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Efficiently Explaining CSPs with Unsatisfiable Subset Optimization

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Abstract

We build on a recently proposed method for stepwise explaining the solutions to Constraint Satisfaction Problems (CSPs) in a human understandable way. An explanation here is a sequence of simple inference steps where simplicity is quantified by a cost function. Explanation generation algorithms rely on extracting Minimal Unsatisfiable Subsets (MUSs) of a derived unsatisfiable formula, exploiting a one-to-one correspondence between so-called *non-redundant explanations* and MUSs. However, MUS extraction algorithms do not guarantee subset minimality or optimality with respect to a given cost function. Therefore, we build on these formal foundations and address the main points of improvement, namely how to generate explanations *efficiently* that are provably *optimal* (with respect to the given cost metric). To this end, we developed (1) a hitting set-based algorithm for finding the optimal constrained unsatisfiable subsets; (2) a method for reusing relevant information across multiple algorithm calls; and (3) methods for exploiting domain-specific information to speed up the generation of explanation sequences. We have experimentally validated our algorithms on a large number of CSP problems. We found that our algorithms outperform the MUS approach in terms of *explanation quality* and *computational time* (on average up to 56 % faster than a standard MUS approach).

1. Introduction

Building on old ideas to explain domain-specific propagation performed by constraint solvers (Sqalli & Freuder, 1996; Freuder, Likitvivatanavong, & Wallace, 2001), we recently introduced a method that takes as input a *satisfiable* set of constraints and explains the solution finding process in a human understandable way (Bogaerts et al., 2020). Explanations in this work are sequences of simple inference steps that involve as few constraints and previously derived facts as possible. Each explanation step derives at least one new fact implied by a combination of constraints and previously derived facts.

The explanation steps of Bogaerts et al. (2020) are heuristically optimised with respect to a given cost function that should approximate human understandability, e.g. taking into account the number of constraints and facts considered, as well as an estimate of their cognitive complexity. For example, when evaluating explanations for logic grid puzzles, the given clues of the puzzle are considered more difficult than simpler reasoning tricks, that are present in all instances of such puzzles and therefore have a higher cost.

In practice, the explanation generation algorithms presented in Bogaerts et al. (2020) rely heavily on calls to *Minimal Unsatisfiable Subsets* (MUS) (Marques-Silva, 2010) of a derived unsatisfiable formula, exploiting a one-to-one correspondence between so-called *non-redundant explanations* and MUSs.

However, the algorithm of Bogaerts et al. (2020) has two main weaknesses. First, it provides *no guarantees on the quality* of the generated explanations due to internally relying on the computation of $\subseteq$-minimal unsatisfiable subsets, which are often suboptimal with respect to the given cost function. Second, it suffers from *performance problems*: the lack of optimality is partly overcome by calling a MUS algorithm on increasingly larger subsets of constraints for each candidate fact to explain. However, using multiple MUS calls per literal in each iteration quickly leads to efficiency problems, causing the explanation generation process to take several hours, even for simple puzzles designed to be solvable by humans.

Contributions In this paper, we tackle the limitations discussed above. We develop algorithms that aid explaining in Constraint Satisfaction Problems and improve the state of the-art in the following ways:

- We develop algorithms that compute (cost-)**Optimal** Unsatisfiable Subsets (from now on called OUSs) based on the well-known hitting-set duality which is also used to compute cardinality-minimal MUSs (Ignatiev et al., 2015; Saikko et al., 2016).

- We observe that in the explanation setting, many of the individual calls for MUSs (or OUSs) can actually be replaced by a single call that searches for an optimal unsatisfiable subset **among subsets satisfying certain structural constraints**. We formalize and generalize this observation by introducing the *Optimal **Constrained** Unsatisfiable Subsets (OCUS)* problem. We then show how $O(n^2)$ calls to MUS/OUS can be replaced by $O(n)$ calls to an OCUS oracle, where n denotes the number of facts to explain.

- We develop techniques for further **optimizing** the O(C)US algorithms, exploiting domain-specific information coming from the fact that we are in the *explanation-generation context*. Such optimizations include (i) the development of methods for **information re-use** between consecutive O(C)US calls; as well as (ii) an explanation-specific version of the OCUS algorithm.

- Finally, we extensively **evaluate** our approaches on a large number of CSP problems.

Paper Structure The rest of this paper is structured as follows. In Section 2, we discuss work related to efficiently computing unsatisfiable subsets. Section 3 introduces the theoretical foundations of our implicit hitting set approach. Section 4 motivates our work, and Section 5 introduces the OCUS problem and a hitting set-based algorithm for computing OCUSs. Then, in Section 6, we look at 2 other methods for computing the next best explanation in the explanation sequence. In Section 7 we present methods to improve the efficiency of our algorithms, e.g. by making them incremental or by using different methods to extract multiple correction subsets. Finally, in Section 8 we evaluate our approach on a large set of puzzle instances and conclude with some future perspectives.

Publication History This article is an extension of a previous paper presented at the International Joint Conference on Artificial Intelligence 2021 (Gamba, Bogaerts, & Guns, 2021). The current paper extends the previous paper with more detailed examples, extensive experiments on a large data set of puzzles, as well as the novel `Explain-One-Step-OCUS-Split` algorithm for efficiently computing explanations.

2. Related Work

In the last few years, driven by the increasing many successes in Artificial Intelligence (AI), there has been a growing need for **eXplainable Artificial Intelligence (XAI)** (Miller, 2019). In the research community, this need manifests itself through the emergence of (interdisciplinary) workshops and conferences on this topic (Miller et al., 2019; Hildebrandt et al., 2020), as well as American and European incentives to stimulate research in the area (Gunning, 2017; Hamon et al., 2020; FET, 2019).

While the main focus of XAI research has been on explaining black-box machine learning systems (Lundberg & Lee, 2017; Guidotti et al., 2018; Ignatiev et al., 2019). Model-based systems, which are typically considered more transparent, are also in need of explanation mechanisms. For instance, Vassiliades, Bassiliades, and Patkos (2021) surveys the important methods that use argumentation (Modgil et al., 2013) to provide explainability in AI, with for example applications in medical diagnosis (Obeid et al., 2019). Abstract argumentation frameworks introduce an abstract formalism to explain argumentative acceptance (Šešelja & Straßer, 2013; Liao & Van Der Torre, 2020; Ulbricht & Wallner, 2021). Description Logics (Baader, Horrocks, & Sattler, 2004) on the other hand, aim at explaining logical proofs (Alrabbaa et al., 2021; Koopmann, 2021), i.e 'why does phi follow from psi?'.

The main focus of our work lies in providing explainable agency (Langley, Meadows, Sridharan, & Choi, 2017) to Constraint Programming (CP) (Rossi, van Beek, & Walsh, 2006) and Boolean Satisfiability (SAT) (Biere et al., 2009) systems. Advances in solving, as well as hardware improvements, allow for such systems now easily consider millions of alternatives in short amounts of time. Because of this complexity, the question arises of how to generate human-interpretable explanations of the conclusions they make. Explanations have seen a rejuvenation in various subdomains of constraint reasoning (Fox et al., 2017; Čyras et al., 2019; Chakraborti et al., 2017; Bogaerts et al., 2020). In the CP and SAT communities, there has been a strong focus on explaining *unsatisfiable* problem instances (Junker, 2001), for example by extracting a minimal unsatisfiable subset (MUS) from the problem constraints (Liffiton & Sakallah, 2008).

We have recently introduced *step-wise explanations* (Bogaerts et al., 2020) to explain the solution of satisfiable instances, exploiting a one-to-one correspondence between so-called non-redundant explanations and MUSs of a derived program. The focus of Bogaerts et al. (2020) was on explaining Zebra puzzles; building on this work, Espasa, Gent, Hoffmann, Jefferson, and Lynch (2021) investigated interpretable explanations using MUSs for a wide range of puzzles. Our current work is motivated by a concrete algorithmic need: to generate these explanations *efficiently*, we need algorithms that can find MUSs that are optimal with respect to a given cost function, where the cost function approximates human-understandability of the corresponding explanation step.

The closest related work can be found in the literature on generating or enumerating MUSs (Lynce & Silva, 2004; Bacchus & Katsirelos, 2016, 2015; Liffiton, Previti, Malik, & Marques-Silva, 2016). Various techniques are used to find MUSs, including manipulation of resolution proofs produced by SAT solvers (Goldberg & Novikov, 2003; Gershman et al., 2008; Dershowitz et al., 2006), incremental solving to enable/disable clauses and branch-and-bound search (Oh et al., 2004), BDD-manipulation methods (Huang, 2005). Some methods rely on *seed-shrink* algorithms (Bendík & Černá, 2020a, 2020b) which repeatedly start from unsatisfiable *seed* (an unsatisfiable core) and *shrink* the seed to a MUS. Other methods work by means of translation into a so-called Quantified `MaxSAT` (Ignatiev, Janota, & Marques-Silva, 2016), a field that combines the expressiveness of Quantified Boolean Formulas (QBF) (Kleine Büning & Bubeck, 2009) with techniques from Maximum Satisfiability (`MaxSAT`) (Li & Manyà, 2021), or by exploiting the so-called hitting set duality (Ignatiev et al., 2015). To the best of our knowledge, only few works have considered *optimizing* MUSs: the only criterion considered so far is cardinality-minimality (Lynce & Silva, 2004; Ignatiev et al., 2015).

An *abstract* framework for describing hitting set–based algorithms, including optimization, has been developed by Saikko et al. (2016). While our approach can be seen to fit within the framework, the terminology is focused on `MaxSAT` rather than MUS and would complicate our exposition.

3. Background

In this section, we introduce the terminology and concepts related to explanation generation. We present all methods using propositional logic but our results easily generalize to richer languages, such as constraint languages, as long as the semantics is given in terms of a satisfaction relation between expressions in the language and possible states of affairs (assignments of values to variables).

Let Σ be a set of propositional symbols, also called *atoms*; this set is implicit in the rest of the paper. A *literal* is an atom p or its negation $\neg p$. A clause is a disjunction of literals, i.e. $c_1 = x_1 \vee \neg x_2$. A formula $\mathcal{F}$ in conjunctive normal form (CNF) is a conjunction of clauses. Slightly abusing notation, a clause is also viewed as a set of literals and a formula as a set of clauses.

A (partial) interpretation $\mathcal{I}$ is a consistent (not containing both p and $\neg p$) set of literals. Satisfaction of a formula $\mathcal{F}$ by an interpretation is defined as usual (Biere et al., 2009): an interpretation $\mathcal{I}$ *satisfies* $\mathcal{F}$ if $\mathcal{I}$ contains at least one literal from each clause in $\mathcal{F}$. A *model* of $\mathcal{F}$ is an interpretation that satisfies $\mathcal{F}$; $\mathcal{F}$ is said to be *unsatisfiable* if it has no models. An interpretation that satisfies $\mathcal{F}$ is also called a *model* of $\mathcal{F}$. A formula $\mathcal{F}$ is *satisfiable* if it has at least one model and *unsatisfiable* otherwise.

