_n) \rightarrow C \) (respectively \( C \) if no axioms are present).
2. Constants and variables are mapped to integers, to enable more efficient lookup and comparison during the proof search, as needed e.g. for fast unification.
3. As the connection tableaux calculi considered in this paper do not have special rules for equality, equality axioms are added to the problem if equality appears in the original problem. The axioms are: reflexivity, symmetry, transitivity, and:

- For every \( n \)-ary function \( f \), the formula \( x_1 = y_1 \rightarrow \cdots \rightarrow x_n = y_n \rightarrow f(x_1, \ldots, x_n) = f(y_1, \ldots, y_n) \) is introduced.
- For every \( n \)-ary predicate \( P \), the formula \( x_1 = y_1 \rightarrow \cdots \rightarrow x_n = y_n \rightarrow P(x_1, \ldots, x_n) \rightarrow P(y_1, \ldots, y_n) \) is introduced.

4. If the formula has the shape \( P \rightarrow C \), then it is transformed to the equivalent \( (P \land \#) \rightarrow (C \land \#) \). \# is a marker that can be understood to be equivalent to \( \top \). It allows proof search to recognise clauses stemming from the conjecture (see (Otten 2008, sec. 2.1)).

5. Implications and equivalences are expanded, e.g. \( A \rightarrow B \) becomes \( \neg A \lor B \).

6. Quantifiers are pushed inside such that their scope becomes minimal.

7. The formula is negated (to perform a proof by refutation) and converted to negation normal form.

8. The formula is reordered to minimise the number of paths through the matrix.

9. The formula is rectified, i.e. variables are renamed such that any two distinct quantifiers in the formula bind variables with different names.

10. The formula is skolemised. For machine learning, we use consistent Skolemisation as discussed in section 4 instead of outer Skolemisation as performed in the original Prolog version.

3.2 Matrix and Literal Database

The matrix is built from the skolemised formula resulting from subsection 3.1. For the clausal connection prover, this involves a transformation of the formula into clausal normal form. The standard transformation applies distributivity rules of the shape \( A \land (B \lor C) \equiv (A \lor B) \land (A \lor C) \) to the formula until a fix point is reached. In the worst case, this transformation makes the formula grow exponentially. To avoid this, the definitional transformation introduces new symbols (Plaisted and Greenbaum 1986; Otten 2010). Similarly to Skolemisation, the introduced symbols should be consistent across different problems, which is achieved by using a normalised string representation of the clause literals as new symbol names. For the nonclausal connection prover, no clausification is required, as the formula can be directly transformed into the nonclausal matrix. For both clausal and nonclausal matrices, the polarity of literals is encoded by the sign of the integer representing the predicate symbol.

We next explain how the prover efficiently searches for connections. leanCoP and nanoCoP rely on Prolog’s internal literal indexing. For every literal \( L \) a set of contrapositives is stored, where a contrapositive corresponds to branches that have to be opened in order to close the leaf \( L \). Finding a connection then amounts to finding contrapositives for \( L \) such that \( L \) can be unified with the negation of the leaf of the current branch. In the clausal case, the contrapositive for a literal \( L \) in the clause \( C \) is \( C \setminus L \). In the nonclausal case, the contrapositive for \( L \) is a copy of the matrix in which all clauses \( \alpha \)-related to \( L \) are deleted, allowing for the efficient construction of e-clauses. In our implementation, we store contrapositives in a hash table indexed by the root symbols of literals. This allows efficient search for literals that have the same root as the leaf of the current branch, but with opposite polarity.
We also considered storing contrapositives in first-order term indexing structures \cite{Ramakrishnan:2001}. The overall effect on performance of storing contrapositives in a discrimination tree \cite{Greenbaum:1986} on the considered datasets is however minor, as unification with array substitutions (see subsection 3.4) is relatively fast.

### 3.3 Proof Search

In both clausal and nonclausal calculi, proof search is analytic, i.e. the proof tree is constructed bottom-up. As the proof search is not confluent, i.e. making a wrong choice can lead to a dead end, backtracking is necessary for completeness. The proof tree is constructed with a depth-first strategy, which results in an incomplete proof search. To remedy this, iterative deepening is used, where the maximal path length \( \lim \) is increased in every iteration.

The principal implementations of the connection tableaux calculi, leanCoP and nanoCoP, use a number of optimisation techniques, such as regularity, lemmata, and restricted backtracking \cite{Otten:2010}. When backtracking is restricted, as soon as the proof search finds some proof tree to close a branch, no other potential proof trees for that branch are considered any more. While restricted backtracking loses completeness, it significantly increases the number of problems solved for various first-order problem classes.

Prolog allows for a very elegant and succinct implementation of proof search. First attempts to directly integrate machine learning into Prolog leanCoP have suffered from slow speed \cite{Urban:2011}. We later showed \cite{Kaliszyk:2015;Kalisyk:2015a} that implementations of leanCoP in a functional programming language allow for fast machine learning as well as for efficient proof reconstruction in interactive theorem provers. However, implementing proof search with restricted backtracking in a functional language is not straightforward.

In this section, we discuss several implementations of a clausal prover loop that permits restricted backtracking: The simplified version of leanCoP shown in subsection 3.3.1 is the smallest, but also the slowest implementation. Care is taken that all subsequent implementations perform the proof search in precisely the same order as the original Prolog implementation. We then introduce a purely functional implementation in subsection 3.3.2 using lazy lists respectively streams. This version slightly increases code size compared to the Prolog version, but greatly improves performance, as shown in the evaluation in subsection 3.6. We also discuss an approach based on continuations, still purely functional, but more complicated than the stream version. In exchange, this version has slightly better performance than the stream one, likely due to not having to allocate memory for (stream) constructors. The fastest, but also most complicated implementation considered in this paper uses an explicit stack and exceptions for backtracking. However, as it proves only as many problems as the continuation-based solution, we will only briefly discuss it.

#### 3.3.1 Prolog

A simplified version of the original leanCoP in Prolog is given in Listing 1. We explain and relate it to the clausal connection calculus introduced in section 2.

The main predicate \texttt{prove}(\( C, \text{Path}, \text{PathLim} \)) succeeds iff there exists a closed proof tree for \( C, M, \text{Path} \) with a maximal \( \text{Path} \) length of \( \text{PathLim} \). For this, \texttt{prove}
attempts to close the proof tree for the first literal $\text{Lit}$ of $C$ in lines 4–9, and if successful, it continues with the remaining clause $\text{Cla}$ of $C$ in line 10.

Let us detail the proof search for the current literal $\text{Lit}$: Line 4 corresponds to the reduction rule: The branch is closed if the negation of $\text{Lit}$ can be unified with a literal on the $\text{Path}$. Lines 6–8 correspond to the extension rule: The literal database as explained in subsection 3.2 is implemented by the predicate $\text{lit}(L,C)$, which succeeds iff the matrix contains some clause that can be unified with $\{L\} \cup C$. This is used to obtain some contrapositive $\text{Cla1}$ for the negation of $\text{Lit}$. If the path does not exceed the length limit (line 7), new branches are opened for $\text{Cla1}$ in line 8.

Backtracking is handled by the Prolog semantics: For example, if choosing the first matching contrapositive for $\text{Lit}$ leads to the proof search getting stuck, the next contrapositive will be tried by Prolog.

Listing 1: Clausal proof search in Prolog.
Listing 2: A functional leanCoP implementation using lazy lists.

### 3.3.2 Lazy Lists and Streams

Proof search in a functional language can be elegantly implemented as a function from a branch to a lazy list of proofs, where a lazy list is an arbitrarily long list built on demand. However, as the proof search considers every list element maximally once, the memoization done for lazy lists creates an unnecessary overhead. For that reason, streams can be used instead of lazy lists, where a stream is a special case of a lazy list that restricts list elements to be traversed maximally once. As our application uses a common interface for lazy lists and streams, we solely present the lazy list version here.

Listing 2 shows a functional leanCoP implementation using lazy lists. Let us first introduce the semantics of the used constructs:

- $x \& f$ denotes $f\,x$.
- $\lambda x \rightarrow y$ stands for a lambda expressions $\lambda\,x.y$.
- $\text{unify sub lit1 lit2}$ unifies two literals $\text{lit1}$ and $\text{lit2}$ under a substitution $\text{sub}$, returning a new substitution if successful.
- $\text{unifyDB sub lit}$ finds all contrapositives in the literal database which could match the literal $\text{lit}$ under the substitution $\text{sub}$. It returns a list of substitution-contrapositive pairs. It corresponds to the $\text{lit}$ predicate in the Prolog version.
- $\text{mapMaybe f l}$ returns the results of $f$ for the elements of $l$ on which $f$ succeeded.
– `concatMap f l` maps `f` over all elements of `l` and concatenates the resulting list of lists to form a flat list.
– `x ++ y` is the concatenation of two lists `x` and `y`.

