Clause Learning and New Bounds for Graph Coloring

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Abstract. Graph coloring is a major component of numerous allocation and scheduling problems.
We introduce a hybrid CP/SAT approach to graph coloring based on exploring Zykov's tree: for two non-neighbors, either they take a different color and there might as well be an edge between them, or they take the same color and we might as well merge them. Branching on whether two neighbors get the same color yields a symmetry-free tree with complete graphs as leaves, which correspond to colorings of the original graph.
We introduce a new lower bound for this problem based on Mycielskian graphs; a method to produce a clausal explanation of this bound for use in a CDCL algorithm; and a branching heuristic emulating Brelaz on the Zykov tree.
The combination of these techniques in both a branch-and-bound and in a bottom-up search outperforms Dsatur and other SAT-based approaches on standard benchmarks both for finding upper bounds and for proving lower bounds.

1 Introduction

A *coloring* of a graph is a labeling of its vertices such that adjacent vertices have distinct labels. Let a labeling of the graph $G = (V, E)$ be a mapping from its set of vertices V to the integers. A labeling c such that $c(v) \neq c(u)$ for every edge $(uv) \in E$ is a coloring of G, and its cardinality is $|\{c(v) \mid v \in V\}|$. The *chromatic number* $\chi(G)$ of a graph G is the cardinality of its smallest coloring.

The problem of finding a minimum coloring of a graph is NP-hard, but has numerous applications. For instance when allocating frequencies, devices on nearby locations should not be assigned the same frequency to avoid interferences. The chromatic number of this distance-induced graph is therefore the minimum span of frequencies that is required.

One of the oldest and most successful technique for coloring a graph is Brelaz' *Dsatur* algorithm [1]: when branching, the vertex with highest *degree of saturation* is chosen and colored with the lexicographically least candidate. The degree of saturation of a vertex v is the number of assigned colors within its neighborhood $N_G(v)$ in G. In case of a tie, the vertex with largest number of uncolored neighbors is chosen among the tied vertices. This heuristic is often

used within a branch-and-bound algorithm with one variable per vertex whose domain is the set of possible colors. The lower bound usually used in those algorithms is not satisfactory. The standard approach is to use an approximation of the clique number $\omega(G)$ of the graph G (e.g., the size of a maximal clique) since $\omega(G) \leq \chi(G)$. However, this bound offers little guarantee, e.g. triangle-free graphs can have arbitrarily large chromatic number [12]. Moreover, within the search tree explored using Brelaz' heuristic, the clique has to be found only among vertices with degree of saturation equal to the number of colors in the current partial solution (i.e., adjacent to at least one vertex of every color used so far). Finally, this formulation exhibits value interchangeability [19]. One common way to break this symmetry is to arbitrarily color a clique, and never branch on colors larger than $k+1$ when extending a solution with k colors [18, 10, 20].

Satisfiability [9, 11] offers an attractive approach to coloring, in part because it is trivial to encode the problem. In satisfiability, we express problems with Boolean variables $\mathbf{X}$. We say that a literal l is either a variable x or its negation $\overline{x}$. Constraints are disjunctions of literals, written interchangably as sets of literals or as disjunctions, which are satisfied by an assignment if it assigns at least one literal to true. In order to encode graph coloring with satisfiability, one typically relies on *color* variables x_{vi}, where x_{vi} being true means vertex v takes color i. For every edge (uv), there is a binary clause $\overline{x}_{vi} \vee \overline{x}_{ui}$ for every color i. Then, if K is the maximum number of colors, then there is a clause $\bigvee_{1 \leq i \leq K} x_{ui}$. Refinements to this encoding include Van Gelder's log encoding versions, where x_{vj} is true if the j-th bit of the binary encoding of the color taken by vertex v is 1 [17]. However, the use of modern SAT solving techniques like restarting [3, 4] and clause learning [9] are not straightforward to combine with symmetry breaking such as that of van Hentenryck et al. [18]. They can only be easily combined with starting from an arbitrary coloring to a clique, but that is incomplete. The `color6` solver [20] uses symmetry breaking branching but forgoes restarting to maintain complete symmetry breaking.

On the other hand, the search tree induced by Zykov's deletion-contraction recurrence [21] has no color symmetry and using the clique number as lower bound is easier and more powerful than in the color variable formulation.

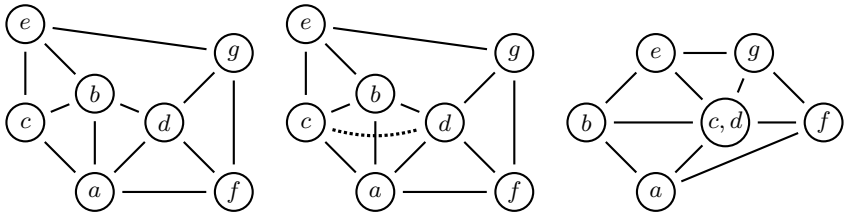
Let $G/(uv)$ be the graph obtained by *contracting* u and v: the two vertices are identified to a single vertex $r(u) = r(v) = u$, every edge (vw) is replaced by $(r(v)w)$ and self edges are discarded. Conversely, let $G + (uv)$ be the graph obtained by adding the edge (uv). The Zykov reccurrence is thus:

$$\chi(G) = \min\{\chi(G/(uv)), \chi(G + (uv))\} \tag{1}$$

Indeed, given a minimum coloring of G, either the vertices u and v have distinct colors and therefore it is also a coloring of $G + (uv)$, or they have the same color and it is a coloring of $G/(uv)$.