A literal l is a *consequence* of a formula $\mathcal{F}$ if l holds in all $\mathcal{F}$'s models. The *maximal consequence* of a formula $\mathcal{F}$, denotes a consequence that holds in all models. If I is a set of literals, we write $\overline{I}$ for the set of negated literals $\{\neg\ell \mid \ell \in I\}$.

Example 1. *Let $\mathcal{C}_1$ be the CNF formula over atoms x_1, x_2, x_3 with the following four clauses:*

$$c_1 := \neg x_1 \vee \neg x_2 \vee x_3 \qquad c_2 := \neg x_1 \vee x_2 \vee x_3 \qquad c_3 := x_1 \qquad c_4 := \neg x_2 \vee \neg x_3$$

An example of an interpretation is $\{\neg x_2, x_3\}$. *The* maximal consequence *of formula* $\mathcal{C}$ *is* $\{x_1, \neg x_2, x_3\}$.

In the following, we introduce key properties on unsatisfiable subsets on which we build our algorithms.

Definition 1. *A* Minimal Unsatisfiable Subset *(MUS) of* $\mathcal{F}$ *is an unsatisfiable subset* $\mathcal{S}$ *of* $\mathcal{F}$ *for which every strict subset of* $\mathcal{S}$ *is satisfiable.* $MUSs(\mathcal{F})$ *denotes the set of MUSs of* $\mathcal{F}$.

Definition 2. *A set* $\mathcal{S} \subseteq \mathcal{F}$ *is a* Maximal Satisfiable Subset *(MSS) of* $\mathcal{F}$ *if* $\mathcal{S}$ *is satisfiable and for all* $\mathcal{S}'$ *with* $\mathcal{S} \subsetneq \mathcal{S}' \subseteq \mathcal{F}$, $\mathcal{S}'$ *is unsatisfiable.*

Definition 3. *A set* $\mathcal{S} \subseteq \mathcal{F}$ *is a* correction subset *of* $\mathcal{F}$ *if* $\mathcal{F} \setminus \mathcal{S}$ *is satisfiable. Such a* $\mathcal{S}$ *is a* minimal correction subset *(MCS) of* $\mathcal{F}$ *if no strict subset of* $\mathcal{S}$ *is also a correction subset.* $MCSs(\mathcal{F})$ *denotes the set of minimal correction subsets of* $\mathcal{F}$.

Each MCS of $\mathcal{F}$ is the complement of an MSS of $\mathcal{F}$ and vice versa.

Definition 4. *Given a collection of sets* $\mathcal{H}$, *a hitting set of* $\mathcal{H}$ *is a set* h *such that* $h \cap C \neq \emptyset$ *for every* $C \in \mathcal{H}$. *A hitting set is* minimal *if no strict subset of it is also a hitting set.*

The next proposition is the well-known hitting set duality (Liffiton & Sakallah, 2008; Reiter, 1987) between MCSs and MUSs that forms the basis of our algorithms, as well as algorithms to compute MSSs (Davies & Bacchus, 2013) and *cardinality-minimal* MUSs (Ignatiev et al., 2015).

Proposition 1. *A set* $\mathcal{S} \subseteq \mathcal{F}$ *is an MCS of* $\mathcal{F}$ *iff it is a* minimal hitting set *of* $MUSs(\mathcal{F})$. *A set* $\mathcal{S} \subseteq \mathcal{F}$ *is a MUS of* $\mathcal{F}$ *iff it is a* minimal hitting set *of* $MCSs(\mathcal{F})$.

Consider the following examples to illustrate the concepts related to unsatisfiability introduced in the previous definitions:

Example 2. *Let* $\mathcal{C}_2$ *be the unsatisfiable CNF formula over atoms* x_1, x_2, x_3 *with the following clauses:*

$$c_1 := \neg x_1 \vee \neg x_2 \vee x_3 \qquad c_2 := \neg x_1 \vee x_2 \vee x_3 \qquad c_3 := \neg x_2 \vee \neg x_3 \qquad c_4 := x_1$$

$$c_5 := \neg x_1 \vee x_2 \qquad c_6 := \neg x_1 \vee \neg x_3$$

In Example 2, the subset of clauses $\{c_1, c_2, c_4, c_6\}$ is an example of a Minimal Unsatisfiable Subset (MUS) and $\{\underline{c_1}\}, \{\underline{c_4}\}, \{\underline{c_2}, c_5\}, \{c_5, \underline{c_6}\}, \{c_3, \underline{c_6}\}$ are examples of minimal correction subsets (MCSs). We observe that MUS $\{c_1, c_2, c_4, c_6\}$ hits at least one clause of each MCS.

4. Motivation

Our work is motivated by the problem of explaining the solution to constraint satisfaction problems, or how to explain the information entailed from it, through a sequence of simple explanation steps. This can be used to teach people problem solving skills; to search for mistakes in the problem formulation that lead to undesired models; to compare the difficulty of related satisfaction problems (through the number and complexity of steps required) and in systems that provide interactive tutoring.

4.1 Step-wise Explanation Generation

Our original explanation generation algorithm (Bogaerts et al., 2020), shown in Algorithm 1, starts from a formula $\mathcal{C}$ (in the application it comes from a high-level CSP), an *initial interpretation* I_0 (here also seen as a conjunction of literals) and a cost function f which quantifies the difficulty of an explanation step, e.g. by means of a weight for each clause.

An *explanation step* is an implication $I' \wedge \mathcal{C}' \implies N$ where

- I' is a subset of already derived literals I;
- $\mathcal{C}'$ is a subset of the constraints of the input formula $\mathcal{C}$; and
- N is a set of literals entailed by I' and $\mathcal{C}'$ which are not yet explained.

The goal is to find a sequence of *simple* explanation steps that explain the *maximal consequence* I_{end}, also referred to as the *end interpretation*, entailed by the given initial interpretation I_0 (line 1). In each explanation step, some literals from I_{end} are explained, resulting in a precision-increasing sequence of interpretations $I_0 \preceq I_1 \preceq \dots I_{end}$. Therefore, the intermediate interpretation I at a given step in this sequence will consist of all the literals "derived so far" and the remaining literals to be explained will explain correspond to $I_{end} \setminus I$.

Algorithm 1: `explain`$(\mathcal{C}, f, I_0)$

```
1  I_end ← propagate(I ∧ C)
2  Seq ← empty sequence
3  I ← I_0
4  while I ≠ Iend do
5  |  S ← Explain-One-Step(C, f, I, I_end)
6  |  I' ← I ∩ S
7  |  C' ← C ∩ S
8  |  N ← propagate(I' ∧ C')
9  |  append (I', C', N) to Seq
10 |  I ← I ∪ N
11 end
12 return Seq
```

The subset returned by `Explain-One-Step` (line 5 of Algorithm 1) is then mapped back to the set of derived literals I' (line 6) and constraints C' (line 7). Finally, at line 8, we propagate the used literals I' and constraints C' present in the found subset to derive new information N' that holds at the intersection of all models of $I' \wedge C'$, i.e., we compute the maximal consequence of $I' \wedge C'$.

Example 3. *Let C be the CNF formula over atoms x_1, x_2, x_3 with the following four clauses:*

$$c_1 := \neg x_1 \vee \neg x_2 \vee x_3 \qquad c_2 := \neg x_1 \vee x_2 \vee x_3 \qquad c_3 := x_1 \qquad c_4 := \neg x_2 \vee \neg x_3$$

Let $I = \{\neg x_2\}$ be the given interpretation *with corresponding maximal consequence $I_{end} = \{x_1, \neg x_2, x_3\}$. $I_{end} \setminus I = \{x_1, x_3\}$ represents the set of remaining literals to explain*

and its negation is denoted by $\overline{I_{end} \setminus I} = \{\neg x_1, \neg x_3\}$. *An example of an explanation step is*

$$\neg x_2 \wedge c_2 \wedge c_3 \implies x_3$$

where we use derived literal $\neg x_2$ *and constraints* c_2 *and* c_3 *to infer* x_3.

Note that all explanations in the examples are expressed in terms of this logical representation, however, the explanations can be translated back to the original input (e.g. natural language clues,, alldifferent constraints, ...).

4.2 Explanation Step

The key part of `Explain-One-Step` is the search for the best explanation step given an interpretation I of the literals derived so far. The procedure depicted in Algorithm 2 shows the gist of how this is done. It takes as input the problem constraints $\mathcal{C}$, a cost function f quantifying the quality of explanations, an interpretation I containing all literals derived so far in the sequence, and the interpretation to be explained I_{end}.

To compute an explanation step, this procedure iterates over the literals to be explained (line 2 of Algorithm 2), computes for each of them an associated MUS (line 3), and then selects the lowest cost one from the found MUSs (line 4). The reason this works is a one-to-one correspondence between MUSs of $\mathcal{C} \wedge I \wedge \neg\ell$ and so-called *non-redundant explanation* of ℓ in terms of (subsets of) $\mathcal{C}$ and I (Bogaerts et al., 2020).

Algorithm 2: `Explain-One-Step`$(\mathcal{C}, f, I, I_{end})$

```
1 S_best ← nil
2 for ℓ ∈ {I_end \ I} do
3 |   S ← MUS(C ∧ I ∧ ¬ℓ)
4 |   if f(S) < f(S_best) then
5 |   |   S_best ← S
6 |   end
7 end
8 return S_best
```

Example 4 (*Example 3 continued*)**.** *For computing a non-redundant explanation of* x_3 *zith given interpretation* $I = \{\neg x_2\}$, *we simply extract a*

$$MUS(\mathcal{C} \wedge I \wedge \neg\ell) = MUS(\mathcal{C} \wedge \{\neg x_2\} \wedge \{\neg x_3\}) = \{c_2, c_3, \{\neg x_2\}, \{\neg x_3\}\}$$

also written as $\neg x_2 \wedge c_2 \wedge c_3 \implies x_3$.

Throughout the paper, we consider cost functions f that map a subset $\mathcal{S} \subseteq \mathcal{C} \wedge I_{end} \wedge \overline{I_{end} \setminus I}$ to a numerical value $f(\mathcal{S})$, namely, a weighted sum on the constraints present in the subset $\mathcal{S}$. $\overline{I_{end} \setminus I}$ refers to the negation of the remaining literals to explain $\{\neg\ell \mid \ell \in I_{end} \setminus I\}$ introduced to compute non-redundant explanation steps with MUSs.

4.3 Concluding Remarks

Experiments have shown that such a MUS-based approach can easily take hours, especially when, at every explanation step, repeated MUS calls are performed for each remaining literal to explain (lines 2-3 of Algorithm 2) to increase the chance of finding a low-cost MUS. Furthermore, MUS extraction algorithms do not guarantee of $\subseteq$-minimality or optimality with respect to a given cost function f. Therefore, in Bogaerts, Gamba, and Guns (2021), we handle the absence of $\subseteq$-minimality and optimality guarantees by heuristically considering increasingly larger subsets of the unsatisfiable formula $(\mathcal{C} \wedge I \wedge \neg l)$.