The main function `prove C Path lim σ` returns a list of substitutions \([σ_1, \ldots, σ_n]\), where every substitution \(σ_i\) corresponds to a closed proof tree for \(C, M, Path\) with a maximal path length smaller than `lim`, where the global initial substitution is `σ` and the final substitution is `σ_i`. Similarly to the Prolog version, `prove` attempts to close the proof tree for the first literal `lit` of `C` in lines 4–8, and the resulting substitutions are used to close the proof trees for the remaining clause `cla` of `C` in line 9. Line 4 corresponds to the reduction rule, and lines 5–8 correspond to the extension rule. As we use lazy lists / streams, a substitution \(σ_i\) is only calculated if proof search failed for all \(σ_j\) with \(j < i\).

```
prove [] path lim sub = [sub]
prove (lit : cla) path lim sub =
  let
    reductions = mapMaybe (unify sub (negate lit)) path
    extensions = unifyDB sub lit & concatMap
      (\ (sub1, cla1) ->
        if lim <= 0 then []
        else prove cla1 (lit : path) (lim - 1) sub1)
  in concatMap (prove cla path lim) (reductions ++ extensions)
```

### 3.3.3 Continuations

Continuation passing style (CPS) allows the implementation of algorithms with complicated control flow in functional languages [Plotkin 1975]. Our CPS implementation shown in [listing 3] defines three functions that call each other mutually: `prove` starts the proof search, `reduce` performs reduction steps and `extend` performs extension steps. Two continuations are passed to the `prove` function: One function `alt` to be called in case the proof search has hit a dead end and needs to backtrack to an alternative, and one function `rem` to be called when a branch has been closed to process the remaining open branches.

### 3.3.4 Stacks

We considered an implementation based on stacks. There, the main prove function has the same arguments as the `prove` function of the stream-based implementation, plus a stack. This stack contains tuples with information about clauses that still have to be processed, together with the depth at which the clauses have been put onto the stack. Once the current clause has been completely refuted, the next tuple is popped from the stack and the clause in the tuple is processed.

3 In this simplified implementation, the actual proof tree is not recorded, in contrast to our actual implementation. The same holds for the Prolog version.
Listing 3: CPS implementation of clausal proof search.

1. `prove [] path lim sub alt rem = rem (sub, alt)`
2. `prove (lit : cla) path lim sub alt rem = reduce path where`
3. `reduce (plit : path) =`
4. `let alt1 () = reduce path`
5. `in case unify sub (negate lit) plit of`
6. `Just sub1 -> prove cla path lim sub1 alt1 rem`
7. `Nothing -> alt1 ()`
8. `reduce [] = extend (unifyDB sub (negate lit))`

9. `extend ((sub1, cla1) : contras) =`
10. `let rem1 (sub, alt) = prove cla path lim sub alt rem`
11. `alt1 () = extend contras`
12. `in`
13. `if lim <= 0 then alt1 ()`
14. `else prove cla1 (lit : path) (lim - 1) sub1 alt1 rem1`
15. `extend [] = alt ()`

3.4 Unification

Unification is one of the most time consuming parts of proof search, therefore it is crucial to represent data, including substitutions, in a way that allows efficient unification.

The simplest approach to represent substitutions is to use association lists from variables to terms. This is done e.g. in the HOL Light implementation of MESON [Harrison 1996]. However, as variable lookup is linear in the number of bound variables, this approach does not scale well. An improvement over this is to use tree-based maps, used for example by Metis [Hurd 2003]. Both solutions however incur a significant overhead in tableaux proof search, where a single large substitution is needed.

In functional languages with efficient support for arrays (e.g. the ML language family, used in many proof systems), it is more efficient to store the substitution in a single global mutable array. As variables can be represented by positive integers, the n-th array element contains the term bound to the variable n. By keeping a stack of variables bound in each prover state, it is also possible to backtrack efficiently: variables removed from the top of the stack are removed from the global array. This way, backtracking can be done as if the substitution was contained in a purely functional data structure, however allowing for more efficient unification.

3.5 Clause Processing Order

Proof search processes clauses and matrices in a certain order <, such that for any elements a, b of the same clause or matrix, a is processed before b iff a < b. The order < is usually derived from the structure of the formula obtained in subsection 3.1.

For nonclausal proof search, we have evaluated different ways to order β-clauses: The original nanoCoP processes the β-clause of a clause C w.r.t. a literal L (see [Definition 4]) using the order <_L, where a <_L b iff a contains L or a < b. The reconstruction of proofs created in this order requires some postprocessing; this motivated our usage of the regular < for β-clauses.
Given an order, we can write sets as ordered sequences \( [X_1, \ldots, X_n] \), where for all \( i < n \), \( X_i < X_{i+1} \). Clauses and matrices can thus be shown as horizontal respectively vertical sequences. We use this notation for an example to illustrate the influence of the ordering.

**Example 2** Let \( M \) contain a clause

\[
C = \begin{bmatrix}
M_1 \\
C_1 \\
M_2 \\
M_3
\end{bmatrix}
\]

Then the \( \beta \)-clauses of \( C \) w.r.t. \( L \) ordered by \( < \) and \( \leq L \) are \( \beta_\prec \) and \( \beta_\prec L \):

\[
\beta_\prec = \begin{bmatrix}
M_1 \\
C_1 \\
M_2 \\
M_3
\end{bmatrix} \quad \beta_\prec L = \begin{bmatrix}
M_2 \\
M_3 \\
C_1 \\
M_1
\end{bmatrix}
\]

One can see that when using \( \beta_\prec L \), the neighbours \( M_2 \) and \( M_3 \) of \( L \) are processed first, unlike when using \( \beta_\prec \).

### 3.6 Evaluation

We evaluate our work on several first-order problem datasets:

- **TPTP** (Sutcliffe 2009b) is a large benchmark for automated theorem provers. It became standard due to its usage in the yearly CASC competition (Sutcliffe 2016). The contained problems are based on different logics and originate from various domains. In our evaluation we use the nonclausal first-order problems of TPTP 6.3.0.

- **MPTP2078** (Alama et al. 2014) contains 2078 problems exported from the Mizar Mathematical Library. This dataset is particularly suited for symbolic machine learning since symbols are shared between problems. It comes in the two flavours “bushy” and “chainy”: In the “chainy” dataset, every problem contains all facts stated before the problem, whereas in the “bushy” dataset, every problem contains only the premises required in Mizar to prove that problem.

- **Miz40** contains the problems from the Mizar library for which at least one ATP proof has been found using one of the 14 combinations of provers and premise selection methods considered in (Kaliszyk and Urban 2015b). The problems are translated to untyped first-order logic using the MPTP infrastructure (Urban 2004). Symbol names are also used consistently in this dataset, and the problems are minimised using ATP-based pseudo-minimisation, i.e., re-running the ATP only with the set of proof-needed axioms until this set no longer becomes smaller. This typically leads to even better axiom pruning and ATP-easier problems than in the Mizar-based pruning used for the “bushy” version above.

- **HOL Light**: We translate theorems proven in HOL Light to FOL, following a similar procedure as (Kaliszyk and Urban 2014). We export top-level theorems
Table 1: Evaluation datasets and number of contained first-order problems.

| Dataset | TPTP | MPTP | Miz40 | HL-top | HL-meson | FS-top | FS-meson |
|---------|------|------|-------|--------|----------|--------|----------|
| Problems | 7492 | 2078 | 32524 | 2498   | 1108     | 27111  | 39979    |

as well as theorems proven by the MESON tactic. We consider the theorems proven in the core of HOL Light (HL) as well as those proven by the Flyspeck project (FS), which finished in 2014 a formal proof of the Kepler conjecture (Hales et al. 2017).

We use a 48-core server with AMD Opteron 6174 2.2GHz CPUs, 320 GB RAM, and 0.5 MB L2 cache per CPU. Each problem is always assigned one CPU. As strategy scheduling is not a focus of this work, we evaluate all provers with disabled strategy scheduling.

We evaluated several prover configurations in Table 2. As state of the art, we used the ATPs Vampire 4.0 (Kovács and Voronkov 2013) and E 2.0 (Schulz 2013), which performed best in the first-order category of CASC-J8 (Sutcliffe 2016). Vampire and E are written in low-level languages (C respectively C++), implement the superposition calculus, and perform premise selection with SInE (Hoder and Voronkov 2011). Furthermore, Vampire integrates several SAT solvers (Biere et al. 2014), and E automatically determines proof search settings for a given problem. We ran E with --auto --auto-schedule and Vampire with --mode casc. In addition, we evaluated the ATP Metis (Hurd 2003): It implements the ordered paramodulation calculus (having inference rules for equality just like the superposition calculus), but is considerably smaller than Vampire and E and is implemented in a functional language, making it more comparable to our work.

We implemented functional-style versions of leanCoP 2.1 and nanoCoP 1.0 in the functional programming language OCaml, using the techniques introduced such as efficient control flow (subsection 3.3), array-based substitutions (subsection 3.4), alternative clause processing orders (subsection 3.5), and consistent Skolemisation (section 4). Our functional OCaml implementations are fleanCoP and fnanoCoP, whereas the original Prolog versions are pleanCoP and pnanoCoP. The Prolog versions were run with ECLiPSe 5.10. A prover configuration containing “+x” or “−x” means that feature x was enabled respectively disabled. “cut” denotes restricted backtracking, “conj” stands for conjecture-directed search, and $\beta_{\leq L}$ refers to the default $\beta$-clause ordering shown in subsection 3.5. leanCoP was evaluated without definitional classification, see subsection 3.2. The OCaml implementations use streams to control backtracking (see subsection 3.3.2) and arrays as substitutions.