Example 1. Figure 1 illustrates the Zykov reccurrence. From the graph G in Figure 1a, we obtain the graph $G + (cd)$ shown in Figure 1b by adding the edge

(cd) and the graph $G/(cd)$ shown in Figure 1c. One of these two graphs has the same chromatic number as G.



(a) G (b) $G + (cd)$ (c) $G/(cd)$

Fig. 1: Zykov reccurrence

This branching scheme was successfully used in a branch-and-price approach to coloring [10]. In the context of satisfiability, Schaafsma et al. showed that a clause encoding of Zykov formulation is not efficient [14]. For every non-edge (uv), the *edge* variable e_{uv} stands for the decision of contracting the vertices ($e_{uv} = 1$), or adding the edge ($e_{uv} = 0$). A difficulty is that a cubic number of clauses are required, three for every triplet u, v, w, in order to forbid that exactly two of the variables e_{uv}, e_{uw} and e_{vw} are true. This encoding proved too heavy and as a result less efficient than the formulations using color variables. However, Schaafsma et al. introduced a novel and clever way of taking advantage of Zykov's idea: when learning a clause involving color variables, one can compactly encode all symmetric clauses using a single clause that only uses edge variables and propagates the same as if all the symmetric clauses were present.

In this work, we propose a constraint programming formulation of coloring in section 2 that also uses the Zykov branching scheme. We use the idea of integrating constraint programming into clause learning satisfiability solvers by simply having each propagator label each pruning or failure by a clausal *reason* or *explanation* [6, 13] to alleviate the cost of keeping the edge variables consistent (section 2.1) and to integrate a lower bound based on either cliques (section 2.2) or a more general bound based on Mycielskians (section 2.3). Together with effective branching heuristics (section 2.4) and search strategies that emphasize either upper or lower bounds (section 2.5), we get a solver that clearly outperforms the state of the art in satisfiability-based coloring (section 3).

2 Clause-learning Approach

In our approach, similar to that Schaafsma et al., we use a model which leads to the exploration of the tree resulting from application of the Zykov recurrence. We have one Boolean variable e_{uv} for each non-edge of the input graph, that is for every $(uv) \notin E$. When e_{uv} is true, the vertices v and u are contracted, hence

assigned the same color, and are separated otherwise, hence assigned different colors. We somewhat abuse notation in the sequel and write clauses using variables e_{uv} even when $(uv) \in E$ and assume that the variable is set to false at the root of the search tree.

With every (partial) assignment A to the edge variables, we can associate a graph G_A. For the empty assignment, we have $G_\emptyset = G$. For non-empty assignments it is the graph that results from contracting all vertices u, v of G for which A contains e_{uv} and adding an edge between all pairs of vertices u, v of G for which A contains $\overline{e}_{uv}$. When e_{uv} and e_{vw} are both true, this means that we contract u and v and then contract w and $r(v)$ and similarly for false literals. The operation of contracting vertices is associative and commutative, so we get the same graph G_A regardless of the order in which we process the literals in A.

The property of having the same color is transitive, so if e_{uv} and e_{vw} are true, then so is e_{uw}. Similarly, if e_{uv} is true and e_{vw} is false, then e_{uw} must also be false. We enforce this using the constraint

$$\textsc{Triangle}(\{e_{uv} \mid (uv) \notin E\}) \tag{2}$$

We can enforce GAC on this constraint using a decomposition of size $O(|V|^3)$:

$$(\overline{e}_{uv} \vee \overline{e}_{vw} \vee e_{uw}) \;\; \forall \text{ distinct } u, v, w \in V \tag{3}$$

Enforcing unit propagation on this decomposition therefore takes $O(|V|^3)$ time, amortized over a branch of the search tree. In our implementation, we have opted instead for a dedicated propagator for this, described in section 2.1, whose complexity over a branch is only $O(|V|^2)$.

The model also includes a constraint Coloring which is satisfied by any assignment that corresponds to a coloring with fewer than k colors.

$$\textsc{Coloring}(\{e_{uv} \mid (uv) \notin E\}, k) \tag{4}$$

This constraint is clearly NP-hard. We describe two incomplete propagators for it in sections 2.2 and 2.3. The first computes either the well known clique lower bound (section 2.2) and the second a novel, stronger, bound (section 2.3). If that bound meets or exceeds k, the propagator fails and produces an explanation. Neither of these bounds is cheap to compute, hence the propagator runs at a lower priority than unit propagation and the Triangle constraint.

Although we have experimented with pruning in this propagator, the pruning rules we have found tend to be ineffective, in the sense that they generate very little pruning, barely reduce the overall search effort, and increase the overall runtime.

Discussion. Clearly, our approach is closely related to that of Schaafsma et al. However, there are some important differences. First, since we do not need

the color variables to compute the size of the coloring, we completely eliminate the need for the clause rewriting scheme that they implement and get color symmetry-free search with no additional effort. In addition, since we our model uses a CP/SAT hybrid, we can use a constraint to compute a lower bound at each node, thus avoiding a potentially large number of conflicts.