Hence, there is a need for algorithmic improvements to make it more practical. We see three main points of improvement, all of which are addressed by our generic OCUS algorithm presented in the next section.

- First, since the algorithm is based on `MUS` calls, there is no guarantee that the explanation found is indeed optimal (with respect to the given cost function). Performing multiple MUS calls is only a heuristic used to circumvent the restriction that *there are no algorithms for cost-based unsatisfiable subset* ***optimization***.
- Second, this algorithm uses `MUS` calls for every literal $\ell \in I_{end} \setminus I$ to explain separately. The goal of all these calls is to find a single unsatisfiable subset of $\mathcal{C} \wedge I \wedge \overline{(I_{end} \setminus I)}$ that contains *exactly one literal* from $\overline{(I_{end} \setminus I)} = \{\neg\ell \mid \ell \in I_{end} \setminus I\}$. This raises the question of whether it is possible *to compute a single (optimal) unsatisfiable subset* ***subject to constraints***, where in our case, the constraint is to include exactly one literal from $\overline{(I_{end} \setminus I)}$.
- Third, the algorithm that computes an entire explanation sequence makes use of repeated calls to `Explain-One-Step`, and will therefore solve many similar problems. This raises the question of ***incrementality****: can we reuse the computed data structures to achieve speedups in later calls?*

In the next section, we introduce the concept of *Optimal Constrained Unsatisfiable Subsets* to address the first two main points of improvement. We address the third point in Section 7 along with other optimizations to speed up the generation of explanation *sequence*.

5. Optimal Constrained Unsatisfiable Subsets

In this section, we address the first two challenges highlighted at the end of Section 4.3, namely (1) the *lack of optimality guarantees* when relying on MUS extraction methods (and heuristics) to compute an explanation step, and (2) whereas the optimal explanation of a single literal can be formalized as an *optimal* MUS (with respect to a given objective), finding the optimal next explanation step over all literals remains an open question. To tackle these, we introduce the concept of an *Optimal Constrained Unsatisfiable Subset (OCUS)* and propose an algorithm for computing one.

Definition 5. *Let $\mathcal{F}$ be a formula, $f : 2^{\mathcal{F}} \to \mathbb{N}$ a cost function and p a predicate $p : 2^{\mathcal{F}} \to \{true, false\}$. We call $\mathcal{S} \subseteq \mathcal{F}$ an* Optimal Constrained Unsatisfiable Subset (OCUS) *of $\mathcal{F}$ (with respect to f and p) if*

- $\mathcal{S}$ *is unsatisfiable,*
- $p(\mathcal{S})$ *is true*
- *all other unsatisfiable* $\mathcal{S}' \subseteq \mathcal{F}$ *for which* $p(\mathcal{S}')$ *is true satisfy* $f(\mathcal{S}') \geq f(\mathcal{S})$.

Proposition 2. *Let* $\mathcal{F}$ *be a CNF formula,* p *be a predicate specified as a CNF over (meta)-variables indicating the inclusion of clauses of* $\mathcal{F}$*, and* f *be a cost-function obtained by assigning a weight to each such meta-variable, then the problem complexity of finding an OCUS is* Σ_2^P-complete.

Proof. If we assume that the predicate p is specified itself as a CNF over (meta)-variables indicating the inclusion of clauses of $\mathcal{F}$, and f is obtained by assigning a weight to each such meta-variable, then the complexity of the problem of finding an OCUS is the same as that of the SMUS (cardinality-minimal or 'Smallest' MUS) problem (Ignatiev et al., 2015): the associated decision problem is Σ_2^P-complete. Hardness follows from the fact that SMUS is a special case of OCUS; containment follows - intuitively - from the fact that this can be encoded as an $\exists\forall$-QBF using a Boolean circuit encoding of the costs. □

In the next sections, we first explain how OCUS can be used to compute an explanation step and then propose an algorithm for computing OCUSs using the well-known hitting set duality between MUSs and MCSs (Liffiton & Sakallah, 2008; Reiter, 1987).

5.1 `Explain-One-Step` with OCUS

`Explain-One-Step` implicitly uses an "exactly one of" constraint on the set of literals to explain $\{\ell \in I_{end} \setminus I\}$, and the way this is done is by considering each literal ℓ from that set separately. It searches for a good, but not necessarily *optimal* CUS (an Unsatisfiable Subset that satisfies the Constraint in question). However, the goal is to find an optimal one. Therefore, when considering the procedure `Explain-One-Step` from the perspective of OCUS defined above, the task of the procedure is to compute an OCUS of the formula $\mathcal{F} := \mathcal{C} \wedge I \wedge \overline{I_{end} \setminus I}$ where p is the predicate that holds for subsets containing *exactly one* literal of $\overline{I_{end} \setminus I}$. The pseudocode for this is shown in Algorithm 3.

Algorithm 3: `Explain-One-Step-OCUS`$(\mathcal{C}, f, I, I_{end})$

1 $\mathcal{F} \leftarrow \mathcal{C} \wedge I \wedge \overline{I_{end} \setminus I}$
2 $p \leftarrow (S \mapsto \#(S \cap \overline{I_{end} \setminus I}) = 1)$
3 $\mathcal{S}, status \leftarrow$ `OCUS`$(\mathcal{F}, f, p)$
4 **if** $status \neq FAILURE$ **then return** $\mathcal{S}$
5 **else return** $\emptyset$

Explaining 1 Literal per Step. We define the 'exactly one' constraint p as the equality constraint shown on line 2 of Algorithm 3. p evaluates to *true* if the size of the intersection of the negated literals to explain $I_{end} \setminus I$ with the subset $\mathcal{S}$ of $\mathcal{F}$ considered is equal to 1, otherwise p evaluates to *false*.

The call to `OCUS` on line 3 of `Explain-One-Step-OCUS` will never lead to the *FAILURE* case, since an OCUS is guaranteed to exist for the input cost function f, predicate p and formula $\mathcal{F}$ we are considering. Failure may occur for a different predicate p. For example, consider the predicate $p : (\mathcal{S} \mapsto f(S) \leq v)$ of Algorithm 5, which evaluates to true if a subset $\mathcal{S}$ has a value less than a given bound v. In this case it can lead to failure if no OCUS exists for a given bound v.

In the next section, we provide the details on how to compute an OCUS on line 3.

5.2 Computing an OCUS

In order to compute an OCUS of a given formula, we propose to build on the hitting set duality of Proposition 1. For this, we will assume to have access to a solver `CondOptHittingSet` that can compute hitting sets of a given collection of sets that are *optimal* (w.r.t. a given cost function f) among all hitting sets *satisfying a condition* p. The choice of the underlying hitting set solver will thus determine which types of cost functions and constraints are possible.

In our implementation, we use a cost function f which is encoded as a linear term (weighted sum), where e.g. constraints are given a larger weight than already derived literals. For example, (unit) clauses representing previously derived facts can be given small weights, and regular clauses can be given large weights, so that explanations are penalized for including clauses when previously derived facts can be used instead. Condition p can be easily encoded as a linear constraint (see Eq. (8) for an example), thus allowing the use of highly optimized mixed integer programming (MIP) solvers to compute optimal hitting sets. In the following, we explain how the conditional optimal hitting set problem `CondOptHittingSet` can be encoded into MIP to reason over combinations of clauses and literals (hitting sets) of the unsatisfiable formula.

Hitting Set Problem Given $\mathcal{F}$, we define a MIP decision variable d_c for every clause $c \in \mathcal{F}$, and write $D = \{d_c \mid c \in \mathcal{F}\}$ for the set of all such variables. We assume a given collection of sets-to-hit $\mathcal{H}$. The goal is to find a hitting set $h \subseteq D$ that hits every set-to-hit at least once (Eq. (3)), satisfies predicate p (Eq. (2)), and minimizes $f(D)$ (Eq. (1)). The `CondOptHittingSet` formulation is as follows:

$$\underset{h \subseteq D}{\text{minimize}} \quad f(h) \tag{1}$$

$$s.t. \quad p(h) \tag{2}$$

$$\sum_{c \in H} d_c \geq 1, \qquad \forall H \in \mathcal{H} \tag{3}$$

$$d_c \in \{0, 1\}, \qquad \forall d_c \in D \tag{4}$$

In the case of `OCUS`, every set-to-hit corresponds to a correction subset of $\mathcal{F}$.

OCUS Algorithm Our generic algorithm for computing OCUSs is depicted in Algorithm 4. It combines the hitting set-based approach for MUSs of Ignatiev et al. (2015) with the use of a MIP solver for (weighted) hitting sets as proposed for maximum satisfiability by Davies and Bacchus (2013). The key novelty is the ability to add structural constraints

to the hitting set solver, without impacting the duality principles of Proposition 1, as we will show.

Algorithm 4: OCUS$(\mathcal{F}, f, p)$

```
1  H ← ∅
2  while true do
3  |  S, status ← CondOptHittingSet(H, f, p)
4  |  if status = FAILURE then return (∅, status)
5  |  if ¬SAT(S) then
6  |  |  return (S, status)
7  |  end
8  |  K ← CorrSubsets(S, F)
9  |  H ← H ∪ K
10 end
```

The algorithm alternates calls to a hitting set solver with calls to a SAT oracle on a subset $\mathcal{S}$ of $\mathcal{F}$. In case the SAT oracle returns true, i.e., subset $\mathcal{S}$ is satisfiable, $\mathcal{K}$ a set of subsets of $F \setminus S$ is returned by CorrSubsets and added to the collection of sets-to-hit $\mathcal{H}$.

Smallest MUS of Ignatiev et al. (2015) The key differences with the SMUS algorithm are the calls to a CondOptHittingSet solver (resp. MinimumHS) and the CorrSubsets (resp. grow) procedure. In the SMUS algorithm, the purpose of grow is to expand a satisfiable subset $\mathcal{S}$ of $\mathcal{F}$ further such that its complement, a correction subset, is as small as possible. Shrinking the correction subset as a result of grow finds stronger constraints on the sets-to-hit, since it restricts the choice of clauses to be selected.

In our algorithm we make use of the CorrSubsets procedure which returns a non-empty *set* of correction subsets. In the case of OCUS, the calls for hitting sets will also take into account the cost (f), and the meta-level constraints (p). As such, It is not clear a priori which properties a good CorrSubsets function should have here. In Section 5.3, we propose different domain-specific methods for enumerating multiple correction subsets.

For the *correctness* of the algorithm, all we need to know is that for a given satisfiable subset $\mathcal{S}$, CorrSubsets returns a *non-empty* set of correction subsets $\mathcal{K}$, where $\forall\ \mathcal{C} \in \mathcal{K} : \mathcal{C} \subseteq (F \setminus S)$. At any given step, if $\mathcal{S}$ is satisfiable, $\mathcal{H}$ is guaranteed to grow, since a non-empty set of correction subsets $\mathcal{K}$ is returned that is disjoint from $\mathcal{S}$. Therefore $\mathcal{K}$ cannot be present in $\mathcal{H}$. The *completeness* and *soundness* of the algorithm follow from the fact that the algorithm is guaranteed to terminate since there is a countable number of correction subsets of $\mathcal{F}$, and from Theorem 6, which states that what is returned is indeed a solution and that a solution will be found if it exists.