The results are shown in Table 2. The OCaml versions clearly outperform the Prolog versions in almost all cases. The most impressive result is achieved by leanCoP+cut+conj on the chainy dataset: The OCaml version proves 58.8% more problems than its Prolog counterpart, thus even passing E. $\beta_{\leq L}$ seems to have an effect mostly when cut is enabled. However, the result depends greatly on the

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4 As part of exporting theorems solved by MESON, we perform some of the original MESON preprocessing, such as propositional simplification, Skolemisation, fixing of function arities and so on. This preprocessing may solve the problem, in which case we do not export the problem at hand.
Table 2: Comparison of provers without machine learning.

| Prover             | TPTP | Bushy | Chainy | Miz40  | FS-top | FS-meson |
|--------------------|------|-------|--------|--------|--------|----------|
| Vampire            | 4404 | 1253  | 656    | 30341  | 6358   | 39760    |
| E                  | 3664 | 1167  | 287    | 26003  | 7382   | 39740    |
| Metis              | 1376 | 500   | 75     | 18519  | 3537   | 38625    |
| flleanCoP+cut+conj | 1859 | 670   | 289    | 12204  | 3980   | 35738    |
| flleanCoP+cut−conj | 1782 | 598   | 244    | 11796  | 3520   | 30668    |
| flleanCoP−cut+conj | 1617 | 499   | 192    | 7826   | 3849   | 35204    |
| flleanCoP−cut−conj | 1534 | 514   | 164    | 11115  | 3492   | 36334    |
| pleanCoP+cut+conj  | 1673 | 606   | 182    | 11243  | 3664   | 35234    |
| pleanCoP+cut−conj  | 1621 | 548   | 153    | 11227  | 3305   | 30416    |
| pleanCoP−cut+conj  | 1428 | 453   | 145    | 7287   | 3671   | 34437    |
| pleanCoP−cut−conj  | 1374 | 460   | 123    | 10442  | 3415   | 35499    |
| fnanoCoP+cut       | 1724 | 511   | 192    | 12332  | 3178   | 30327    |
| fnanoCoP+cut−β<\text{L} & 1776 & 547 & 233 & 11197 & 3182 & 30216 \\
| fnanoCoP−cut       | 1567 | 542   | 151    | 13316  | 1993   | 37938    |
| fnanoCoP−cut−β<\text{L} & 1559 & 541 & 152 & 13173 & 1991 & 37923 \\
| pnanoCoP+cut       | 1585 | 480   | 112    | 11921  | 2970   | 30272    |
| pnanoCoP−cut       | 1485 | 510   | 126    | 12943  | 1986   | 38015    |

Table 3: Impact of implementation on efficiency of clausal proof search on the bushy MPTP2078 dataset with 10s timeout, restricted backtracking (+cut), no definitional CNF, and conjecture-directed search (+conj).

| Implementation | Solved | Inferences |
|----------------|--------|------------|
| Prolog         | 606    | -          |
| Lazy list      | 639    | 878199349  |
| Stack (list substitution) | 648 | 1253862954 |
| Stream         | 670    | 1702827032 |
| Continuation   | 681    | 2200272406 |
| Stack          | 681    | 2490100879 |

dataset: On the chainy dataset, disabling $\beta_{<\text{L}}$ solves 21.3% more problems, but on the Miz40 dataset, it solves 8.8% less.

We evaluated different proof search implementation styles in Table 3 and Table 4. Here, inferences denote the number of successful unifications performed by some prover on all problems within 10 seconds timeout. This metric is not available for the Prolog versions, as they do not print the number of inferences performed so far when prematurely terminated.

To measure the impact of the substitution structure, we evaluated the best-performing implementation, i.e. the stack-based one, using a list-based substitution instead of an array-based substitution, see Table 3. This decreased the number of inferences by 50%, showing that the performance of the substitution structure is crucial for fast proof search.

Unless noted otherwise, we will use the stream-based implementation with array-based substitution in the remainder of this paper.
Table 4: Impact of implementation on efficiency of nonclausal proof search on the bushy MPTP2078 dataset with 10s timeout and restricted backtracking (+cut).

| Implementation   | Solved | Inferences |
|------------------|--------|------------|
| Prolog           | 480    | -          |
| Lazy list        | 504    | 374849495  |
| Streams          | 511    | 495368962  |

4 Consistent Skolemisation

First-order Skolemisation introduces new function symbols. For machine learning algorithms, it is beneficial to introduce names consistently across problems, meaning that Skolem terms originating from the same axiom in two different problems should be syntactically equivalent. Consistent Skolemisation methods have been studied in the context of the δ-rule in tableaux methods, e.g. (Beckert et al. 1993). (Giese and Ahrendt 1999) pointed out that the Skolem terms introduced may lead to rather large formulae, which can be solved by structure sharing. However, in our setting, structure sharing across different problems is not possible, which makes it necessary to find different approaches. In previous work (Kaliszyk and Urban 2015a), consistent Skolemisation was part of the clausification procedure. The implementation of nonclausal proof search motivated a more general consistent Skolemisation method. To recognise the same Skolem term across different problems, it is necessary to capture by the Skolem term only the part of the formula that defines the existential variable. For this, we propose a consistent Skolemisation method based on ε-terms.

Let us first introduce the setting for this section: Let \( \Delta \) be a rectified formula in negation normal form that is to be skolemised. Furthermore, let the size of a formula \( F \) be the length of the string representation of \( F \), and denote it by \( |F| \).

**Definition 5 (Skolemisation)** The Skolemisation of a formula \( \Delta \) yields a formula equisatisfiable to \( \Delta \), not containing any existential quantifiers. To this end, Skolemisation replaces any subterm in \( \Delta \) of the shape \( \exists x.F \) by \( F[t/x] \), where \( t \) is called the Skolem term for \( x \).

Replacing existentially quantified variables with ε-terms using the defining property of ε-terms

\[
\exists x. P(x) \leftrightarrow P(\varepsilon x. P(x)),
\]

we obtain a formula equivalent to the original one (Hilbert and Bernays 1939). However, recursively replacing existential quantifiers by ε-terms can lead to an exponential size of the skolemised formula. To show this, we are going to define two kinds of ε-Skolemisation and show that they both produce exponentially large output. In particular, the blowup is caused by the introduction of new Skolem names that contain other Skolem names.

**Definition 6** Let \( F \) a subformula of \( \Delta \) such that \( F \) is of the shape \( \exists x.G \). A naïve ε-Skolemisation step replaces \( F \) in \( \Delta \) by \( G[(\varepsilon x.G)/x] \).

Naïve ε-Skolemisation (NeS) of a formula \( \Delta \) repeatedly applies naïve ε-Skolemisation steps until the formula does not contain any more existential
quantifiers. To fix the order of Skolemisation steps, let outside-in NeS replace subformulas only if they are not subformulas of an existential quantification, and inside-out NeS replace subformulas only if they do not have subformulas containing existential quantifiers. We now give an example for which both outside-in and inside-out NeS produce exponentially large skolemised formulas.

Example 3 Let \( \phi_n \) be a formula recursively defined by \( \phi_0 = P(x_0, x_0) \) and \( \phi_{n+1} = \exists x_n. (P(x_{n+1}, x_{n+1}) \rightarrow \phi_n) \).

Lemma 1 Inside-out NeS of \( \phi_n \) produces a formula exponential in \( n \).
Proof Denote the inside-out NeS of \( \phi_n \) as \( \text{sk}(\phi_n) \). Then \( \text{sk}(\phi_0) = P(x_0, x_0) \) and \( \text{sk}(\phi_{n+1}) = P(x_{n+1}, x_{n+1}) \rightarrow \text{sk}(\phi_n)[t_n/x_n] \), where \( t_n = \epsilon x_n. (P(x_{n+1}, x_{n+1}) \rightarrow \text{sk}(\phi_n)) \) is the Skolem term corresponding to \( x_n \). For every \( n \), \( \text{sk}(\phi_n) \) contains at least two occurrences of \( x_n \), and the Skolem term \( t_n \) corresponding to \( x_n \) is larger than \( |\text{sk}(\phi_n)| \). Therefore, for every \( n \), \(|\text{sk}(\phi_{n+1})| > 2|\text{sk}(\phi_n)|\).

Lemma 2 Outside-in NeS of \( \phi_n \) produces a formula exponential in \( n \).
Proof Let \( \Delta = \forall x_m. \phi_m \) be the formula to be skolemised. Then the Skolem terms corresponding to \( x_n \) can be given by

\[
s_n = \begin{cases} 
  x_m & \text{if } n = m \\
  \epsilon x_n. P(s_{n+1}, s_{n+1}) \rightarrow \phi_n & \text{otherwise}
\end{cases}
\]

For any \( n < m \), because every Skolem term \( s_n \) contains two occurrences of \( s_{n+1} \), we have that \(|s_n| > 2|s_{n+1}|\). As the base case \( s_m \) is greater than zero, we have that \(|s_0|\) is exponential in \( m \).

The example above motivates a new consistent Skolemisation method that produces quadratic output and is also applicable to nonclausal search. For this, let us define some notation first: \( \mathcal{F}\text{Var}(F) \) denotes the free variables of \( F \), and \( \mathcal{F}\text{Var}_Q(F) \) respectively \( \mathcal{F}\text{Var}_Q(x)(F) \) denote the free variables in a subformula \( F \) of \( \Delta \) that are universally respectively existentially bound in \( \Delta \). \( \Delta^x \) is the subformula of \( \Delta \) that binds the variable \( x \), i.e. if \( \Delta \) has a subformula \( \exists x.F \), then \( \Delta^x \) is \( \exists x.F \). Furthermore, the transitive universal respectively existential free variables of \( F \) are denoted by

\[
\mathcal{F}\text{Var}_Q^*(F) = \mathcal{F}\text{Var}_Q(F) \cup \bigcup_{x \in \mathcal{F}\text{Var}_Q(F)} \mathcal{F}\text{Var}_Q^*(\Delta^x),
\]

where \( Q \in \{\forall, \exists\} \).