The approach of Schaafsma et al. does not enforce triangle consistency except through the color variables (so that $X_v = X_u \iff e_{uv}$). In contrast, the triangle propagator maintains GAC on this constraint, without having to encode channeling between the edge variables and the color variables.

The main drawback of this model is that we need a large number of variables. This is especially problematic for large, sparse graphs, where the number of non-edges is quadratic in the number of vertices and significantly larger than the number of edges. Indeed, in 4 of the 125 instances we used in our experimental evaluation, our solver exceeded the memory limit.

The approach of Schaafsma et al. does not have the same limitation, as they introduce variables only when they are needed to rewrite a learnt clause. It is possible that this approach of lazily introducing variables can be adapted to our model, but this, as well as other ways of reducing the memory requirements, remains future work.

2.1 Triangle consistency propagation

The propagator for the TRIANGLE constraints works as follows: for each vertex v, we keep a bag $b(v)$ to which it belongs. Initially, $b(v) = \{v\}$ for all v. When we set e_{uv} to true, we set $e_{u'v'}$ to true for all $v' \in b(v), u' \in b(u)$. We also set $e_{u'v'}$ to false for all $v' \in b(v)$ and $u' \in N(b(u) \setminus N(b(v))$.[3] Finally, we set $B = b(u) \cup b(v)$ and update $b(v') = B$ for all $v' \in B$. In the case where we set e_{uv} to false, we set $e_{u'v'}$ to false for all $v' \in b(v), u' \in b(u)$.

A small but important optimization is that if the propagator is invoked for e_{uv} becoming true (resp. false) but u and v are already in the same bag (resp. already separated) then it does nothing. This ensures that it touches each non-edge exactly once, hence its complexity is quadratic over an entire branch. This is also optimal, since in the worst case every non-edge must be set either as a decision or by propagation.

This propagator uses the clauses (3) as explanations. The mapping from actions that it performs to explanations is fairly straightforward, using the vertices involved in the literal that woke the propagator as "pivots". For example, if $b(v) = \{v, v'\}$, $b(u) = \{u, u'\}$ and it is woken on the literal e_{uv}, it sets $e_{uv'}$ using $(\overline{e}_{vv'} \vee \overline{e}_{uv} \vee e_{uv'})$ as the reason and then $e_{u'v'}$ using $(\overline{e}_{uv'} \vee \overline{e}_{uu'} \vee e_{u'v'})$.

2.2 Clique-based lower bound.

As we already discussed, an important advantage of the edge-variable based model is that computing a lower bound for the current subproblem is as easy as

[3] We abuse the neighborhood notation and write $N(S)$ for $\bigcup_{u \in S} N(u)$.

for the entire problem. For example, if the partial assignment in the current node is A, the clique number of the graph G_A is a lower bound for the subproblem.

In order to find a large clique we use the following greedy algorithm. Let o be an ordering of the vertices, so we visit all vertices in the order $v_{o_1}, \ldots, v_{o_n}$. We maintain an initially empty list of cliques. For each vertex, we add to all the cliques which admit it and if no clique admits it we put it in a new singleton clique. When this finishes, we iterate over the vertices one more time and add them to all cliques which admit them, because in the first pass a vertex v was not evaluated against cliques which were created after we processed v. We then pick the largest among these cliques as our lower bound.

If the lower bound meets or exceeds the upper bound k, the propagator reports a conflict. We construct a clausal conflict as follows: each vertex v of the current graph is the result of the contraction of 1 or more vertices of the original graph. In keeping with the notation for the triangle consistency propagator, we call this the *bag* $b(v)$. We arbitrarily pick one vertex $r(v)$ from the bag of each vertex v in the largest clique C, and set the explanation to

$$\bigvee_{v,u \in C} e_{r(v)r(u)} \tag{5}$$

We have experimented with producing explanations with mixed-sign literals and found that they tend to be much shorter and speed up search in terms of number of conflicts per second, but significantly increase the overall effort required, both in runtime and number of conflicts.

Preprocessing and vertex ordering. We tried a few different heuristics for ordering the vertices of the graph, including the inverse of the degeneracy order [7], which tends to produce large cliques [2, 5]. However, we found that it works best to sort the vertices in order of decreasing bag size.

Lin et al [8] recently proposed a reduction rule for graph coloring instances, which allowed them to reduce the size of large, sparse graphs.

Proposition 1 ([8]). *Let G be a graph with $\chi(G) \geq k$ and let I be an independent set of G such that for all $v \in I$, $d(v) \leq k$. Then, $k-1 \leq \chi(G \setminus I) \leq \chi(G)$ and if $\chi(G \setminus I) = k-1$ then $\chi(G) = k$.*

The rule of proposition 1 can be used with any lower bound and applied iteratively until no more reduction is possible. Besides the obvious advantage of producing a smaller instance, this reduction also helps improve the lower bound found by a heuristic maximal clique algorithm. The reason is that whatever heuristic we use for finding a maximal clique may make a suboptimal choice and this preprocessing step removes some obviously suboptimal choices from consideration.

We have used this result for preprocessing, as Lin et al. did, but observed very little benefit in our instance set, which comprises smaller and denser graphs than the one that they used. We also used it, however, to improve the ordering

for the greedy algorithm by placing such vertices at the end of the ordering. As we will show in section 3, this has a small but measurable impact.