Theorem 6. *Let $\mathcal{H}$ be a set of correction subsets of $\mathcal{F}$. If $\mathcal{S}$ is a hitting set of $\mathcal{H}$ that is f-optimal among the hitting sets of $\mathcal{H}$ that satisfy a predicate p, and $\mathcal{S}$ is unsatisfiable, then $\mathcal{S}$ is an OCUS of $\mathcal{F}$. If $\mathcal{H}$ has no hitting sets satisfying p, then $\mathcal{F}$ has no OCUSs.*

Proof. For the first claim, it is clear that $\mathcal{S}$ is unsatisfiable and satisfies p. Hence all we need to show is the f-optimality of $\mathcal{S}$. If there would exist some other unsatisfiable subset $\mathcal{S}'$ that satisfies p with $f(\mathcal{S}') \leq f(\mathcal{S})$, we know that $\mathcal{S}'$ would hit every minimal correction set

of $\mathcal{F}$, and hence also every set in $\mathcal{H}$ (since every correction set is the superset of a minimal correction set). Since $\mathcal{S}$ is f-optimal among hitting sets of $\mathcal{H}$ that satisfy p, and since $\mathcal{S}'$ also hits $\mathcal{H}$ and satisfies p, it must be that $f(\mathcal{S}) = f(\mathcal{S}')$.

The second claim follows immediately from Proposition 1 and the fact that an OCUS is an unsatisfiable subset of $\mathcal{F}$. □

Perhaps surprisingly, the correctness of the proposed algorithm does *not* depend on the monotonicity properties of f nor p. In principle, any (computable) cost function and condition on the unsatisfiable subsets can be used. In practice, however, one is bound by the limitations of the chosen hitting set solver.

As an illustration, we provide an example of one call to `Explain-One-Step-OCUS` (Algorithm 3) and the corresponding `OCUS`-call in detail (Algorithm 4) for our running example:

Example 5 (*continued*)**.** *Recall the 4 previously introduced clauses from our running example* $C := c_1 \wedge c_2 \wedge c_3 \wedge c_4$ *with:*

$$c_1 := \neg x_1 \vee \neg x_2 \vee x_3 \qquad c_2 := \neg x_1 \vee x_2 \vee x_3 \qquad c_3 := x_1 \qquad c_4 := \neg x_2 \vee \neg x_3$$

Consider a call to `Explain-One-Step-OCUS` *with* $I = \emptyset$ *and* $I_{end} = \{x_1, \neg x_2, x_3\}$*. We add the following three new clauses, which represent the complement of the literals to be derived* $\overline{I_{end} \setminus I}$*:*

$$\{\neg x_1\} \qquad \{x_2\} \qquad \{\neg x_3\}$$

The cost function f *is defined as a linear sum*

$$f(\mathcal{S}) = \sum_{c \in \mathcal{S}} w_i \cdot c_i \tag{5}$$

over the following clause weights:

$$\begin{aligned} &\textbf{Clause weights: } w_{c_1} = 60 \qquad w_{c_2} = 60 \qquad w_{c_3} = 100 \qquad w_{c_4} = 100 \\ I \wedge \overline{I_{end} \setminus I} &\textbf{ weights: } w_{\neg x_1} = 1 \qquad w_{x_2} = 1 \qquad w_{\neg x_3} = 1 \end{aligned}$$

We encode the same cost function in the MIP encoding as a weighted sum using the corresponding decision variables as follows:

$$f(\mathcal{S}) = \sum_{c \in \mathcal{S}} w_c \cdot d_c \tag{6}$$

To ensure that we only explain one literal at a time, we add predicate p *as*

$$p(S) := \#(S \cap \{\neg x_1, x_2, \neg x_3\}) = 1 \tag{7}$$

The MIP encoding of the predicate p *corresponds to*

$$p(h) := \sum_{c \in \overline{I_{end} \setminus I}} d_c = d_{\{\neg x_1\}} + d_{\{x_2\}} + d_{\{\neg x_3\}} = 1 \tag{8}$$

At Line 3 of `Explain-One-Step-OCUS`*,* $\mathcal{F}$ *is constructed, consisting of :*

$$\mathcal{F} = C \wedge I \wedge \overline{(I_{end} \setminus I)} = c_1 \wedge \cdots \wedge c_4 \wedge \neg x_1 \wedge x_2 \wedge \neg x_3 \tag{9}$$

Finally, to generate an explanation step, we call `OCUS` *on formula* $\mathcal{F}$ *with the given cost function* f *and* exactly-one *constraint* p*:*

$$\texttt{OCUS}(\mathcal{F}, f, p) \tag{10}$$

In this small example, the `CorrSubsets`$(\mathcal{S}, \mathcal{F})$ *procedure simply returns* $\{F \setminus S\}$*.*

Step	$\mathcal{S}$	SAT($\mathcal{S}$)	$\mathcal{H} \leftarrow \mathcal{H} \cup$ CorrSubsets($\mathcal{S}, \mathcal{F}$)
			$\emptyset$
1.	$\{\neg x_3\}$	*true*	$\{\{c_1, c_2, c_3, c_4, \neg x_1, x_2\}\}$
2.	$\{\neg x_1\}$	*true*	$\{\ldots, \{c_1, c_2, c_3, c_4, x_2, \neg x_3\}\}$
3.	$\{x_2\}$	*true*	$\{\ldots, \{c_1, c_2, c_3, c_4, \neg x_1, \neg x_3\}\}$
4.	$\{c_1, x_2\}$	*true*	$\{\ldots, \{c_2, c_3, c_4, \neg x_1, \neg x_3\}\}$
5.	$\{c_2, x_2\}$	*true*	$\{\ldots, \{c_1, c_3, c_4, \neg x_1, \neg x_3\}\}$
6.	$\{c_1, \neg x_3\}$	*true*	$\{\ldots, \{c_2, c_3, c_4, \neg x_1, x_2\}\}$
7.	$\{c_2, \neg x_1\}$	*true*	$\{\ldots, \{c_1, c_3, c_4, x_2, \neg x_3\}\}$
8.	$\{c_1, \neg x_1\}$	*true*	$\{\ldots, \{c_2, c_3, c_4, x_2, \neg x_3\}\}$
9.	$\{c_2, \neg x_3\}$	*true*	$\{\ldots, \{c_1, c_3, c_4, \neg x_1, x_2\}\}$
10.	$\{c_4, x_2\}$	*true*	$\{\ldots, \{c_1, c_2, c_3, \neg x_1, \neg x_3\}\}$
11.	$\{c_3, x_2\}$	*true*	$\{\ldots, \{c_1, c_2, c_4, \neg x_1, \neg x_3\}\}$
12.	$\{\mathbf{c_3}, \mathbf{\neg x_1}\}$	*false*	

Table 1: Example 5 - Intermediate steps when computing an `OCUS` for `Explain-One-Step-OCUS` where `CorrSubsets`$(\mathcal{S}, \mathcal{F}) = \{\mathcal{F} \setminus \mathcal{S}\}$.

Table 1 breaks down the intermediate steps of algorithm 4 for generating an OCUS of given $\mathcal{F}$*,* f *and* p*. First, the collection of sets-to-hit* $\mathcal{H}$ *is initialized as the empty set. At each iteration, the hitting set solver searches for a cost-minimal assignment that hits all sets in* $\mathcal{H}$ *and that contains exactly one of* $\{\neg x_1, x_2, \neg x_3\}$ *(due to* p*). If the hitting set is unsatisfiable, it is guaranteed to be an OCUS.*

The first iterations show that the `OCUS` *algorithm first hits all the literals of* $\overline{I_{end} \setminus I}$ *(steps 1-3 of Table 1) and then starts combining one literal of* $\overline{I_{end} \setminus I}$ *with the remaining clauses until an OCUS is found (step 12). Finally, step 12 of Table 1 signifies that using clause* c_3 *we can derive* x_1*, and more formally* $c_3 \implies x_1$*.*

Incremental MIP Solver The `OCUS` algorithm requires repeatedly computing hitting sets over an increasing collection of sets-to-hit. Initializing the MIP solver once and keeping it warm throughout the `OCUS` iterations allows it to reuse information from previous solver calls to solve the current hitting set problem. Similar to Davies and Bacchus (2013), we

notice a speed-up between 3 to 5 times by keeping the solver warm[1] compared to initializing a new MIP solver instance at every iteration.

As can be seen in Table 1, the `OCUS` algorithm requires many intermediate steps to find an OCUS. Note, for example, that the computed correction subsets contain more than 1 literal to explain that are not relevant for explaining the literal in the current hitting set. Taking step 2 as an example, if $\{\neg x_1\}$ is a hitting set, its corresponding correction subset $\{c_1, c_2, c_3, c_4, x_2, \neg x_3\}$ contains $\{x_2, \neg x_3\}$ which cannot be taken.

Even though our running example has a rather small number of clauses, `OCUS` needs to combine an increasingly large number of literals and clauses to find an OCUS. Next, we investigate how to efficiently grow a given satisfiable subset in order to reduce the size of the corresponding correction subset. By imposing stronger restrictions on the hitting sets, we will be able to reduce the number of sets to hit.

5.3 Computing Correction Subsets

The `CorrSubsets` procedure generates a set of correction subsets starting from a given satisfiable subset $\mathcal{S}$ of an unsatisfiable formula $\mathcal{F}$. However, calling `Explain-One-Step-OCUS` on our running example has shown that a naive 'No grow':

$$\texttt{CorrSubsets}(\mathcal{S}, \mathcal{F}) \leftarrow \{\mathcal{F} \setminus \mathcal{S}\} \tag{11}$$

drastically increases the number of sets-to-hit required compared to using the model provided by the `SAT` solver. This last observation suggests that the satisfiable subset $\mathcal{S}$ should be *efficiently grown* into a *larger satisfiable subset* before computing the complement:

$$\texttt{CorrSubsets}(\mathcal{S}, \mathcal{F}) \leftarrow \{\mathcal{F} \setminus \texttt{Grow}(\mathcal{S}, \mathcal{F})\} \tag{12}$$

5.3.1 Growing satisfiable subsets using domain-specific information

The goal of the `Grow` phase of the `CorrSubsets` procedure (see Eq. (12)) is to turn $\mathcal{S}$ into a larger satisfiable subformula of $\mathcal{F}$. The effect of this is that the complement added to $\mathcal{H}$ will be smaller, and hence imposes stronger restrictions on the hitting sets.

There are multiple conflicting criteria that determine what makes an effective 'grow' procedure. On the one hand, we want our subformula to be as large as possible (which would ultimately correspond to computing a maximal satisfiable subformula), but on the other hand, we also want the procedure to be very efficient, as it is called in every iteration.