Definition 7 (Consistent \( \epsilon \)-Skolemisation) Let \( x \) be an existentially quantified variable in \( \Delta \). The \( \epsilon \)-defining formula of \( \Delta^x \) is \( \max\{\Delta^y \mid y \in \mathcal{F}\text{Var}_Q^*(\Delta^x)\} \). The consistent \( \epsilon \)-Skolem term for \( x \) is \( \epsilon x.F \), where \( F \) is the \( \epsilon \)-defining formula of \( \Delta^x \) with all quantifiers for \( \mathcal{F}\text{Var}_Q^*(\Delta^x) \) and \( x \) removed. Consistent \( \epsilon \)-Skolemisation of a formula \( \Delta \) replaces any subformula of \( \Delta \) of the shape \( \exists x.F \) by \( F[t/x] \), where \( t \) is the consistent \( \epsilon \)-Skolem term for \( x \).
Example 4 Let
\[ \Delta = \forall x_1 \exists y_1. (P(x_1, y_1) \implies (\forall x_2 \exists y_2. P(x_2, y_2)) \land (\forall x_3 \exists y_3. Q(x_3, y_3, y_1))). \]
The \(\epsilon\)-defining formula of \(\Delta^{y_1}\) and \(\Delta^{y_2}\) is \(\Delta^{y_3}\) and of \(\Delta^{y_2}\), it is \(\Delta^{y_2}\). The consistent \(\epsilon\)-Skolem term for \(y_n\) is \(s_n\), where

\[
\begin{align*}
    s_1 &= \epsilon y_1. P(x_1, y_1) \implies (\forall x_2 \exists y_2. P(x_2, y_2)) \land (\forall x_3 \exists y_3. Q(x_3, y_3, y_1)) & \mathcal{FVar}(s_1) = \{x_1\} \\
    s_2 &= \epsilon y_2. P(x_2, y_2) & \mathcal{FVar}(s_2) = \{x_2\} \\
    s_3 &= \epsilon y_3. \exists y_1. P(x_1, y_1) \implies (\forall x_2 \exists y_2. P(x_2, y_2)) \land Q(x_3, y_3, y_1) & \mathcal{FVar}(s_3) = \{x_1, x_3\}
\end{align*}
\]

Theorem 1 Consistent \(\epsilon\)-Skolemisation of a formula \(\Delta\) yields a formula equivalent to \(\Delta\).

Proof Let us consider an arbitrary existentially quantified variable \(x\) in \(\Delta\). Let \(D\) be the \(\epsilon\)-defining formula of \(\Delta \epsilon\). We can move all universal quantifiers corresponding to \(\mathcal{FVar}(\Delta \epsilon)\) in front of \(D\), yielding \(\forall y_1. D_1\). Note that \(\mathcal{FVar}(D_1) = \mathcal{FVar}(\Delta \epsilon)\) and \(y_1 = \mathcal{FVar}(\Delta \epsilon) \setminus \mathcal{FVar}(D)\). Furthermore, we can move the existential quantifier for \(x\) in front of \(D_1\), resulting in \(\forall y_2. \exists x. D_2\). Now, we can use the defining property of \(\epsilon\)-terms to obtain \(\forall y_3. D_2[t/x]\), where \(t = \epsilon x. D_2\). Finally, we can move back the quantifiers from \(y_3\) to their original places to yield \(D_3\). (\(D_3\) could have been equally obtained by removing the quantifier \(\exists x\) from \(D\) and replacing \(x\) by \(\epsilon x. D_2\).) As all free variables of every such \(\epsilon\)-term \(t\) are universally quantified, we can execute the operations above to replace in arbitrary order every existentially quantified variable with its corresponding \(\epsilon\)-term. As all the operations preserve equivalence of the formula, this yields a formula equivalent to \(\Delta\), and we can see that it is exactly the outcome of consistent \(\epsilon\)-Skolemisation.

Lemma 3 Consistent \(\epsilon\)-Skolemisation of a formula \(\Delta\) yields a formula of size smaller than \(|\Delta|^2\).

Proof The maximal size of a consistent \(\epsilon\)-Skolem term is \(|\Delta|\), and as there are less than \(|\Delta|\) occurrences of existentially quantified variables in \(\Delta\), replacing them yields a formula of size smaller than \(|\Delta|^2\).

To obtain a first-order formula from consistent \(\epsilon\)-Skolemisation, we replace every consistent \(\epsilon\)-Skolem term of the shape \(\epsilon x. F\) with \(f_{\epsilon x.f}(\mathbf{y})\), where \(\mathbf{y}\) is \(\mathcal{FVar}(\epsilon x. F)\) (and thus also \(\mathcal{FVar}(\Delta^{\epsilon})\)). Here, \(\lfloor t \rfloor\) denotes a normalisation of \(t\) such that for any \(t_1\) and \(t_2\), if \(t_1\) is \(\alpha\)-equivalent to \(t_2\), then \(\lfloor t_1 \rfloor = \lfloor t_2 \rfloor\). We use this normalisation to recognise equivalent Skolem terms even if their variables are differently named. Due to the introduction of new function symbols, this yields a formula equisatisfiable to \(\Delta\).

The following corollary states under which conditions variables that are existen- tial bound at different locations will be consistently skolemised to the same function symbol. Note that this result holds across different formulas and problems.

Corollary 1 (Consistency) Two existentially quantified variables are mapped to the same first- order function symbol iff their corresponding \(\epsilon\)-Skolem terms are \(\alpha\)-equivalent.

Proof Follows from \[\text{Definition 7}\].
5 Naive Bayesian Internal Guidance

The order in which extension steps are tried can have a significant effect on the performance of proof search. In this section, we propose the use of Naive Bayesian probability to guide the use of extension steps based on an intermediate proof state.

We generally call methods that implement guidance inside ATPs internal guidance methods. In the particular case of machine learning guidance, such methods are historically motivated by the relative success of the external guidance methods used mainly for premise selection outside of the core ATP systems [Blanchette et al. 2016a; Urban et al. 2008; Kaliszyk and Urban 2014]. Internal guidance methods aim to estimate the utility of actions according to the system’s knowledge of the world and previous experiences. In our setting, a positive experience is when in a certain tableau branch, an extension step used a contrapositive that contributed to the final proof. We use this information to prefer contrapositives in branches that are similar to branches where the contrapositives were previously useful.

To measure the similarity between tableau branches, we characterise them by features [Kaliszyk et al. 2015b], which we explain in subsection 5.1. In subsection 5.2 we then calculate the utility of a contrapositive in the current branch, given knowledge about its utility in previous proofs. In subsection 5.3 we motivate the integration of machine learning methods in the prover and introduce the prover FEMaLeCoP, which we evaluate in subsection 5.4.

5.1 Tableau Branch Characterisation

The words of the connection tableaux calculus \( \langle C, M, Path \rangle \) correspond to a set of tableau branches sharing the active Path. Therefore, to characterise a branch, we use as its features the set of symbols occurring in the active path. We weigh the symbols by the number of times they appeared in all problems, giving higher weight to rarer symbols via inverse document frequency (Jones 1973), as well as by the distance between the current depth and the depth the symbols where put onto the path, giving higher weight to symbols more recently processed.

5.2 Naive Bayes

Given a set of contrapositives that are applicable in a tableau branch, we wish to obtain an ordering of the contrapositives such that trying the contrapositives in the given order minimises the time spent to find a proof. In this subsection, we show how to order the set of applicable contrapositives by a formula \( nb \) that is based on Naive Bayesian probability, as used for premise selection [Kaliszyk and Urban 2015b].

First, let us denote the knowledge about the usage of contrapositives in previous proofs by \( F(l_i) \), which is the multiset of sets of features characterising the tableau branches in which the usage of \( l_i \) contributed to the final proof. \( |F(l_i)| \) is the total number of times that \( l_i \) was used in previous proofs.

Example 5 \( F(l_1) = \{ \{ f_1, f_2 \}, \{ f_2, f_3 \} \} \) means that the contrapositive \( l_1 \) was used twice in previous proofs; once in a proof state characterised by the features \( f_1 \) and \( f_2 \), and once when features \( f_2 \) and \( f_3 \) were present.
Let $P(l_i, f)$ denote the probability that a contrapositive $l_i$ from a set of applicable contrapositives is useful in a tableau branch characterised by features $f$. Using Bayes’ theorem together with the (naive) assumption that features are statistically independent, we derive

$$P(l_i | f) = \frac{P(l_i)P(f | l_i)}{P(f)} = \frac{P(l_i)}{P(f)} \prod_{f_j \in f} P(f_j | l_i).$$

To increase numerical stability, we calculate the logarithm of the probability

$$\ln P(l_i | f) = \ln P(l_i) - \ln P(f) + \sum_{f_j \in f} \ln P(f_j | l_i).$$

In the final formula $\text{nb}(l_i, f)$ to rank contrapositives, we modify $\ln P(l_i | f)$ as follows:

- We add a term to disadvantage features not present in $f$ that occurred in previous situations where the contrapositive was useful.
- We weigh the probability of any feature $f$ by its inverse document frequency $i(f)$ to give more weight to rare features.
- We drop the term $\ln P(f)$, as we compare only values for fixed features $f$.
- We weigh the individual parts of the sum with constants $\sigma_1$, $\sigma_2$, and $\sigma_3$.