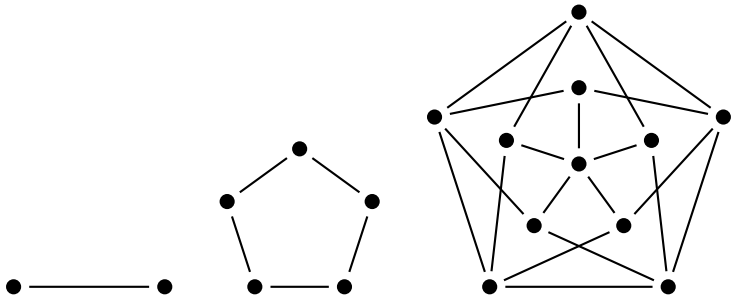
2.3 Mycielski-based Bound

Although being a useful bound in practice, the clique number is both hard to compute and gives no guarantees on the quality of the bound. We propose here a new lower bound inspired by *Mycielskian graph*.

Definition 1 (Mycielskian graph [12]). *The Mycielskian graph $\mu(G)$=($\mu(V)$,$\mu(E)$) of G =(V,E) is defined as follows:*

- *$\mu(V)$ contains every vertex in V, and $|V|+1$ additional vertices, constituted of a set $U = \{u_i \mid v_i \in V\}$ and another distinct vertex w.*
- *For every edge $v_iv_j \in E$, $\mu(E)$ contains v_iv_j, v_iu_j and u_iv_j. Moreover, it contains all the edges between U and w.*

The Mycielskian $\mu(G)$ of a graph G, has the same clique number, however its chromatic number is $\chi(G) + 1$. Indeed, consider a coloring of $\mu(G)$. For any vertex $v_i \in V$, we have $N(v_i) \subseteq N(u_i)$, and therefore we can safely use the same color v_i as for u_i. If follows that at least $\chi(G)$ colors are required for the vertices in U, and since $N(w) = U$, then w requires a $\chi(G) + 1$-th color. Mycielski introduced these graphs to demonstrate that triangle-free graphs can have arbitrarilly large chromatic numbers, hence the clique number does not approximate the chromatic number.



(a) M_2 (b) M_3 (c) M_4

Fig. 2: A 2-clique $M_2 = \mu(\emptyset)$, its Mycielskians $M_3 = \mu(M_2)$ and $M_4 = \mu(M_3)$

The principle of our bound is a greedy procedure that can discover embedded "pseudo" Mycielskians. Indeed, the class of embedded graphs that we look for is significantly broader than set of "pure" Mycielskians $\{M_2, M_3, M_4, \ldots\}$. First, we look for a partial subgraph. Therefore, trivially, Mycielskians with extra edges also provide valid lower bounds. Moreover, we use as starting point

a (potentially large) clique. Finally, the method we propose can also find Mycielskians modulo some vertex contractions. Clearly, those are also valid lower bounds since contracting vertices is equivalent to adding equality constraints to the problem.

Let $N_G(v)$ be the neighborhood of v in the graph G. Suppose that we have a partial subgraph $H = (V_H, E_H)$ of G such that $\chi(H) \geq k$. This can be for example a clique of size k. We define

$$S_v = \{u \mid N_H(v) \subseteq N_G(u)\} \tag{6}$$

Suppose that there exists a vertex w with at least one neighbor in every set S_v:

$$w \in \cap_{v \in V_H} N_G(S_v) \tag{7}$$

and let $u(v)$ be any element of S_v such that $u(v) \in N_G(w)$ and $U = \{u(v) \mid v \in V\}$, then:

Lemma 1. *The graph*

$$H' = (V \cup U \cup \{w\}, E \cup \bigcup_{v \in V} N_H(v) \times u(v) \cup \bigcup_{u \in U} \{(u, w)\})$$

is such that $\chi(H') \geq k + 1$.

Proof. The proof follows from the facts that H' is the Mycielskian graph of H possibly with contracted vertices, and is embedded in G.

Suppose first that, for every $v \in V$ we have $u(v) \neq v$ and $w \notin V$. Then it is easy to see that $H' = \mu(H)$ by using $u(v_i)$ for the vertex u_i, and w for itself, in Definition 1.

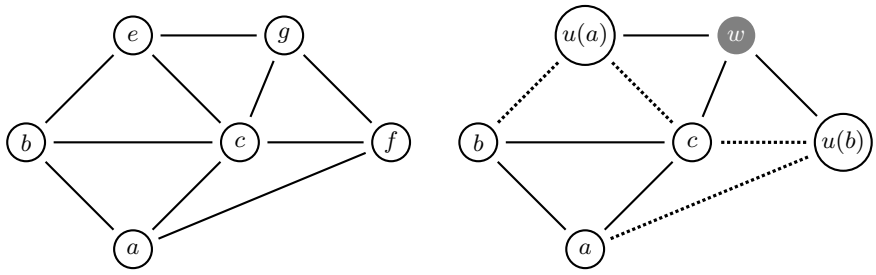
Suppose now that $H' \neq \mu(H)$. This can only be because either:

- For some vertex v_i of H, we have $u(v_i) = v_i$. In this case, consider the graph $\mu(H)$ and contract u_i and v_i. The resulting graph $\mu(H)/(u_i v_i)$ has a chromatic number at least as high as $\mu(H)$. However, it is isomorphic to H'.
- The vertex w is the vertex v_i from the original subgraph H. Here again contracting v_i and w in $\mu(H)$ yields H'.