In the case of explanations, we make the following observations:

- Our formula at hand (using the notation from the `Explain-One-Step-OCUS` algorithm) consists of three types of clauses: (1) (translations of) the problem constraints (this is $\mathcal{C}$) (2) literals representing the assignment found (this is I), and (3) the negations of literals not yet derived (this is $\overline{I_{end} \setminus I}$).
- $\mathcal{C}$ and I together are satisfiable, with assignment I_{end}, and *mutually supportive*, by this we mean that making more clauses in $\mathcal{C}$ true, more literals in I will automatically become true and vice versa.

1. We use the same setup as in the experiment section: a single core on a 10-core INTEL Xeon Gold 61482 (Skylake), a memory-limit of 8GB. The code is written on top of PySAT 0.1.7.dev1 (Ignatiev, Morgado, & Marques-Silva, 2018), for MIP calls, we used Gurobi 9.1.2, and for the SAT calls MiniSat 2.2.

- The constraint p enforces that each hitting set will contain **exactly** one literal of $\overline{I_{end} \setminus I}$

Since the restrictions on the third type of elements of $\mathcal{F}$ are already strong, it makes sense to search for a *maximal* satisfiable subset of $\mathcal{C} \cup I$ with hard constraints that $\mathcal{S}$ should be satisfied, using a call to an efficient (partial) `MaxSAT` solver.

Furthermore, we can initialize this call as well as any call to a `SAT` solver with the polarities for all variables set to the value they take in I_{end}.

We evaluate different grow strategies as part of the `CorrSubsets`$(\mathcal{S}, \mathcal{F})$ procedure in the experiments section including:

`SAT` extracts a satisfying model from the `SAT` solver to turn $\mathcal{S}$ into a larger satisfiable subset. This grow will be considered the baseline for comparing the other grow-variants.

`SubsetMax-SAT` extends the satisfiable subset computed by `SAT` by looping over every remaining clause $c \in \mathcal{F} \setminus \mathcal{S}$. If $\mathcal{S} \cup \{c\}$ is satisfiable, then clause c is added to $\mathcal{S}$ as well as any other clause from $c' \in \mathcal{F} \setminus \mathcal{S} \cup \{c\}$ that is satisfied in the model found by the SAT solver.

`Dom.-spec. MaxSAT` grows a satisfiable subset $\mathcal{S}$ with a `MaxSAT` solver using only the previously derived facts and the original constraints.

`MaxSAT Full` grows satisfiable subset $\mathcal{S}$ with a `MaxSAT` solver using the full unsatisfiable formula $\mathcal{F}$.

In the experiments, we omit the 'No grow' procedure where the complement $\{\mathcal{F} \setminus \mathcal{S}\}$ is returned by `CorrSubsets`. Not growing produces large sets-to-hit as seen in Table 1 of the running example. Additional experiments comparing the effectiveness of the naive 'No grow' to growing with the `SAT` solver procedure shows that 'No grow' leads to significantly longer `OCUS` runtimes.

Finally, Table 1 showed that `OCUS` has to combine an increasingly large number of literals and clauses. In the next section, we analyse whether we can break the more general OCUS problem into smaller subproblems, similar to Algorithm 2, where instead of searching for a MUS, we search for an *Optimal Unsatisfiable Subset* (OUS) and select the best one.

6. Multiple Optimal Unsatisfiable Subsets

Preliminary experiments have shown that most of the time ($\sim 90\%$ of the time) is spent searching for hitting sets when generating an explanation step with `OCUS`. The main reason for this is that the hitting set solver needs to consider an increasingly large collection of sets-to-hit, potentially searching over an exponential number of literals and clauses (see Table 1 of Example 5).

In this section, we first analyze if instead of working OCUS-based, we can split up the `OCUS`-call into individual calls that compute Optimal Unsatisfiable Subsets (OUSs) for every literal by replacing a MUS call to OUS in Algorithm 2.

6.1 Bounded OCUS

Since OUS, without an additional predicate, is a special case of OCUS, we can take advantage of Proposition 1 and reuse the `OCUS` algorithm with a trivially true p, i.e., $\texttt{OUS}(\mathcal{F}, f) := \texttt{OCUS}(\mathcal{F}, f, \mathbf{t})$ for each $\mathcal{F}$ and f. However, the switch from `MUS` to `OUS` in Algorithm 2 still requires looping over every literal and computing the OUS, potentially introducing overhead compared to the single `OCUS` call. However, we can use the OUS obtained in one iteration, to infer a bound on the score that must be achieved in subsequent OUS calls.

Upper Bound Every MUS or OUS computed at Line 3 of Algorithm 2 provides an upper bound on the cost, which should be improved in the next iteration. By keeping track of the best candidate explanation, its corresponding cost can be considered the current best upper bound on the cost of the OUSs of the remaining literals to explain.

Lower Bound Every hitting set computed inside the `OUS` algorithm produces a lower bound on the best cost that can be obtained, even the satisfying ones. Indeed, the candidate hitting set returned on line 3 of Algorithm 4 is guaranteed to be the lowest-cost one. Consequently, the cost of the best candidate explanation so far can be used as an early stopping criterion: if the cost of the current hitting set is larger than the cost of the best explanation so far, `OUS` will not be able to find a better (cheaper) unsatisfiable subset $\mathcal{S}$ for that literal.

In fact, such a *bounded OCUS* call is naturally obtained by doing an `OCUS` call with as constraint $p(S) := f(\mathcal{S}) \leq f(\mathcal{S}_{best})$.

Bounded OCUS-based Explanations `Explain-One-Step-OCUS-Bounded` in Algorithm 5 uses calls to the `OCUS` algorithm for every individual literal to compute the next best explanation step. The algorithm keeps track of the current best OCUS candidate $\mathcal{S}_{best}$. This $\mathcal{S}_{best}$ is only updated if the `OCUS` algorithm is able to find an OCUS that is cheaper than the current upper bound $f(\mathcal{S}_{best})$. Predicate $f(\mathcal{S}) \leq f(\mathcal{S}_{best})$ of the `OCUS`-call at line 4 of Algorithm 5 allows us to ensure that the cost of the hitting set does not exceed the upper bound. In case it does happen, the hitting set solver will return a failure message meaning that a better candidate explanation cannot be computed for that literal given the current interpretation I.

Algorithm 5: `Explain-One-Step-OCUS-Bounded`$(\mathcal{C}, f, I, I_{end})$

```
1 S_best ← nil
2 S^ℓ_best ← nil for each ℓ        (or from previous iteration)
3 for ℓ ∈ {I_end \ I} sorted by f(S^ℓ_best) do
4 |   S^ℓ_best, status ← OCUS((C ∧ I ∧ ¬l), f, f(S) ≤ f(S_best))
5 |   if status ≠ FAILURE then
6 |   |   S_best ← S^ℓ_best
7 |   end
8 end
9 return S_best
```

Literal Sorting Obtaining a good upper-bound quickly can further reduce runtime. We can heuristically aid this by keeping track of S^{ℓ}_{best} across explanation steps, and then use its score $f(S^{\ell}_{best})$ to sort the literals at line 3. The literal sorting ensures we first try the cheapest S^{ℓ}_{best} from a previous explanation step since these are more likely to provide a good upper bound on the cost of the next candidate OCUS.

6.2 Interleaving OCUS Calls for Different Literals: a Special-case OCUS Algorithm

The case to avoid for `Explain-One-Step-OCUS-Bounded` is that an `OCUS` call for a literal takes many hitting set iterations, and returns an 'expensive' OCUS with lower-cost OCUSs to be found for other literals.

Conceptually, one should only do hitting set iterations for the most promising literal, one that is most likely to produce an OCUS with the lowest cost. Indeed, this is what the original `OCUS` algorithm with an 'exactly one of' constraint is built for: to choose freely among all possible hitting sets across the different literals in order to find the globally optimal next candidate OUS.

For this special case, where the constraint p is that exactly one of a set of literals must be chosen, we can manually decompose the problem to iteratively search for the best hitting set across the independent problems. In such an approach, we do not repeatedly call (bounded) `OCUS` until optimality, but do one hitting-set iteration at a time; each time continuing with one hitting-set iteration of the most promising literal.

This is shown in Algorithm 6. Every literal to explain ℓ is associated with: (1) its current *collection of sets to hit* $\mathcal{H}_\ell$; and (2) corresponding *optimal hitting set* $\mathcal{S}_\ell$ (initially the empty set for both) as well as (3) it's corresponding *cost* $f(\mathcal{S}_\ell)$. These are stored in a priority queue, sorted by the cost.

Algorithm 6: `Explain-One-Step-OCUS-Split`$(\mathcal{C}, f, I, I_{end})$

```
1  queue ← InitializePriorityQueue((ℓ, ∅, ∅) : 0 | ∀ℓ ∈ I_end \ I)
2  while (ℓ, S_ℓ, H_ℓ) ← queue.pop() do
3  |  if ¬SAT(S_ℓ) then
4  |  |  return S_ℓ
5  |  end
6  |  K ← CorrSubsets(S_ℓ, (C ∧ I ∧ ¬ℓ))
7  |  H_ℓ ← H_ℓ ∪ K
8  |  S_ℓ ← OptHittingSet(H_ℓ, f)
9  |  queue.push((ℓ, S_ℓ, H_ℓ) : f(S_ℓ))
10 end
```

`Explain-One-Step-OCUS-Split` repeatedly extracts the best literal-to-explain and corresponding hitting set out of the priority queue. Similar to Algorithm 4, if the corresponding hitting set is unsatisfiable, it is guaranteed to be the cost-minimal OUS. This is because the queue ensures that this hitting set is the lowest scoring hitting set across all literals and because each hitting set is guaranteed to be an optimal hitting set of its collected sets-to-hit $\mathcal{H}_\ell$. If, on the other hand, the hitting set is satisfiable, a number of correction subsets are

extracted from the literal-specific unsatisfiable formula and added to its respective collection of sets to hit. Finally, a new hitting set is computed and this information is pushed back into the priority queue.

The intermediate steps of `OCUS` depicted in Table 1 of Example 5 shows that `OCUS` needs to consider *many combinations of clauses and literals* for *all literals to explain*. Whereas `OCUS_Split` reasons over a smaller unsatisfiable formula containing literals relevant for the literal to explain, and only expands the most promising literal. In the experiments, we compare which `Explain-One-Step-`* configuration (`OCUS`, `OCUS_Bound`, or `OCUS_Split`) is the fastest for computing explanations.

In the following section, we analyse how to exploit the fact that OCUS and its variants have to be called repeatedly on an unsatisfiable formula that is incrementally extended when generating a sequence of explanations. We then consider how to reduce the number and size of sets-to-hit, e.g. to include only information relevant to each literal-to-explain, and how to generate small (p-)disjoint correction subsets from a given hitting set.

7. Efficiently Computing Optimal Explanations

Up until now, we have investigated how to speed-up the generation of an explanation step from the perspective of OCUS as an oracle. In the following, we discuss optimizations applicable to the `O(C)US` algorithms that are specific to explanation sequence generation, though they can also be used when other forms of domain knowledge are present.