The resulting formula is

$$\text{nb}(l_i, f) = \sigma_1 \ln P(l_i) + \sigma_2 \sum_{f_j \in f} i(f_j) \ln P(f_j | l_i) + \sigma_3 \sum_{f_j \in \bigcup F(l_i) \backslash f} i(f_j) \ln (1 - P(f_j | l_i)).$$

We are now going to describe how to calculate $P(l_i)$ as well as $P(f_j | l_i)$. First, we calculate the unconditional contrapositive probability as

$$P(l_i) = \frac{|F(l_i)|}{\sum_{l_j \in l} |F(l_j)|}.$$

In practice, as the denominator of the fraction is the same for all $l_i$, we drop it, similarly to $P(f)$ above. To obtain the conditional feature probability, we distinguish whether a feature $f_j$ already appeared in conjunction with a contrapositive $l_i$. If so, then its probability is the ratio of times $f_j$ appeared when $l_i$ was used and all times that $l_i$ was used. Otherwise, the probability is estimated to be a minimal constant probability $\mu$:

$$P(f_j | l_i) = \begin{cases} \sum_{l' \in F(l_i)} 1_{l' \in l'}(f_j) / |F(l_i)| & \text{if } \exists l' \in F(l_i), l_j \in l' \\ \mu & \text{otherwise} \end{cases}$$

Here, $1_A(x)$ denotes the indicator function that returns 1 if $x \in A$ and 0 otherwise.
5.3 Implementations

The Machine Learning Connection Prover (MaLeCoP) was the first leanCoP-based system to explore the feasibility of machine-learnt internal guidance (Urban et al. 2011). MaLeCoP relies on an external machine learning framework (using by default the SNoW system (Carlson et al. 1999)), providing several machine learning algorithms, namely Naive Bayes and shallow neural networks based on perceptrons or winnow cells. During proof search, MaLeCoP sends features of its current branch to the framework, which orders the proof steps applicable in the current branch by their expected utility. The usage of a general framework eases experiments with different methods, but the prediction speed of MaLeCoP’s underlying advisor system together with the communication overhead was several orders of magnitude lower than the raw inference speed of leanCoP. This was to some extent countered by fast query caching mechanisms and a number of strategies trading the machine-learnt advice for raw speed, yet the real-time performance of the system remained relatively low.

This motivated the creation of the Fairly Efficient Machine Learning Connection Prover (FEMaLeCoP), which improved speed by integrating a fast and optimised Naive Bayesian classifier as shown in subsection 5.2 into the prover (Kaliszyk and Urban 2015a). Naive Bayes was chosen because learning data can be easily filtered for the current problem, making the calculation of Naive Bayesian probabilities for a given branch efficient for each applicable contrapositive. FEMaLeCoP efficiently calculates the Bayesian probabilities of a given set of contrapositives by saving contrapositive statistics directly in the literal database. Performance is further improved as branch features are not fully recalculated in every new branch, but updated from the previous branch.

5.4 Evaluation

The evaluation involves generation of training data with leanCoP, followed by running FEMaLeCoP with the training data on the same problems. We run both leanCoP and FEMaLeCoP on the bushy MPTP2078 dataset with a timeout of 60s, nondefinitional clausification, conjecture-directed search and restricted backtracking. Both leanCoP and FEMaLeCoP considered in this evaluation are implemented in OCaml using continuation passing style, see subsection 3.3.3.

leanCoP proves 574 problems. From the resulting proofs, the information is extracted which contrapositive contributed in which tableau branch. This information is combined for all proofs to a format that allows efficient retrieval of learning data for given contrapositives.

With the training data generated from the leanCoP proofs, we run FEMaLeCoP on the same problems as leanCoP. While the inference rate drops by about 40%, FEMaLeCoP proves 640 problems. The union of leanCoP and FEMaLeCoP proves 664 problems, adding 90 problems (15.7%) to the problems solved by leanCoP. A more thorough evaluation of Naive Bayesian machine learning integrated with other internal guidance components will be performed in the next section.

7 The leanCoP version evaluated here uses a different clause order than the versions in subsection 3.3 which explains the different baseline performance.
In this section, we describe how to expand a proof search tree using Monte Carlo Tree Search (MCTS).

For an intuition of the relationship between different proof search strategies, see Figure 6: Iterative deepening considers all potential proof trees of a certain depth before considering trees of higher depth. Restricted backtracking uniformly discards a set of potential proof trees. MCTS allows for a more fine-grained proof search, searching different regions of the search space more profoundly than others, based on heuristics.

We introduce MCTS and propose a set of heuristics adapted to proof search. Then, we show an implementation of the method, closing with an evaluation.

6 Monte Carlo Proof Search

Monte Carlo Tree Search (MCTS) is a method to search potentially infinite trees by sampling random tree paths (called simulations) [Browne et al. 2012]. The outcome of simulations is then used to estimate the quality of tree nodes, and MCTS steers search towards nodes with higher quality estimates.

Definition 8 (Tree) A tree is a tuple \((N, n_0, \rightarrow)\), where \(N\) is a set of tree nodes, \(n_0 \in N\) is the root node, and \(\rightarrow \in N \times N\) is a cycle-free relation, i.e. there is no \(n \in N\) such that \(n \rightarrow^{+} n\). We write that \(n'\) is a child of \(n\) iff \(n \rightarrow n'\). Every \(n \in N\) is the child of maximally one node in \(N\).

We consider proof search as traversal of a (usually infinite) tree \((N, n_0, \rightarrow)\), such that \(N\) is the set of derivations (tableaux), \(n_0\) is a derivation that consists of some word \((C, M, Path)\) corresponding to the matrix \(M\) of a given problem, and \(n \rightarrow n'\) iff \(n'\) can be obtained from \(n\) by applying a single calculus rule. If \(n \rightarrow n'\) by a single application of the extension rule using the contrapositive \(c\), then we write \(n \xrightarrow{\text{ext}(c)} n'\). Proof search succeeds when we find a leaf node of \(N\) that is a proof.

\(\rightarrow^{+}\) is the transitive closure of \(\rightarrow\).
Let $\rho \in N \to \mathbb{R}$ be a reward function that estimates the distance of an unclosed derivation in the proof search tree from a closed derivation. Then we can use Monte Carlo Tree Search to traverse the proof search tree, giving preference to regions that yield higher rewards. For this, we first define Monte Carlo trees:

**Definition 9 (Monte Carlo tree)** A Monte Carlo tree $T$ for a tree $(N, n_0, \rightarrow)$ is a tuple $(N_T, \rightarrow_T, \rho_T)$, where $\rightarrow_T \subseteq \rightarrow^*$ and $\rho_T \in N \to \mathbb{R}$ is a mapping. We write that $n'$ is a $T$-child of $n$ if $n \rightarrow_T n'$. The initial Monte Carlo tree $T_0$ is $(N_{T_0}, \rightarrow_{T_0}, \rho_{T_0})$ with $N_{T_0} = \{n_0\}$, $\rightarrow_{T_0} = \emptyset$ and $\rho_{T_0}(n) = 0$ for all $n$.

A single iteration of Monte Carlo Tree Search takes a Monte Carlo tree $T$ and returns a new tree $T'$ as follows:

1. **Selection**: A node $n \in N_T$ with $n_0 \rightarrow_T^* n$ is chosen with a child selection policy, see subsection 6.2.
2. **Simulation**: A child $n_1$ of $n$ is randomly chosen with child probability $P(n_1 \mid n)$ to be the simulation root, see subsection 6.3. (Every tree node is chosen maximally once to be a simulation root, to guarantee the exploration of the tree.) From $n_1$, a sequence of random transitions $n_1 \rightarrow \cdots \rightarrow n_s$ is performed, where for every $i < s$, $n_{i+1}$ is randomly selected with child probability $P(n_{i+1} \mid n_i)$.
3. **Expansion**: A node $n_e$ from $n_1 \rightarrow \cdots \rightarrow n_s$ is selected with the expansion policy, see subsection 6.5. The node $n_e$ is added as a child to $n$ with reward $\rho(n_s)$ (see subsection 6.4) to yield the new tree $T'$:

   $N_{T'} = N_T \cup \{n_e\}$ \hspace{1cm} $\rightarrow_{T'} = \rightarrow_T \cup \{(n, n_e)\}$ \hspace{1cm} $\rho_{T'} = \rho_T \cup \rho(n_e \mapsto \rho(n_s))$

In the next sections, we show heuristics for the child selection policy, child probability, reward, and expansion policy.

### 6.2 Child Selection Policy

UCT (Upper Confidence Bounds for Trees) is a frequently used child selection policy for Monte Carlo Tree Search (Kocsis and Szepesvári 2006). It uses $\text{visits}_T(n)$, which is the number of $T$-descendants of $n$, and $\bar{\rho}_T(n)$, which is the average $T$-descendant reward of $n$.

$$\text{visits}_T(n) = |\{n' \mid n \rightarrow_T^* n'\}|$$

$$\bar{\rho}_T(n) = \frac{\sum\{\rho_T(n') \mid n \rightarrow_T^* n'\}}{\text{visits}_T(n)}$$

Given a node $n$, UCT ranks every $T$-child $n'$ of $n$ with

$$\text{uct}(n, n') = \bar{\rho}_T(n') + C_p \sqrt{\frac{\ln \text{visits}_T(n)}{\text{visits}_T(n')}}$$

Here, $C_p$ is called the exploration constant, where small values of $C_p$ prefer nodes with higher average descendant reward and large values of $C_p$ give more weight to

---

9 Frequently, MCTS is described to have a backpropagation step that adds rewards to the ancestors of the newly added nodes. We omit this step, adapting the child selection policy instead.
nodes with fewer visits. In the UCT formula, division by zero is expected to yield \( \infty \), so if a node \( n \) has unvisited children, one of them will be selected by UCT.