Notice that there is not a third case where w is taken among U since, for any $v \in V_H$, we have $u(v) \notin \cap_{v \in V_H} N_G(S_v)$ because $u(v)$ is not a neighbor of itself.

Finally, it is easy to see that H' is embedded in G since the edges added to H' are all edges of G □

Example 2. Figure 3a shows the graph $G/(cd)$ obtained by contracting vertices c and d in the graph G of Figure 1. Let H be the clique $\{a, b, c\}$. We have $S_a = \{a, e\}$, $S_b = \{b, f\}$ and $S_c = \{c\}$. Furthermore, $N_G(\{a, e\}) \cap N_G(\{b, f\}) \cap N_G(\{c\}) = \{b, c, g\} \cap \{a, e, c, g\} \cap \{a, b, e, g, f\} = \{g\}$, from which we can conclude that this graph has chromatic number at least 4. As shown in Figure 3b, when



(a) $H = G/(cd)$ (b) Trace of Algorithm 1 on H

Fig. 3: Embedded Mycielski

called with $H = \{a, b, c\}$ Algorithm 1 will extend it with a first layer $U = \{e, c, f\}$ and an extra vertex $w = g$. Notice that the graph obtained by adding the edge (cd) has a 4-clique (see Figure 1). Therefore, the graph G in Figure 1a also has a chromatic number of at least 4.

Algorithm 1 greedily extends a partial subgraph $H = (V_H, E_H)$ of the graph G (with $\chi(H) \geq k$) into a larger partial subgraph $H' = (V'_H, E'_H)$, following the above principles. As long as this succeeds, in the outermost loop, we replace H by H' and iterate. The computed bound k is equal to $\chi(H)$ plus the number of successful iterations.

We compute the sets S_v (Equation 6) and the set W of nodes with at least one neighbor in every S_v in Loop 1. Then, if it is possible to extend H (Line 4), we compute the pseudo Mycielskian (V'_H, E'_H) as shown in Lemma 1 and replaces H with it in Line 5 before starting another iteration.

Complexity. One iteration of Algorithm 1 requires $O(|V_H| \times |V|)$ bitset operations (Line 2 is 1 'AND' operation and Line 3 is $O(|V|)$ 'OR' operations and 1 'AND'). The second part of the loop, starting from Line 4, runs in $O(|V_H|^2)$ time. Typically, the number of iterations is very small. In the worst case, it cannot be larger than $\log |V|$ since the number of vertices in H is (more than) doubled at each iteration. It follows that Loop 1 is executed at most $2|V|$ times, and therefore, the worst case time complexity is $O(|V|^2)$ bitset operations (hence $O(|V|^3)$ time).

Explanation. Similarly to the clique based lower bound, the explanations that we produce here correspond to the set of all edges in the graph H:

$$\bigvee_{(v,u) \in E_H} e_{uv} \tag{8}$$

Adaptive application of the Mycielskian bound. In our experiments, we found that trying to find a Mycielskian subgraph in every node of the search tree

Algorithm 1: MycielskiBound$(k, H = (V_H, E_H), G = (V, E))$

```
while |V_H| < |V| do
    W ← V;
    ∀v ∈ V_H  S_v ← {v};
1   foreach v ∈ V_H do
        foreach u ∈ V do
2           if N_H(v) ⊆ N_G(u) then  S_v ← S_v ∪ {u} ;
3       W ← W ∩ N_G(S_v);
4   if W ≠ ∅ then
        k ← k + 1;
        (V'_H, E'_H) ← (V_H, E_H);
        w ← any element of W;
        foreach v ∈ V_H do
            V'_H ← V'_H ∪ { any element of (N_G(w) ∩ S_v)};
            E'_H ← E'_H ∪ {(wu)} ∪ {u × N_H(v)};
5       (V_H, E_H) ← (V'_H, E'_H);
    else break;
    return k;
```

was too expensive and did not pay off in terms of total runtime. Therefore, we adapted a heuristic proposed by Stergiou [15] which allows us to apply this stronger reasoning less often. In particular, we only compute the clique lower bound by default. But everytime there is a conflict, whether by unit propagation or by bound computation, we compute the Mycielskian lower bound in the next node. If that causes a conflict, we keep computing this bound until we backtrack to a point where even the stronger bound does not detect a bound violation. This has the effect that we compute the cheaper clique lower bound most of the time, but learn clauses based on the stronger bound.

2.4 Branching heuristic

Brelaz' branching heuristic remains extremely competitive for finding good colorings, as evidenced by the performance of `Dsatur` in our experimental evaluation (section 3). Moreover, Schaafsma et al. observed that branching on color variables was significantly better than branching on edge variables.

But adding the color variables is not really desirable. First, it adds the overhead of propagating the reified equality constraints. Second, adequately and efficiently channeling them with edge variables is not trivial, as witnessed by the fact that symmetry breaking constraints can improve the propagation back to edge variables. So it would be preferable to get the benefit of the more effective branching heuristic without needing to introduce color variables.