7.1 Incremental OCUS Computation

Inherently, generating a sequence of explanations still requires many O(C)US calls. Indeed, a greedy sequence construction algorithm calls an `Explain-One-Step` variant repeatedly with a growing interpretation I until $I = I_{end}$. All of these calls to `Explain-One-Step`, and hence O(C)US, are done with very similar input (the set of constraints does not change, and the I slowly grows between two calls). For this reason, it makes sense that information computed during one of the earlier stages can be useful in later stages as well. The main question is:

> Suppose two `OCUS` calls are done, first with inputs $\mathcal{F}_1$, f_1, and p_1, and later with $\mathcal{F}_2$, f_2, and p_2; *how can we make use as much as possible of the data computations of the first call to speed-up the second call?*

The answer is surprisingly elegant. The most important data `OCUS` keeps track of is the collection $\mathcal{H}$ of correction subsets that need to be hit.

7.1.1 Bootstrapping $\mathcal{H}$ with Satisfiable Subsets

This collection in itself is not useful for transfer between two calls, since – unless we assume that $\mathcal{F}_2$ is a subset of $\mathcal{F}_1$ – there is no reason to assume that a set in $\mathcal{H}_1$ is also a correction subset of $\mathcal{F}_2$ in the second call. However, each set H in $\mathcal{H}$ is the complement (with respect to the formula at hand) of a *satisfiable subset* of constraints, and each subset of a satisfiable subset is satisfiable as well. Thus, instead of storing $\mathcal{H}$, we can keep track of a set of *satisfiable subsets* **SSs**; as the intermediate results of calls to `CorrSubsets`.

When a second call to OCUS is performed, we can then initialize $\mathcal{H}$ as the complement of each of these satisfiable subsets with respect to $\mathcal{F}_2$, i.e.,

$$\mathcal{H} \leftarrow \{\mathcal{F}_2 \setminus \mathcal{S} \mid \mathcal{S} \in \mathbf{SSs}\}. \tag{13}$$

The effect of this is that we *bootstrap* the hitting set solver with an initial set $\mathcal{H}$.

7.1.2 Incrementality with MIP

For hitting set solvers that natively implement incrementality, such as modern Mixed Integer Programming (MIP) solvers, we can generalize this idea further: we know that all calls to $\texttt{OCUS}(\mathcal{F}, f, p)$ will be cast with $\mathcal{F} \subseteq \mathcal{C} \cup I_{end} \cup \overline{I_{end} \setminus I_0}$, where I_0 is the start interpretation. To compute the conditional hitting set for a specific $\mathcal{C} \cup I \cup \overline{I_{end} \setminus I} \subseteq \mathcal{C} \cup I_{end} \cup \overline{I_{end} \setminus I_0}$, we need to ensure that the hitting set solver only uses literals in $\mathcal{C} \cup I \cup \overline{I_{end} \setminus I}$. For incremental hitting set solvers, this means updating the constraint p at every explanation step to include (1) only literals from interpretation I at the current explanation step, and (2) the 'exactly-one' constraint for explaining one literal at a time.

Since our implementation uses a MIP solver for computing hitting sets (see Section 3), and we know the entire formula from which elements must be chosen,we initialize the MIP solver once with all relevant decision variables of $\mathcal{C} \cup I_{end} \cup \overline{I_{end} \setminus I_0}$.

Bear in mind that retracting a constraint p to replace it with an updated one (in the next explanation call) is non-trivial for MIP solvers. Therefore, we assign an infinite weight in the cost function to all literals of $I_{end} \setminus I$ and update their weights as soon as they have been derived according to the given cost function. In this way, the MIP solver will automatically maintain and reuse previously found sets-to-hit in each of its computations.

Next, we investigate how to speed-up the generation of an OCUS using an appropriate CorrSubsets method when domain-specific information is available. Through our running example we will look at the impact of incremetality and a better CorrSubsets procedure.

7.1.3 Efficiently Generating an Explanation Sequence with Incremental OCUS

In the following example, we illustrate the efficiency of *incrementality with MIP* together with the *SAT grow* to speed up generating an OCUS-based explanation sequence.

Example 6 (*continued*)**.** *Consider the previously introduced clauses of our running example C:*

$$c_1 := \neg x_1 \vee \neg x_2 \vee x_3 \qquad c_2 := \neg x_1 \vee x_2 \vee x_3 \qquad c_3 := x_1 \qquad c_4 := \neg x_2 \vee \neg x_3$$

To define the input for the MIP-incremental OCUS with initial interpretation $\mathcal{I} = \emptyset$, we extend C with the new clauses representing the final interpretation $I_{end} = \{\{x_1\}, \{\neg x_2\}, \{x_3\}\}$ and the complement thereof $\overline{I_{end} \setminus \mathcal{I}} = \{\{\neg x_1\}, \{x_2\}, \{\neg x_3\}\}$. For the MIP-incremental variant of OCUS, p remains the same. The cost function f_I is defined as a weighted sum over the following weights:

Clause weights:	$w_1 = 60$	$w_2 = 60$	$w_3 = 100$	$w_4 = 100$
$I \wedge \overline{I_{end} \setminus I}$ **weights:**	$w_{\neg x_1} = 1$	$w_{x_2} = 1$	$w_{\neg x_3} = 1$	
$I_{end} \setminus I$ **weights:**	$w_{x_1} = \infty$	$w_{\neg x_2} = \infty$	$w_{x_3} = \infty$	

Note how the literals that haven't been derived yet ($I_{end} \setminus I$) are given an infinite weight according to Section 7.1.2 for incrementality purposes. Therefore, f_I will be updated at every explanation step whenever interpretation I changes. The incremental `OCUS`*-call is now:*

$$\texttt{OCUS}(\mathcal{C} \wedge I_{end} \wedge \overline{(I_{end} \setminus I)}, f_I, p) \tag{14}$$

In this example, the `Grow` *procedure uses the model provided by the* `SAT` *solver to grow a given subset $\mathcal{S}$. The* `CorrSubsets` *procedure simply returns*

$$\mathcal{K} = \texttt{CorrSubsets}(\mathcal{S}, \mathcal{F}) = \{\mathcal{F} \setminus \texttt{Grow}(\mathcal{S}, \mathcal{F})\} \tag{15}$$

The following tables (Tables 2 to 4) summarize the intermediate steps to compute an OCUS-based explanation sequence for our running example. The literals that cannot be selected by the hitting set solver have been struck out because they have not been derived yet.

Step	$\mathcal{S}$	SAT($\mathcal{S}$)	Grow($\mathcal{S}, \mathcal{F}$)	$\mathcal{H} \leftarrow \mathcal{H} \cup \mathcal{K}$
				$\emptyset$
1.	$\{\neg x_3\}$	*true*	$\{c_1, c_2, c_4, \neg x_1, \neg x_2, \neg x_3\}$	$\{\{c_3, \cancel{x_1}, x_2, \cancel{x_3}\}\}$
2.	$\{x_2\}$	*true*	$\{c_1, c_2, c_3, x_1, x_2, x_3\}$	$\{..., \{c_4, \neg x_1, \cancel{\neg x_2}, \neg x_3\}\}$
3.	$\{\neg x_1\}$	*true*	$\{c_1, c_2, c_4, \neg x_1, \neg x_2, x_3\}$	$\{..., \{c_3, \cancel{x_1}, x_2, \neg x_3\}\}$
4.	$\{c_4, x_2\}$	*true*	$\{c_1, c_2, c_4, \neg x_1, x_2, \neg x_3\}$	$\{..., \{c_3, \cancel{x_1}, \cancel{\neg x_2}, \cancel{x_3}\}\}$
5.	$\{c_3, \neg x_3\}$	*true*	$\{c_1, c_3, c_4, x_1, \neg x_2, \neg x_3\}$	$\{..., \{c_2, x_2, \cancel{x_3}, \neg x_1\}\}$
6.	$\{c_3, \neg x_1\}$	*false*	-	-

Table 2: *Example (continued).* Explanation step 1 ($\mathbf{c_3} \implies \mathbf{x_1}$) of the explanation sequence generated with `Explain-One-Step-OCUS` with incremental MIP solving (see Section 7.1.2).

Observation 1. ***(An effective grow)*** *The most striking aspect of Table 2 compared to Table 1 is the number of steps required to find an OCUS that is greatly reduced, i.e. from 12 steps to 6, as a result of choosing an effective grow.*

For the next explanation step, since x_1 has been explained, we adapt the weights of the clauses $\{x_1\}$ and $\{\neg x_1\}$ to $w_{x_1} = 1$ and $w_{\neg x_1} = \infty$ respectively.

Observation 2. ***(Incrementality)*** *In the intermediate* `OCUS` *steps of explanation step 2 (Table 3), we observe the effect of incrementality from the number of steps required to find an OCUS. Recall that in the MIP setting, $\mathcal{F}$ is constructed overall literals of I_{end} and $\overline{I_{end} \setminus I}$, and hence stays the same throughout all explanation steps. Therefore, the correction subsets of the previous explanation steps can be reused as is. Using the previously computed sets-to-hit ensures that the* `OCUS` *algorithm starts from a good candidate OCUS. If the same* `OCUS`*-call is performed without bootstrapping the previous sets-to-hit, the number of intermediate steps is higher, i.e. 5 instead of 2.*

Finally, for the last explanation step, we adapt the weights to reflect the current interpretation and that we only want to explain $\neg x_2$ ($w_{x_3} = 1$ and $w_{\neg x_3} = \infty$).

Step	$\mathcal{S}$	SAT($\mathcal{S}$)	Grow ($\mathcal{S}$, $\mathcal{F}$)	$\mathcal{H} \leftarrow \mathcal{H} \cup \mathcal{K}$
				$\{\{c_3, x_1, x_2, \neg x_3\}$, $\{c_3, x_1, x_2, \cancel{x_3}\}$, $\{c_4, \cancel{\neg x_1}, \cancel{\neg x_2}, \neg x_3\}$, $\{c_3, x_1, \cancel{\neg x_2}, \cancel{x_3}\}$, $\{c_2, x_2, \cancel{x_3}, \cancel{\neg x_1}\}\}$
1.	$\{c_2, x_1, \neg x_3\}$	*true*	$\{c_2, c_3, c_4, x_1, x_2, \neg x_3\}$	$\{..., \{c_1, \cancel{x_3}, \cancel{\neg x_2}\}\}$
2.	$\{c_1, c_2, x_1, \neg x_3\}$	*false*		

Table 3: *Example (continued).* Explanation step 2 ($\mathbf{c_1} \wedge \mathbf{c_2} \wedge \mathbf{x_1} \implies \mathbf{x_3}$) of the explanation sequence generated with `Explain-One-Step-OCUS` *incremental*.