The UCT child selection policy \( cs_T(n) \) recursively traverses the Monte Carlo tree \( T \) starting from the root \( n_0 \). \( cs_T(n) \) chooses the \( T \)-child of \( n \) with maximal UCT value and recurses, unless \( n \) has no \( T \)-child, in which case \( n \) is returned:

\[
cs_T(n) = \begin{cases} 
  cs_T \left( \arg \max_{n' \mid n \rightarrow T n'} \text{uct}(n, n') \right) & \text{if } \exists n', n \rightarrow T n' \\
  n & \text{otherwise}
\end{cases}
\]

### 6.3 Child Probability

The child probability \( P(n' \mid n) \) determines the likelihood of choosing a child node \( n' \) of \( n \) in a simulation. We show three different methods to calculate the child probability.

- **The baseline probability** assigns equal probability to all children, i.e. \( P(n' \mid n) \propto 1 \).
- **The open branches probability** steers proof search towards derivations with fewer open branches, by assigning to \( n' \) a probability inversely proportional to the number of open branches in \( n' \). Therefore, \( P(n' \mid n) \propto 1/(1 + |b_0(n')|) \), where \( b_0(n) \) returns the open branches in \( n \).
- **The Naive Bayes probability** attributes to \( n' \) a probability depending on the calculus rule applied to obtain \( n' \) from \( n \): In case the extension rule was not used, the node obtains a constant probability. If the extension rule was used, the formula \( \text{NB} \) introduced in subsection 5.2 is used, requiring contrapositive statistics from previous proofs. However, as \( \text{NB} \) is not a probability, we use it to rank contrapositives by the number of contrapositives with larger values of \( \text{NB} \):

\[
\text{rank}_{\text{NB}}(n, c) = \left\{ c' \mid n \xrightarrow{\text{ext}(c')} n', \text{NB}(c', f(n)) \geq \text{NB}(c, f(n)) \right\},
\]

where \( f(n) \) denotes the features of the derivation \( n \). Then, we assign to nodes as probability the inverse of the Naive Bayes rank:

\[
P(n' \mid n) \propto \begin{cases} 
  1/\text{rank}_{\text{NB}}(n, c) & \text{if } n \xrightarrow{\text{ext}(c')} n' \\
  1 & \text{otherwise}
\end{cases}
\]

### 6.4 Reward

The reward heuristic estimates the likelihood of a given derivation to be closable. This is in contrast to most prover heuristics (such as child probability) that only compare the quality of children of the same node. We use our reward heuristics to evaluate the last node \( n \) of a simulation.

Several heuristics in this section require a normalisation function, for which we use a strictly increasing function \( \text{norm} : [0, \infty) \rightarrow [0,1) \) that fulfills \( \lim_{x \to \infty} \text{norm}(x) = 1 \) and \( \text{norm}(0) = 0 \). For example, \( \text{norm}(x) = 1 - (x + 1)^{-1} \).

- **The branch ratio reward** determines the reward to be the ratio of the number of closed branches and the total number of branches, i.e. \( \rho(n) = |b_c(n)|/|b(n)| \).
– The **branch weight reward** is based on the idea that many open branches with large literals are indicators of a bad proof attempt. Here, the size $|l|$ of a literal is measured by the number of symbol occurrences in $l$. Furthermore, the closer to the derivation root a literal appears, the more characteristic we consider it to be for the derivation. Therefore, the reward is the average of the inverse size of the branch leafs, where every leaf is weighted with the normalised depth of its branch.

$$\rho(n) = \frac{1}{|b_o(n)|} \sum_{b \in b_o(n)} \frac{\text{norm(depth(b))}}{|\text{leaf}(b)|}$$

– The **machine-learnt closability reward** assumes that the success ratio of closing a branch in previous derivations can be used to estimate the probability that a branch can be closed in the current derivation. This needs the information about attempted branches in previous derivations, and which of these attempts were successful. We say that a literal $l$ stemming from a clause $c$ is attempted to be closed during proof search when $l$ lies on some branch. The attempt is successful iff proof search manages to close all branches going through $l$. Given such data from previous proof searches, let $p(l)$ and $n(l)$ the number of successful respectively unsuccessful attempts to close $l$. We define the unclosability of a literal $l$ as $\frac{n(l)}{p(l) + n(l)}$. However, the less data we have about a literal, the less meaningful our statistics will be. To account for this, we introduce weighted unclosability: We assume that a literal that never appeared in previous proof searches is most likely closable, i.e. its weighted unclosability is 0. The more often a literal was attempted to be closed, the more its weighted unclosability should converge towards its (basic) unclosability. Therefore, we model the probability of $l$ to be closable as

$$P(l \text{ closable}) = 1 - \frac{n(l)}{p(l) + n(l)}.$$  

Finally, the closability of a derivation is the mean closability of all leafs of open branches of the derivation, i.e. the final reward formula is

$$\rho(n) = \sum_{b \in b_o(n)} P(\text{leaf}(b) \text{ closable}) / |b_o(n)|.$$ 

To measure the efficiency of a reward heuristic, we introduce **discrimination**. Assume that an MCTS iteration of the Monte Carlo tree $T$ starts a simulation from the node $n_p$ and finds a proof. Then the discrimination of $T$ is the ratio of the average reward on the Monte Carlo tree branch from the root node $n_0$ to $n_p$ and the average reward of all Monte Carlo tree nodes. Formally, let the average reward of a set of nodes $N$ be $\overline{\rho}_T(N) = \frac{\sum_{n \in N} \rho_T(n)}{|N|}$. Then the discrimination of $T$ is

$$\overline{\rho}_T\left(\left\{ n \mid n_0 \rightarrow_T^* n, n \rightarrow_T^* n_p \right\}\right) / \overline{\rho}_T\left(\left\{ n \mid n_0 \rightarrow_T^* n \right\}\right).$$

6.5 Expansion Policy

The expansion policy determines which node $n_e$ of a simulation $n_1 \rightarrow \cdots \rightarrow n_s$ is added to the Monte Carlo tree. We implement two different expansion policies:

– The **default expansion policy** adds $n_1$, i.e. the simulation root, to the MC tree.
The minimal expansion policy picks \( n_e \) to be the smallest of the simulation nodes w.r.t. a given norm \( |\cdot| \), such that for all \( i \), \( |n_e| \leq |n_i| \). If multiple \( n_e \) are admissible, the one with the smallest index \( e \) is picked. We consider two norms on nodes:

1. The first norm measures the number of open branches.
2. The second norm measures the sum of depths of open branches.

The minimal expansion policy is similar to restricted backtracking in the sense that it restricts proof search to be resumed only from certain states, thus resulting in an incomplete search.

6.6 Implementation

We implemented Monte Carlo proof search (MCPS) based on leanCoP, where leanCoP builds the search tree and MCTS chooses which regions of the tree to search. Unlike for the traditional leanCoP, the depth of the search tree is not limited. To guarantee nonetheless that simulations terminate, simulations are stopped after a fixed number of simulation steps \( s_{\text{max}} \).

While it is possible to run MCPS from the root node until a proof is found, we have found it to perform better when it serves as advisor for leanCoP. We show this in [Listing 3](#) assuming for a simpler presentation that the default expansion policy from [subsection 6.5](#) is used: MCPS as performed by `mcps lit path sub` attempts to close the branch containing the literals in `path` and the literal `lit` as leaf. The result is a lazy list `mc` of Monte Carlo iterations, where an iteration consists of a Monte Carlo tree and possibly a proof discovered during the simulation performed in the iteration. The first \( \text{maxIterations} \) are considered: When \( \text{maxIterations} \) is set to 0, proof search behaves like leanCoP, and in case it is set to \( \infty \), the whole proof search is performed in the MCPS part. As MCPS is performed lazily, MCPS is performed for less than \( \text{maxIterations} \) iterations when it discovers some proof contributing to the final closed derivation. Here, the lazy list characterisation introduced in [subsubsection 3.3.2](#) turns out to be permit a very concise implementation as well as an easy integration of techniques such as restricted backtracking. As soon as all proofs discovered during MCPS were considered, the tree \( T \) of the final Monte Carlo iteration `last mc` is obtained and the children of the root of \( T \) are sorted by decreasing average \( T \)-descendant reward \( \rho_T \). Finally, the last applied proof step of each child is processed like in the lazy list implementation.

The array substitution technique from [subsection 3.4](#) requires that the proof search always backtracks only to states whose substitution is a subset of the current state’s substitution. However, because this requirement is not fulfilled for MCPS, we use association lists for substitutions.