In order to get behavior similar to that of Brelaz' heuristic in the edge variable model, we proceed as follows: we pick a maximal clique C in the current graph. We pick the vertex v that maximises $|N(v) \cap C|$, breaking ties by highest $|N(v) \setminus C|$, and an arbitrary vertex $u \in N(v) \cap C$ [4]. We then set e_{uv} to true. This uses the current maximal clique to implicitly construct a coloring and uses that to choose the next vertex to color as Brelaz' heuristic does. If the assignments e_{uv} are refuted for all $u \in C$, then v is adjacent to all vertices in C and so $C \cup \{v\}$ is a larger clique, which corresponds to using a new color in Brelaz' heuristic.

This branching strategy can be more flexible than committing to a coloring by assigning the color variables. For example, unit propagation on learned clauses as we exlore a branch of the search tree can make it so that the maximal clique C' at some deep level is not an extension of the maximal clique C at the root of the tree, i.e., $C \not\subseteq C'$. The Brelaz heuristic on the color variables commits to using C at the root, hence cannot take advantage of the information that C' is a larger clique. The modification that we present here achieves this.

2.5 Solution strategies

Previous satisfiability-based approaches to coloring have mostly ignored the optimization problem of finding an optimal coloring of a graph and instead attack the decision problem of whether a graph is colorable with k colors. In our setting, we have the flexibility to do both. In particular, we implemented two search strategies: branch-and-bound and bottom-up. The former uses a single instance of a solver, finds a solution and then tightens the upper bound in the Coloring constraint and continues searching. This is similar to the top-down approach one would use when solving a series of decision problems, starting from a heuristic upper bound and decreasing that until we generate an unsatisfiable instance, in which case we have identified the optimum. The advantage of the branch-and-bound approach is that it does not discard accumulated information between solution: learned clauses and heuristic scores for variables. Moreover, it more closely resembles the typical approach used in constraint programming systems.

The other approach we implemented is bottom-up: start from a lower bound (such as those described in section 2.2 or 2.3) and keep increasing until we find a satisfiable instance, which gives the optimum. This has none of the advantages of the branch-and-bound approach, as it is not safe to reuse clauses from a more constrained problem in one that is less constrained. Moreover, it cannot generate upper bounds before it finds the optimum. But it gains from the fact that the more constrained problems it solves may be easier. One particular behavior we have observed is that sometimes the lower bound computed at the root coincides with the optimum and finding is quite easy with the bottom-up strategy, but finding that solution with branch-and-bound can be very hard.

[4] We assume the graph is connected, otherwise u may not always exist.

3 Experimental Evaluation

We implemented several variations of our approach using MiniCSP[5] as the underlying CDCL CSP solver, and retained two, one for each of the solution strategies described in section 2.5.[6] The former, `cdcl`, is a branch-and-bound algorithm, using Brelaz branching. The latter, `cdcl`↑, is a bottom-up algorithm, using VSIDS. In both cases, we use the adaptive application of the Mycielskian bound, as explained in section 2.3. When computing the Mycielskian bound, we apply Algorithm 1 on all of the maximal cliques, and keep the best outcome.

We compared with the state-of-art SAT-based solver `color6` [20], a very efficient clause-learning algorithm for graph coloring proposed recently by Zhou et al. Similarly to our approach, it is based on a SAT solver (namely `zChaff`), however, it uses the color-based formulation. It was shown to outperform the state of the art on many instances. As `color6` solves satisfiability instances only (testing whether a coloring with a specific number of colors exists), we implemented a branch-and-bound wrapper on top of it, denoted `color6`, as well as well as a wrapper that implements the bottom-up strategy, denoted `color6`↑. We used the lower and upper bounds computed by our approach (respectively the maximal clique algorithm described in section 2.2 and a greedy run of Brelaz) as initial bounds for `color6` and `color6`↑.

Moreover, we also compared with an implementation of `Dsatur` by Trick, and an integer programming formulation in `CPLEX`. The model we used for `CPLEX` is the trivial one using binary color variables (one for each vertex and each color), and one binary inequality per edge. However, observe that `CPLEX` actually computes maximal cliques in its preprocessing, so providing it with clique inequalities would have been useless. Moreover, we initialized the upper bound with the same method as for `color6`, and also arbitrarily fixed the colors of one maximal clique in order to break symmetries.

Unfortunately, we could not compare our method to the method of Schaafsma et al. (`Minicolor`) directly. Indeed, its implementation, generously provided by the authors, is difficult to use in the type of extensive experiments of the type we performed. Firstly, the algorithm is restricted to instances with at most 32 colors. Secondly it solves the satisfiability problem $\chi(G) \leq K$ and uses a file converter. Finally, the changes made to `Minisat`'s code do not seem to be robust and we experienced several occurrences of assertion failures.

We used 125 benchmark instances from Trick's graph coloring webpage (`http://mat.gsia.cmu.edu/COLOR/color.html`) and described in the proceedings of the workshop COLOR02 [16]. In the subsequent tables, however, we omit 22 of these instances that were trivial for every approach we used (i.e., that solved by every method to optimality). Every method was run with a time limit of one hour and a memory limit of 3.5GB[7] on 4 nodes, each with 35 Intel Xeon CPU E5-2695 v4 2.10GHz cores running Linux Ubuntu 16.04.4.