Step	$\mathcal{S}$	SAT($\mathcal{S}$)	Grow ($\mathcal{S}$, $\mathcal{F}$)	$\mathcal{H} \leftarrow \mathcal{H} \cup \mathcal{K}$
				$\{\{c_3, x_1, x_2, \cancel{\neg x_3}\}$, $\{c_3, x_1, x_2, x_3\}$, $\{c_4, \cancel{\neg x_1}, \cancel{\neg x_2}, \cancel{\neg x_3}\}$, $\{c_3, x_1, \cancel{\neg x_2}, x_3\}$, $\{c_2, x_2, x_3, \cancel{\neg x_1}\}$, $\{c_1, x_3, \cancel{\neg x_2}\}\}$
1.	$\{c_4, x_2, x_3\}$	*false*		

Table 4: *Example (continued).* Explanation step 3 ($\mathbf{c_4} \wedge \mathbf{x_3} \implies \neg\mathbf{x_2}$) of the explanation sequence generated with `Explain-One-Step-OCUS` *incremental*.

Observation 3. ***(Disjoint Correction Subsets)*** *Observe set-to-hit* $\{c_4, \cancel{\neg x_1}, \cancel{\neg x_2}, \cancel{\neg x_3}\}$ *in the collection of previously compute sets-to-hit of Table 4. Given the current interpretation and the literal* $\neg x_2$ *to explain, only* c_4 *can* <u>*and*</u> *has to be taken. The phenomenon of a set being disjoint from another with respect to* p *is what we call in Definition 7 p-disjointness. In this case, subset* $\{c_4, \cancel{\neg x_1}, \cancel{\neg x_2}, \cancel{\neg x_3}\}$ *is p-disjoint from the other sets-to-hit for the hitting set solver. Therefore, it poses a stronger restriction on the sets-to-hit.*

Definition 7. *Two sets* S_1 *and* S_2 *are p-disjoint if every set that hits both* S_1 *and* S_2 *and satisfies* p *contains* $s_1 \in S_1$ *and* $s_2 \in S_2$ *with* $s_1 \neq s_2$.

Example 6 shows that *incrementality with MIP* and *growing the satisfiable subset* $\mathcal{S}$ are effective at reducing the size and the number of sets-to-hit when computing a sequence of explanations using `Explain-One-Step-OCUS`. Next, in section 7.1.4, we take advantage of Definition 7 to enumerate multiple correction subsets that are p-disjoint of each other during the `CorrSubsets` procedure.

7.1.4 Correction Subsets Enumeration

Our `OCUS` algorithm repeatedly alternates between computing hitting sets and correction subsets. The increasingly large collection of sets-to-hit makes finding optimal hitting sets much more expensive compared to the `CorrSubsets` procedure, which solely relies on finding

correction subsets from a given satisfiable subset. Additionally, in the last explanation step of Example 6, we saw that one of the sets-to-hit ($\{c_4, \cancel{\neg x_1}, \cancel{\neg x_2}, \cancel{\neg x_3}\}$) was p-disjoint to the others, imposing a strong restriction on the hitting set solver. The question is:

> Can we cheaply find *multiple*, ideally *p-disjoint*, correction subsets and thereby add multiple sets-to-hit in one go?

Inspired by Marques-Silva, Heras, Janota, Previti, and Belov (2013), we depict a `CorrSubsets` procedure in Algorithm 7 that computes a collection of correction subsets $\mathcal{K}$ starting from a given subset of constraints $\mathcal{S}$ (either the empty set or a computed hitting set). The `CorrSubsets` procedure will repeatedly compute a satisfiable subset $\mathcal{S}' \supseteq \mathcal{S}$, and add its complement to the collection of disjoint MCSes $\mathcal{K}$ and to $\mathcal{S}$, ensuring that the constraints in the correction subset cannot be present in the next correction subset (disjoint), until no more satisfiable subsets can be found.

Algorithm 7: `CorrSubsets`$(\mathcal{S}, \mathcal{F})$

```
1 K ← ∅
2 S' ← S
3 while SAT(S') do
4 |   C ← F \ Grow(S', F)
5 |   S' ← S' ∪ C
6 |   K ← K ∪ {C}
7 end
8 return K
```

For simple constraints p, Algorithm 7 is directly applicable and will be able to compute *disjoint* correction subsets. However, for more complicated p constraints, this easily degrades into computing only a single correction subset.

7.1.5 Correction Subsets Enumeration with Incremental MIP

If Algorithm 7 is directly applied to the MIP incremental `OCUS` variant that considers the whole formula $\mathcal{C} \wedge I_{end} \wedge \overline{(I_{end} \setminus I)}$, both the literal-to-explain and its negation will be present at line 5 leading to UNSAT. In a given explanation step, only the base constraints $\mathcal{C}$, the current interpretation I, and the literals of $\overline{(I_{end} \setminus I)}$ can be hit by the hitting set solver. Therefore, we project subset $\mathcal{S}'$ onto the base constraints, the current interpretation, and the negated literals to explain. This extra step is executed right after line 5 of Algorithm 7:

$$\mathcal{S}' \leftarrow \mathcal{S}' \cap (\mathcal{C} \cup I \cup \overline{I_{end} \setminus I})$$

By incorporating *explanation-specific* information, we are able to enumerate extra correction subsets that are p-disjoint.

Example 7 (Example 6 continued)**.** *Consider the same setting as in Example 6 with given initial interpretation $\mathcal{I} = \emptyset$ and $I_{end} = \{x_1, \neg x_2, x_3\}$. Table 5 illustrates the efficiency of the incremental variant of the `CorrSubsets` algorithm starting from hitting set $\mathcal{S} := \{\neg x_3\}$*

Step	$\mathcal{S}'$	$\texttt{SAT}(\mathcal{S}')$	$\mathcal{S}' \leftarrow \texttt{Grow}(\mathcal{S}, \mathcal{F})$	$\mathcal{K} \leftarrow \mathcal{K} \cup \{\mathcal{F} \setminus \mathcal{S}'\}$
				$\emptyset$
1.	$\{\neg x_3\}$	*true*	$\{c_1, c_2, c_4, \neg x_1, \neg x_2, \neg x_3\}$	$\{\{c_3, \cancel{x_1}, x_2, \cancel{x_3}\}\}$
2.	$\{c_3, x_2, \neg x_3\}$	*true*	$\{c_2, c_3, c_4, x_1, x_2, \neg x_3\}$	$\{..., \{c_1, \neg x_1, \cancel{\neg x_2}, \cancel{x_3}\}\}$
3	$\{c_1, c_3, \neg x_1, x_2, \neg x_3\}$	*false*		

Table 5: *Example 6 (continued).* Correction Subset enumeration starting from hitting set $\{\neg x_3\}$ with *MIP-incremental* `OCUS`.

as in the first step of our running example (Table 2 of Example 6). This example uses the ***SAT****-based* ***Grow*** *of Section 5.3.1.*

The MIP-based incremental variant of ***OCUS*** *uses unsatisfiable formula $\mathcal{F}$ defined as $\mathcal{C} \wedge I_{end} \wedge \overline{(I_{end} \setminus I)}$. For given interpretation $I = \emptyset$, the $\mathcal{F}$ corresponds $\mathcal{F} := \mathcal{C} \wedge \{x_1\} \wedge \{\neg x_2\} \wedge \{x_3\} \wedge \{\neg x_1\} \wedge \{x_2\} \wedge \{\neg x_3\}$.*

Taking a closer look at step 1 of Table 5, $\neg x_3$ is present in $\mathcal{S}$ and x_3 is in the corresponding correction subset. If we were to add it directly to $\mathcal{S}$, the algorithm would stop at the next iteration since $\mathcal{S}$ would be unsatisfiable. However, x_3 (and x_1) cannot be selected by the hitting set solver, and therefore should not be added. By adding only the clauses from $\{\mathcal{F} \setminus \mathcal{S}\}$ projected onto $(\mathcal{C} \cup I \cup \overline{I_{end} \setminus I})$, i.e. c_3 and x_2, we are able to enumerate ***multiple*** *correction subsets that are p-disjoint for the hitting set solver.*

Example 7 depicts the effectiveness of enumerating multiple correction subsets that are p-disjoint by projecting the correction subset onto the unsatisfiable formula for the current interpretation $(\mathcal{C} \cup I \cup \overline{I_{end} \setminus I})$. In the rest of the paper, we consider correction subset enumeration with a `SAT`-based grow as the baseline approach. We refer to it as *Multi-****SAT****.*

8. Experiments

In this section, we validate the *qualitative improvement* of computing explanations that are optimal with respect to a cost function as well as the *performance improvement* of the different versions of our algorithms.

Experimental Setup

Our experiments[2] were run on a compute cluster where each explanation sequence was assigned a single core on a 10-core INTEL Xeon Gold 61482 (Skylake) processor with a time limit of 60 minutes and a memory-limit of 8GB. The code is written on top of PySAT 0.1.7.dev1 (Ignatiev et al., 2018). For the MIP calls, we used Gurobi 9.1.2, for SAT calls MiniSat 2.2 and for `MaxSAT` calls RC2 as bundled with PySAT. In the MUS-based approach, we used PySAT's deletion-based MUS extractor MUSX (Marques-Silva, 2010).

2. The code for all experiments is made available at `https://github.com/ML-KULeuven/ocus-explain`.

Regarding the benchmark dataset, we rely on a set of generated Sudoku puzzles of increasing difficulty (different amount of given numbers), the Logic Grid puzzles of Bogaerts et al. (2021), as well as the instances from Espasa et al. (2021).[3]

When generating an explanation sequence for these puzzles, the unsatisfiable subsets identify which constraints and which previously derived facts should be combined to derive new information. Similar to Gamba et al. (2021), for Logic Grid puzzles, we assign a cost of 60 for puzzle-agnostic constraints; 100 for puzzle-specific constraints; and a cost of 1 for facts. For all other puzzles, we assign a cost of 60 when using a constraint and a cost of 1 for facts. In Table 12 of Appendix A, we summarize the average number of clauses (avg. # clauses), the average number of literals to explain (avg. # lits-to-explain) as well as the number puzzles (n) in the benchmark data set for each puzzle family.

Research Questions Our experiments are designed to answer the following research questions:

- Q1 What is the effect of using an *optimal* unsatisfiable subset, on the quality of the generated step-wise explanations?
- Q2 What is the impact of information **re-use** on the efficiency of `OCUS`?
- Q3 What are the time-critical components of `OCUS`?
- Q4 How does more advanced extraction of correction subsets and extraction of multiple correction subsets affect performance?
- Q5 What is the efficiency of a single step O(C)US
  - (a) from an instantaneous (time-to-first) explanation point of view?
  - (b) from a step-wise (single next explanation) solving point of view?

8.1 Explanation Quality

To evaluate the effect of optimality on the quality of the generated explanations, we reimplemented a MUS-based explanation generator based on Algorithm 2. Before presenting the results, we want to stress that this is *not* a fair comparison with the implementations of Bogaerts et al. (2020) and Espasa et al. (2021), where a heuristic is used that relies on *even more* calls to `MUS` in order to avoid the quality problems we will illustrate below. While in both cases this would yield better explanations, it comes at the expense of computation time, thereby leading to several hours to generate the explanation of a single puzzle.