6.7 Evaluation

We evaluated the presented heuristics on the bushy MPTP2078 problems, with definitional clausification and a timeout of 10s for each problem. Before evaluation, we collected training data for the machine learning heuristics by running leanCoP on all bushy problems with a timeout of 60s.
Listing 4: Monte Carlo Proof Search as advisor.

```haskell
prove [] path lim sub = [sub]
prove (lit : cla) path lim sub =
let
    mc = take maxIterations (mcps lit path sub)
    proofs1 = mapMaybe getProof mc
    proofs2 = last mc & root & children & sortOn avgReward & concatMap
        (\ child -> case lastStep child of
            Reduction sub1 -> [sub1]
            Extension (sub1, cla1) ->
            if lim <= 0 then []
            else prove cla (lit : path) (lim - 1) sub1)
        in concatMap (prove cla path lim) (proofs1 ++ proofs2)
```

Table 5: Comparison of Monte Carlo heuristics. Iterations, simulation steps and discrimination ratio are averages on the 196 problems solved by all configurations.

| Configuration               | Iterations | Sim. steps | Discr. | Solved |
|----------------------------|------------|------------|--------|--------|
| Base                       | 116.46     | 1389.82    | 1.37   | 332    |
| Uniform probability        | 949.62     | 17539.59   | 1.31   | 237    |
| NB probability             | 528.39     | 8014.03    | 1.35   | 248    |
| Random reward              | 104.88     | 1167.98    | 1.12   | 334    |
| Branch weight reward       | 108.13     | 1268.88    | 1.19   | 364    |
| ML closability reward      | 108.52     | 1151.61    | **2.30** | **367** |
| Default exp. pol.          | 371.81     | 4793.58    | 1.38   | 328    |
| Minimal exp. pol. 2        | 224.72     | 2769.12    | 1.40   | 348    |

The base configuration of monteCoP uses the open branches probability (see sub-section 6.3), the branch ratio reward (see sub-section 6.4), and the minimal expansion policy 1 (see sub-section 6.5), where the maximal simulation depth $s_{max} = 50$, the exploration constant $C_p = 1$, and the maximal number of MCTS iterations $maxIterations = \infty$. For any heuristic $h$ not used in the base configuration, we replaced the default heuristic with $h$ and evaluated the resulting configuration. The results are shown in Table 5. We can see that the heuristics that most improve the base configuration are the machine-learnt closability reward and the minimal expansion policy 2.

We explored a range of values for several numeric parameters, for which we show results in Figure 7: The maximal number of MCTS iterations $maxIterations$ performs best between 20 and 40, see Figure 7a. Below 20, MCTS can not provide any meaningful quality estimates, and above 40, the quality estimates do not significantly improve any more, while costing computational resources. The exploration constant $C_p \approx 0.75$ gives best results, where the machine-learnt closability reward achieves a local optimum, see Figure 7b. At such an optimum, exploration and exploitation combine each other best, therefore the existence of such an optimum is a sanity check for reward heuristics (which the branch ratio reward does not pass). The maximal simulation depth $s_{max} \approx 20$ seems to perform best, see Figure 7c. Above this value, the number of solved problems decreases, since the number of actually performed simulation steps decreases, as shown in Figure 7d. This might be explained by the
fact that at higher simulation depths, the computational effort to calculate the set of possible steps increases, for example because the substitution contains more and larger elements.

![Graphs showing parameter influence](image)

(a) Maximal number of MCTS iterations. 
(b) Exploration.

(c) Maximal simulation depth. 
(d) Simulation steps / Maximal simulation depth.

**Fig. 7: Parameter influence.**

We adapted the base configuration to use the best heuristics from Table 5 and the best values for parameters discussed in Figure 7, yielding \( s_{\text{max}} = 20 \), \( C_p = 0.75 \), and \( \text{maxIterations} = 27 \). This improved configuration solves 538 problems, compared to 509 solved by the best single leanCoP strategy.

## 7 Clausal and Nonclausal Proof Certification

In this section, we show how to certify connection tableaux proofs by reconstructing them in HOL Light. To abstract from the technical details, we give translations for both clausal and nonclausal versions of connection proofs to LK (Gentzen 1935). As the implementation can be used for regular proof search in HOL Light, we evaluate its performance on HOL Light problem sets.
7.1 Converting HOL to FOL Problems

To use leanCoP respectively nanoCoP as a proof tactic in HOL Light, it is necessary to convert a given proof goal from HOL to FOL. For this, we reuse a large part of the MESON (Harrison 1996) infrastructure, such as instantiation of higher-order axioms. Once we are left with a first-order problem \((A_1 \land \cdots \land A_n) \rightarrow C\), we transform it similarly to subsection 3.1. From the resulting formula, we create a matrix \(M\) and a literal database as explained in subsection 3.2 and search for a proof. The resulting proof consists of a connection proof tree and a global substitution \(\sigma\). Given this information, we want to construct a proof of \(M \vdash \bot\), which is written in LK as \(M \vdash\).

We show such a translation method both from clausal and nonclausal proofs to LK in the next sections.

7.2 Connection Calculi for Proof Translation

In the presentation of the connection calculi in Otten (2011), all proof rules have a fixed number of premises. To ease the translation of proofs, we present slightly reformulated versions of the calculi. We introduce the following notation for rules with an arbitrary number of premises:

\[
\frac{\bigwedge_i P_i}{C} \quad \equiv \quad \frac{P_1 \ldots P_n}{C}
\]

The reformulated calculi for translation are shown in Figure 8 and Figure 9. The words of the original calculi were \(\langle C, M, Path \rangle\). In the reformulated calculi, the words are \(\langle X, M, Path \rangle\), where \(X\) denotes an arbitrary clause element, i.e. a matrix or a literal. Furthermore, in the new calculi, the axiom rule becomes obsolete. Proofs can be trivially translated between the connection calculi in this chapter and those shown in section 2.

Example 6 Consider Example 1 on page 4. For the matrices \(M\) respectively \(M'\), proofs in the connection calculi for translation are given in Figure 10 respectively Figure 11.
where \( \{ X_1, \ldots, X_n \} \) is copy of \( C \in M \)

where \( \sigma(L) = \sigma(L') \)

where \( \{ X_1, \ldots, X_n \} \) is the \( \beta \)-clause of \( C_2 \) wrt. \( L' \), \( C_2 \) is copy of \( C_1 \), \( C_1 \) is e-clause of \( M \) wrt. \( Path \cup \{ L \} \), \( C_2 \) contains \( L' \) with \( \sigma(L) = \sigma(L') \)

where \( \{ X_1, \ldots, X_n \} \in M' \)

\[\Gamma, C_1, C_1 \land \ldots \land C_n \vdash \Delta \quad \land \text{L} \]

Furthermore, we use an LK rule \( \bot \text{L} \) which derives \( \bot \) from two complementary literals in the context:

\[\Gamma, A, \neg A \vdash \bot \text{L} \]
Let us start with the two rules that are translated the same way for clausal and nonclausal proofs, namely the start and the reduction rule. The translation of these rules is shown in Figure 12.

For the start rule, the translation obtains the formula corresponding to the clause \( C \) with the \( \land \) rule, and instantiates it with the \( \forall \) rule. The substitution \( \sigma \) is used to determine the instantiations, where fresh names are invented when a variable is unbound in the substitution. Then, the sequent is split into several subsequents \( X_i, M \vdash \), which represent the translations of the connection proofs for \( \langle X_i, M, \{} \rangle \).

7.3.1 Clausal Proof Translation

The translation of the clausal extension rule (shown in Figure 8) is given in Figure 13. First, \( L, M, Path \vdash \) is transformed to the equivalent \( M, P \vdash \), where \( P = Path \cup \{ L \} \).

Structurally, the remaining translation resembles that of the start rule, with the exception that it additionally closes a proof branch containing the negated literal \( L \).

7.3.2 Nonclausal Proof Translation

We now proceed with the translation of nonclausal connection proofs, using the calculus introduced in Figure 2. The LK context in the translation of nonclausal proofs now has the shape \( X, M, Path \). \( X \) refers to either a literal or a matrix, whereas \( X \)

---

In the clausal setting, \( X_i \) could be written as \( L_i \), but as the same rule is used in the nonclausal setting, where \( X_i \) can represent either a literal or a matrix, we write \( X_i \) for the common rules.
| Connection Calculus | LK |
|---------------------|----|
| $\bigwedge (X_i, M, \text{Path})$ | $\bigvee L$ |
| $M', M, \text{Path}$ | Decomposition |
| where $\{X_1, \ldots, X_n\} \in M'$ | $\left[ X_1, M', \text{Path} \vdash \right] \ldots \left[ X_n, M', \text{Path} \vdash \right] \bigvee L$ |

Fig. 14: LK translation of the decomposition rule.

$$M_i = \left\{ \begin{array}{ll} c_i \left[ \begin{array}{c} X_{1,1} \\ \vdots \\ M_{i+1} \\ \vdots \\ X_{i,n} \end{array} \right] & \text{if } i \leq m \\ \left[ \begin{array}{c} X_{1,1} \\ \vdots \\ \beta_{i+1} \\ \vdots \\ X_{i,n} \end{array} \right] & \text{if } i > m \end{array} \right\}$$

otherwise \hspace{1cm} otherwise

Fig. 15: Definition of matrix $M_i$, clause $C_i$, and $\beta$-clause $\beta_i$.

represented just literals in subsubsection 7.3.1 Furthermore, we use a set of matrices $M$, instead of a single matrix $M$ as in the clausal case. During translation, $M$ is extended such that for each word $(L, M, \text{Path})$ in the connection calculus and its corresponding LK sequent $L, M, \text{Path} \vdash$, the $\varepsilon$-clauses of $M$ wrt $\text{Path} \cup \{L\}$ are the clauses $C$ for which $C$ in $M'$ and $M' \in M$. We will see this in detail in the explanation for the extension rule.

The LK translation of nonclausal proofs reuses the translations of the start and the reduction rules given in Figure 12. However, occurrences of $M$ in the LK translation are replaced by $M$. The start rule uses $M = \{M\}$, i.e. $M$ contains only the initial problem matrix $M$.

The decomposition rule of the nonclausal calculus can be seen as a generalisation of the start rule. We give its translation to LK in Figure 14.

Let us now consider a nonclausal extension step applied to $(L, M, \text{Path})$. Let $C_i$ denote the $\varepsilon$-clause of $M$ wrt $\text{Path} \cup \{L\}$ that was used for the extension step. By construction of $M$ mentioned above, $C_i$ is some clause in $M_i \in M$. Furthermore, let $\beta_i$ be the $\beta$-clause of $C_i$ wrt $\text{L}$. Then we can find some $m$ such that $M_1, C_i$ and $\beta_i$ can be written as in Figure 15.