[5] Sources available at: `https://bitbucket.org/gkatsi/minicsp`.
[6] Sources available at: `https://bitbucket.org/gkatsi/gc-cdcl/src/master/`.
[7] `cdcl` exceeded the memory limit on 4 instances, and `CPLEX` on 16 instances.

		cdcl			color6			CPLEX			Dsatur		
		opt	ub	lb	opt	ub	lb	opt	ub	lb	opt	ub	lb
DSJ	(14)	0.07	76.00	30.71	0.07	77.57	28.93	0.07	86.07	29.79	0.00	77.86	27.64
FullIns	(14)	1.00	6.79	6.79	0.21	6.79	5.14	0.86	6.93	6.36	0.00	6.79	4.86
Insertions	(11)	0.27	5.18	2.55	0.36	5.18	2.82	0.36	5.18	3.64	0.00	5.18	2.00
abb313GPI	(1)	1.00	9.00	9.00	0.00	14.00	8.00	0.00	14.00	8.00	0.00	10.00	6.00
ash	(3)	1.00	4.00	4.00	0.67	4.67	3.67	0.33	5.67	3.33	0.00	4.33	3.00
flat	(6)	0.00	73.83	11.67	0.00	74.33	10.67	0.00	79.67	10.67	0.00	74.83	9.67
fpsol2	(1)	1.00	65.00	65.00	0.00	65.00	59.00	1.00	65.00	65.00	1.00	65.00	65.00
inithx	(1)	1.00	54.00	54.00	0.00	54.00	43.00	1.00	54.00	54.00	1.00	54.00	54.00
latin_square	(1)	0.00	116.00	90.00	0.00	125.00	90.00	0.00	159.00	90.00	0.00	129.00	90.00
le450	(10)	0.50	15.20	13.00	0.10	15.60	13.00	0.30	19.10	13.00	0.20	16.00	11.70
miles	(5)	1.00	34.80	34.80	0.00	36.40	33.40	1.00	34.80	34.80	1.00	34.80	34.80
mug	(4)	1.00	4.00	4.00	1.00	4.00	4.00	1.00	4.00	4.00	0.00	4.00	3.00
myciel	(5)	1.00	6.00	6.00	0.80	6.00	4.80	0.60	6.00	5.00	0.00	6.00	2.00
qg	(4)	0.75	66.00	57.50	0.25	63.25	57.50	0.25	72.50	57.50	0.25	59.50	57.50
queen	(13)	0.46	12.08	10.85	0.00	15.92	10.62	0.38	12.46	10.77	0.23	12.00	10.62
school1	(1)	1.00	14.00	14.00	0.00	26.00	14.00	1.00	14.00	14.00	0.00	14.00	13.00
wap0	(8)	0.12	46.50	41.25	0.00	47.62	40.00	0.00	51.12	40.00	0.00	48.00	30.38
will199GPI	(1)	1.00	7.00	7.00	0.00	10.00	6.00	1.00	7.00	7.00	0.00	7.00	6.00

Table 1: Comparison with top-down methods (by classes of instances)

The results in Tables 1 and 2 are averaged over instances from the same class and the number of instances in each class is given next to the class name. We show the ratio of instances for which a proof of optimality was found ('opt'), as well as the average upper bound ('ub') and lower bound ('lb'), for every method. The best results for each criterion are highlighted using colors. Table 1 focuses on top-down methods. `cdcl` is better on all but three classes of instances: `Insertions`, `qg` (quasigroup) and `queen`. Moreover, it finds the same coloring as the other methods in the `Insertions` class, and computes strictly more proofs of optimality than other solvers in the the two other classes. Finally, on many classes it is strictly better than the second best solver (considering at least one criterion). Table 2 focuses on the two bottom-up methods. Here again there are far more classes where `cdcl`↑ is better than classes (such as `qg` again) where the opposite is true. Moreover, although `cdcl`↑ finds better lower bounds on two large classes (`DSJ` and `flat`) this does not translates to a higher proof ratio.

Table 3 shows results aggregated across all instances. We report the average ratio of instance proven optimal ('optimal') in the first column. Then in the second to the fifth columns, we report the arithmetic ('avg') and geometric averages ('gavg') for both the lower and upper bounds. Finally, we report the *mean normalised gap to the best upper bound*, and to the best lower bound. Let b (resp. w) be the value found by best (resp. worst) method. In the case of the lower bound, b will be the maximum, while it will be the minimum for the upper bound. The normalised gap $g(x)$ of the outcome x is:

$$g(x) = \begin{cases} 0 & \text{if } b = w \\ (b - x)/(b - w) & \text{otherwise} \end{cases}$$

		cdcl↑			color6↑		
		opt	ub	lb	opt	ub	lb
DSJ	(14)	0.07	86.93	33.79	0.07	86.93	35.79
FullIns	(14)	0.93	6.86	6.71	0.21	7.29	5.43
Insertions	(11)	0.36	5.36	4.27	0.36	5.36	4.09
abb313GPI	(1)	0.00	14.00	9.00	0.00	14.00	8.00
ash	(3)	1.00	4.00	4.00	0.67	4.67	3.67
flat	(6)	0.00	82.17	14.00	0.00	82.17	16.83
fpsol2	(1)	1.00	65.00	65.00	0.00	65.00	59.00
inithx	(1)	1.00	54.00	54.00	0.00	54.00	43.00
latin_square	(1)	0.00	159.00	90.00	0.00	159.00	90.00
le450	(10)	0.80	14.70	13.00	0.20	20.00	13.00
miles	(5)	1.00	34.80	34.80	0.00	36.40	33.40
mug	(4)	1.00	4.00	4.00	1.00	4.00	4.00
myciel	(5)	1.00	6.00	6.00	0.80	6.00	5.60
qg	(4)	0.25	72.50	57.50	0.75	66.00	57.50
queen	(13)	0.46	14.54	10.92	0.00	15.92	10.62
school1	(1)	1.00	14.00	14.00	1.00	14.00	14.00
wap0	(8)	0.12	50.88	41.25	0.00	51.12	40.00
will199GPI	(1)	1.00	7.00	7.00	0.00	10.00	6.00

Table 2: Comparison with bottom-up methods (by classes of instances)

A mean normalised gap of 0 (resp. 1) therefore indicates that the method systematically has the best (resp. worst) outcome.

Overall, the variants of `cdcl` are best for all criteria. `CPLEX` is third best for the number of optimality proofs. Although it requires a lot of memory, and is very poor in terms of solution quality, `CPLEX` often gives good lower bounds. This is not so surprising since the linear relaxation is quite potent on this formulation. For instance at the root node, since we fix the variables of a maximal clique, the lower bound from the linear relaxation can only be higher than that of our method. It should be noted, however, that in many cases it was not able to improve on the initial bounds provided to the model, even when memory was not an issue. `color6`↑ is second best for the lower bound, however, notice that the much larger mean normalised gap to the best lower bound than `cdcl`↑ indicates

method	optimal	ub		lb		gap (ub)	gap (lb)
	avg	gavg	avg	gavg	avg	avg	avg
`cdcl`	0.53398	15.247	30.107	10.790	18.689	0.0909	0.2254
`cdcl`↑	0.53398	16.248	33.427	11.846	19.427	0.4175	0.0740
`CPLEX`	0.41748	16.503	33.388	10.886	18.379	0.4014	0.2562
`color6`↑	0.23301	17.408	34.068	11.527	19.252	0.6408	0.2371
`color6`	0.19417	16.314	31.233	10.040	17.748	0.3201	0.4716
`Dsatur`	0.12621	15.506	30.495	8.754	16.524	0.1450	0.7248

Table 3: Comparison with the state of the art: global results

method	optimal	ub		lb		gap (ub)	gap (lb)
	avg	gavg	avg	gavg	avg	avg	avg
`cdcl`	0.53398	15.247	30.107	10.790	18.689	0.0909	0.2254
`cdcl`↑	0.53398	16.248	33.427	11.846	19.427	0.4175	0.0740
`cdcl`↑ $\setminus M$	0.51456	16.219	33.466	11.738	19.262	0.4175	0.0925
`cdcl`$\setminus M$	0.49515	15.308	30.126	10.364	18.272	0.0929	0.2764
`cdcl`$\setminus M, O$	0.47573	15.469	30.534	10.234	18.282	0.1273	0.2890
`cdcl`↑ $\setminus M, O$	0.45631	16.370	33.476	11.701	19.369	0.4563	0.0988
`cdcl`$\setminus M, O, L$	0.39806	15.521	30.524	10.034	18.184	0.1311	0.3602
`cdcl`↑ $\setminus M, O, L$	0.23301	17.861	34.476	10.724	18.738	0.6311	0.2808

Table 4: Factor analysis: global results

that it was often close but rarely better than our approach. Finally, `Dsatur`, even though extremely simple, is still a very good method to actually find small colorings and is a close second best for the upper bound.

Next, we tried to assess the impact of the new bounds, and of learning. To that purpose, we ran six variants. Let L denote the usage of clause learning, M the mycielskian-based lower bound and O the partition-based vertex ordering used to find maximal cliques, then $X \setminus S$ stands for the solver X where the options in S are turned off. The results reported in Table 4 clearly show the impact of each factor. There is an almost perfect correlation between turning off a feature, and moving down the ranking for any criterion. In particular, clause learning has clearly a very high impact as turning it off systematically and significantly degrades the performances on every criterion. Moreover, using the partition-based vertex ordering also has a very significant impact for such a simple technique. Finally the mycielskian-based lower bound also clearly helps. However, its impact on the upper bound is limited. For instance, with respect to `cdcl`$\setminus M$, it increases the proof ratio by 7.8% and the mean lower bound by 2.3%, but decreases the mean upper bound by only 0.3%.

4 Conclusions

We have presented a CP/SAT hybrid approach to graph coloring. The approach uses a new, sophisticated, lower bound that generalizes the clique bound and is inspired by Mycielskian graphs. We combined it with clause learning and effective primal heuristics for coloring to get a solver that in both its configurations outperforms the previous state of the art in satisfiability-based coloring, constraint programming based coloring, as well as a MIP model of the problem. The main disadvantage of the approach is that it requires one Boolean variable for each non-edge of the graph and hence cannot scale to large sparse graphs.

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