The translation of the nonclausal extension rule is shown in Figure 16. We first transform $L, M, \text{Path} \vdash$ to the equivalent $M^0, P \vdash$, as $M^0 = M$ and $P = \text{Path} \cup \{L\}$. We then determine $M_i \in M$ and put it into the context by contraction (CL).

Now we recursively prove the sequent $M_i, M_{i+1}, P \vdash$. If $M_i$ is the literal $\overline{L}$, we prove the sequent $\overline{L}, M^0, P \vdash$ with the $\bot$ L rule. Otherwise, we proceed as follows: First, we choose the appropriate clause $C_i$ of $M_i$ that corresponds to $\beta_i$. In the same step, we merge $M_i$ with $M^{i-1}$, yielding $M^i$. After the instantiation of $C_i$, the clause elements $X_{i,1}$ to $X_{i,n}$ give rise to several proof branches where all but one are closed by translation of the proof branches of the connection proof. The one
remaining clause element \( M_{i+1} \) gives rise to a sequent \( M_{i+1}, M^i, P \vdash \), which we translate by recursion. This concludes the translation of the extension rule.

**Example 7.** Consider the nonclausal proof given in Figure 10. We show its translation to LK in Figure 17, where boxed sequents indicate words of the original proof. We
Table 6: HOL Light evaluation datasets and number of contained problems.

| Prover        | HL-top | HL-meson | FS-top | FS-meson |
|---------------|--------|----------|--------|----------|
| ME             | 2499   | 1119     | 27112  | 44468    |

Table 7: HOL Light tactic results.

| Prover          | HL-top | HL-meson | FS-top | FS-meson |
|-----------------|--------|----------|--------|----------|
| Metis           | 807    | 1029     | 4626   | 42829    |
| MESON           | 736    | 900      | 4221   | 39227    |
| leanCoP+cut     | 724    | 948      | 3714   | 39922    |
| leanCoP−cut     | 717    | 844      | 3800   | 38528    |
| nanoCoP+cut     | 538    | 802      | 2743   | 34213    |
| nanoCoP−cut     | 550    | 811      | 2351   | 34769    |

use $F$ from Example 1 to define

\[
M_0 = \{F\}, \\
M_1 = M_0 \cup \{\neg P(s^2a) \land (P(sa) \lor \neg Q)\}, \\
M_2 = M_1 \cup \{\neg P(s^3a) \land (P(s^2a) \lor \neg Q)\}.
\]

7.4 Evaluation

We evaluate our HOL Light proof search tactics based on leanCoP and nanoCoP and compare their performance with the Metis (Färber and Kaliszyk 2015) and MESON (Harrison 1996) tactics integrated into HOL Light. Similarly to (Kaliszyk et al. 2015a), we disable splitting for MESON. As evaluation datasets, we use toplevel and MESON goals from core HOL Light as well as from Flyspeck, see Table 6. We use the Git version 08f4461 of HOL Light from March 2017, running every tactic with a timeout of 10s on each problem.

The results are shown in Table 7. As many problems in HOL Light are solved using either MESON or Metis, the problems are likely biased towards these two provers. Furthermore, the fact that both MESON and Metis are clausal might have shaped the design of the theorems in HOL Light towards solvability by clausal provers.

Comparing Table 7 with Table 2, we notice that the stand-alone connection provers perform better than their counterparts integrated in HOL Light. Apart from different preprocessing, this can be explained by different array access performance: Array access is more than 30 times faster in native OCaml programs, compared to programs compiled in OCaml’s toplevel (as used in HOL Light). This heavily affects our connection provers, as fast unification via arrays is critical for their performance, see subsection 3.4.

11 Note that this table mentions a larger number of MESON goals than Table 1. This is because we consider for this evaluation also those problems that are solved by the first-order export.
8 Related Work

A number of related works has already been discussed in previous sections. In particular in section 2, we introduced the connection calculus (Bibel 1991) as a variant of tableaux (Letz and Stenz 2001), we discussed its implementation in the leanCoP theorem prover (Otten and Bibel 2003), a number of improvements introduced in the second version of leanCoP (Otten 2008) including restricted backtracing (Otten 2010), and the nonclausal variant of the connection calculus (Otten 2011) together with its implementation (Otten 2016).

The compact Prolog implementation of theorem provers following the lean architecture made it attractive for many experiments both with the calculus and with the implementation. The intuitionistic version of leanCoP (Otten 2005) became the state-of-art prover for first-order problems in intuitionistic logic (Raths et al. 2007). Connections have also been considered for first-order modal logic in mleanCoP (Otten 2014), for higher-order logic (Andrews 1989) and for linear logic (Galmiche 2000). Various implementation modifications can be performed very elegantly, such as search strategies, scheduling, randomization of the order of proof search steps (Raths and Otten 2008), and internal guidance (Urban et al. 2011; Kaliszyk and Urban 2015a).

A number of early learning and data based approaches to guide automated theorem provers has been surveyed in (Denzinger et al. 1999). The Prover9 hints method (Veroff 1996) allows the user to specify (an often large set of) clauses to treat in a special way. A similarly working watch list has been later integrated in E, along with other learning mechanisms (Schulz 2001). Further methods for guiding the actual proof search of ATPs using machine learning have been considered in the integration of a Naive Bayesian classifier to select next proof actions in Satallax (Färber and Brown 2016), as well as in Enigma (Jakubuš and Urban 2017) where the clause selection in E uses a tree-based n-gram approach to approximate similarity to the learned proofs using a support vector machine classifier. Holophrasm (Whalen 2016) introduces a theorem prover architecture using GRU neural networks to guide the proof search of a tableaux style proof process of MetaMath. TensorFlow neural network guidance was integrated in E (Loos et al. 2017), showing that with batching and hybrid heuristics, it can solve a number of problems other strategies cannot solve. Finally, various reasons as to why the connection calculus is well suited for machine learning techniques, especially deep learning, are considered in (Bibel 2017).

The main use of machine learning in automated and interactive theorem provers today is to reduce original problems before the actual proof search. Machine learning based methods (Kühlwein et al. 2013; Blanchette et al. 2016b) improve on and complement the various ATP heuristics (Hoder and Voronkov 2011) and ITP heuristics (Meng and Paulson 2009). The problem of selecting the most useful lemmas for the given proof, referred to as “premise selection” or “relevance filtering” (Alama et al. 2014) nowadays uses syntactic similarity approaches, simple Naive Bayes and k-NN based classifiers, regression and kernel based methods (Kühlwein et al. 2013), as well as deep neural networks (Irving et al. 2016). This has become especially important in the “large theory bench” division added to the CADE Automated Systems Competition in 2008 (Sutcliffe 2009a), with systems such as MaLARea (Urban et al. 2008) and ET (Kaliszyk et al. 2015a) achieving notable results.

Theorem proving can be seen as a game – for instance, it has been modelled as a two-player game in the framework of game-theoretical semantics (Hintikka 1982).
Monte Carlo Tree Search (MCTS) [Browne et al. 2012] has been found to produce state-of-the-art players for several games, most notably for the two-player game Go (Silver et al. 2016), but also for single-player games such as SameGame (Schadd et al. 2012). It therefore seems reasonable to apply MCTS to the game of theorem proving. One-step lookahead can help Vampire proof search (Hoder et al. 2016), suggesting that MCTS, whose simulation phase can be seen as multi-step lookahead, can effectively guide proof search.

Certification of ATP found proofs has been especially important for the integration of ATPs into interactive proof assistants. Such components provide automation in the form of proof tactics or automated justification for smaller steps. HOL Light includes the certified proof producing model elimination prover MESON [Harrison 1996]. The paramodulation-based prover Metis [Hurd 2003] was designed with a small certified proof core to simplify its integration with interactive theorem provers (Färber and Kaliszyk 2013). Coq includes a proof certifying version of the intuitionistic first-order automated theorem prover JProver (Schmitt et al. 2001) and Matita includes a proof certifying version of an ordered paramodulation prover (Asperti and Tassi 2007). A translation of connection tableaux proofs to expansion trees which can be used for proof certification was studied in (Reis 2015). An alternative approach to proof certification is the usage of verified automated theorem provers (Ridge and Margetson 2005).

9 Conclusion and Future work

We have given an overview of our experiments conducted with connection provers. First, we presented translations to functional programming languages, exploring possibilities to increase the speed of proof search while keeping the implementation as simple as possible. We showed that the number of solved problems can be increased by up to 58.8%, on one dataset beating even E in automatic mode. Next, we discussed machine learning integration in leanCoP via context-sensitive clause ordering and Monte Carlo Tree Search, showing that both these techniques can increase the number of solved problems, despite fewer inferences being performed. Finally, we showed how to translate clausal and nonclausal connection proofs to LK, yielding a usable proof search tactic for HOL Light.

The performed machine learning experiments are promising enough to justify the enhancement of Monte Carlo Proof Search with stronger heuristics, such as neural networks. While we applied Monte Carlo Tree Search to theorem proving as a single-player game, it could also be used to treat theorem proving as two-player game.

The combination of several tools that are small, simple and comprehensible can be more effective than a large, monolithic tool. While the resulting connection provers cannot yet outperform larger systems like Vampire (Kovács and Voronkov 2013) and E (Schulz 2013), we hope that the insight gained by experiments performed in connection provers might be used in their complex counterparts. Connection provers might be candidates for the core of future automated reasoning tools and artificial intelligence experiments.

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