To answer **Q1**, we ran the OCUS-based algorithm as described in Algorithm 3 and compared at every step the cost of the produced explanation with the cost of MUS-based explanation of Algorithm 2. These costs are plotted on a heatmap in Figure 1, where the darkness represents the number of occurrences of the combination at hand.

3. We express our gratitude towards *Matthew. J. McIlree* and *Christopher Jefferson* of St. Andrews University for their help with the extraction of CNF instances from Essence problem specifications (Frisch, Harvey, Jefferson, Martinez-Hernandez, & Miguel, 2008) using Savile Row (Nightingale, Akgün, Gent, Jefferson, Miguel, & Spracklen, 2017), as well as for supplying the problem instances.

We see that the difference in quality is striking in many cases, with the MUS-based solution often missing very cheap explanations (as seen by the darkest squares in the column above cost 60), thereby confirming the need for a cost-based OUS/OCUS approach.

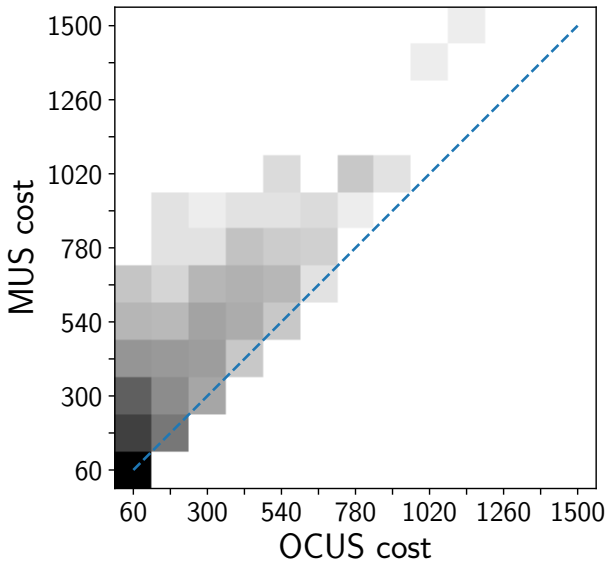


Figure 1: Q1 - Explanation quality comparison of optimal versus subset-minimal explanations in the generated puzzle explanation sequences.

8.2 Information Re-use

To answer **Q2**, we compare the effect of incrementality when generating a sequence of explanations. Next to (1) `OCUS`, we also include (2) the *bounded* `OCUS` (`OCUS_Bound`) algorithm, where we call the `OCUS` algorithm for every literal in every step, but we reuse information by giving it the current best bound $f(S_{best})$ and iterating over the literals that performed best in the previous call first; and (3) the *split* `OCUS` (`OCUS_Split`) approach, where we split up the computations by iteratively selecting the most promising literal and expanding only one hitting set for it, then re-evaluating the most promising literal and so forth.

8.2.1 Incremental versus Non-incremental Explanation Generation

Preliminary experiments have shown that incrementality by keeping track of the hitting sets using the MIP solver significantly outperforms bootstrapping satisfiable subsets. Therefore, in the experiments, we only show results on incrementality using MIP solvers.

For `OCUS`, incrementality (*+Incr*) is achieved by reusing the same MIP hitting set solver throughout the explanation calls, as explained in Section 7.1. Methods `OCUS_Bound` and `OCUS_Split` use a separate hitting set solver for every literal to explain. Each hitting set solver can similarly be made incremental (with respect to its own literal) across the explanation calls (*+Incr.*), or not.

Figure 2 depicts the number of instances fully explained through time before the given 1-hour timeout. In each configuration depicted, we use a single `SAT`-based `Grow` in the

`CorrSubsets` procedure. The same color is used for the same `OCUS` algorithms, with a full line for the incremental version and a dashed line for the non-incremental one.

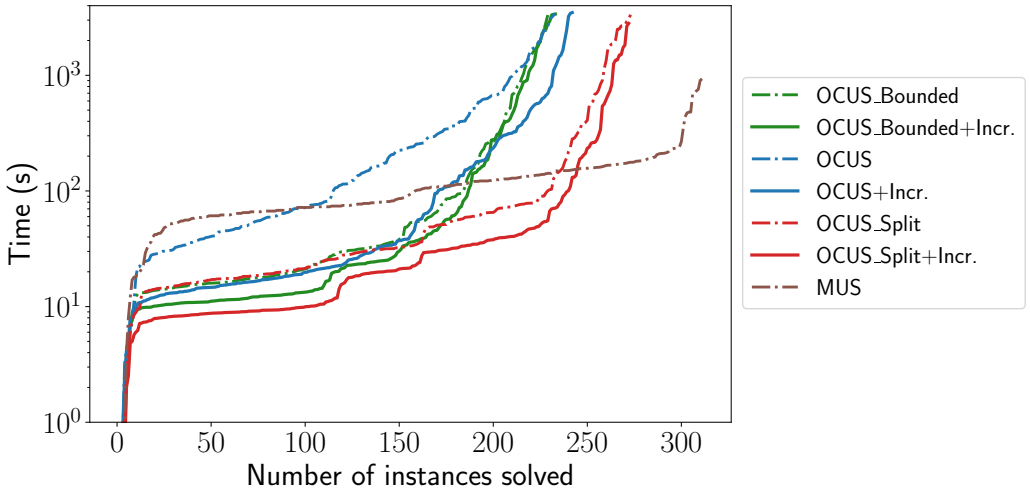


Figure 2: Time to generate a full explanation sequence with a single `SAT` grow call in the `CorrSubsets` procedure for incremental and non-incremental `OCUS` algorithms. Incrementality improves the number of instances solved and the time required to solve them for all O(C)US algorithms.

If we compare all configurations, we see that `OCUS` is faster than the plain `MUS`-based implementation for simpler instances. `MUS` is able to explain more instances than all `OCUS` versions, as it solves a simpler problem (with worse quality results as shown in **Q1**). `OCUS_Bound` is faster than `OCUS` for easier instances but explains about the same number of instances, and `OCUS_Split` is considerably faster and solves the most instances out of all `OCUS` algorithms.

The effect of introducing incrementality produces a speed-up in `OCUS`. For `OCUS_Bound` it is negligible and for `OCUS_Split` there is a speed-up in all but its most difficult instances. In general, we see that the curves of the incremental variants are located somewhat lower. The best runtimes are obtained with `OCUS_Split+Incr.`, that is, using an incremental hitting set solver *for every individual literal-to-explain separately* and only expanding the literal that is most likely to provide a cost-minimal OCUS.

8.2.2 Instance-level Speed-up with Incrementality

Next, we analyze the speed-up of introducing incrementality per instance. Fig. 3 compares the time to generate a full sequence for the incremental variant with the non-incremental version for each puzzle of every `OCUS` configuration. Results in the upper triangle signify an improvement using incrementality, and the lower triangle indicates worse performance with incrementality.

Taking a closer look at the results for `OCUS`, the story is similar to the results of Fig. 2. Many of the instances are explained quickly (around 10 to 20 seconds) by `OCUS+Incr.`, whereas non-incremental `OCUS` takes much longer to explain some instances, even leading to a timeout.

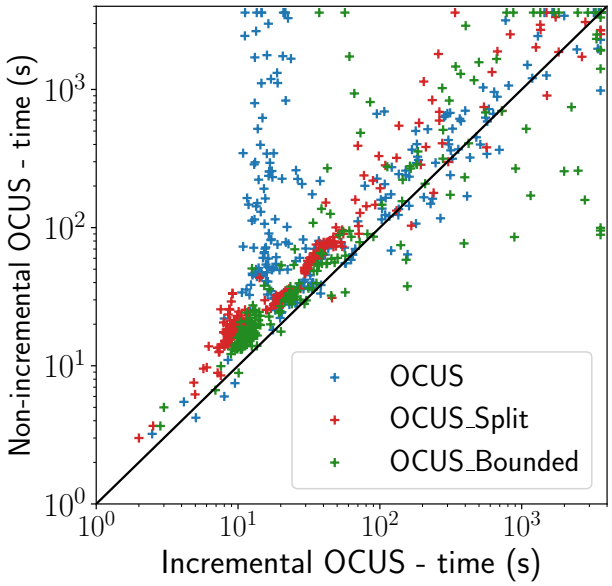


Figure 3: Q2 - Runtime comparison of introducing incrementality on the time to generate a whole explanation sequence with SAT-based Grow.

Incrementality with OCUS_Split and OCUS_Bound produce marginal improvements on the runtime. Most of the instances lie close to the black line. Only a few instances are present in the lower triangle, for the incremental variant of OCUS_Bound. For these instances, OCUS_Bound+Incr. takes on average double the time to generate the first explanation step due to the overhead associated with introducing incrementality. The story is similar for the few instances where OCUS_Split+Incr. is slower than OCUS_Split.

8.3 Runtime Decomposition

To evaluate the time-critical components of OCUS (Q3), we decompose the time spent in each part of the OCUS algorithms in Table 6. We only included the runtimes of instances that do not time out for all methods to allow a fair comparison.

The table depicts for each configuration (1) the number of instances *explained*; (2) %OPT the percentage of time spent in the hitting set solver; (3) %SAT the percentage of time spent in the sat solver: (4) %CorrSS the percentage of time spent in the CorrSubsets procedure; and (5) N_{sth} the average total number of sets-to-hit computed. Each version of the OCUS algorithm uses the SAT-based grow in the CorrSubsets procedure (see Table 7).

Looking closer at the runtime decomposition, we observe that most of the time in all the OCUS algorithms is spent computing the optimal hitting sets. The results in the N_{sth} column (top 3 rows versus incremental bottom 3 rows), highlight the decrease in the amount of sets-to-hit that need to be computed when adding incrementality, in our case, re-using the MIP solver between explanation steps. Indeed, similar to the results of Example 6, the OCUS algorithms do not need to recompute the previously derived sets-to-hit, and will therefore start with a good candidate hitting set at the beginning of an explanation step.

config	explained	%OPT	%SAT	%CorrSS	N_{sth}
OCUS	[233 / 403]	96.65%	3.01%	0.35%	6245
OCUS_Bound	[229 / 403]	86.86%	12.31%	0.83%	9310
OCUS_Split	[273 / 403]	88.58%	10.41%	1.01%	7480
OCUS+Incr.	[242 / 403]	99.16%	0.78%	0.06%	405
OCUS_Bound+Incr.	[233 / 403]	95.95%	3.94%	0.1%	1538
OCUS_Split+Incr.	[272 / 403]	96.28%	3.42%	0.3%	1713
MUS	[311 / 403]	—	—	—	—

Table 6: Runtime decomposition of core parts of O(C)US with the SAT-based grow. On the left, most of the computational time is spent in computing more optimal (constrained) hitting sets, while on the right, the runtime is shifted towards higher quality correction subsets. Incrementality, by re-using the same MIP solver throughout the explanation steps, helps to drastically reduce the average number of sets-to-hit N_{sth}.

8.4 Correction Subset Extraction

As Table 6 table shows, most time is spent computing the optimal hitting sets. Hence, there is potential in reducing its effort by computing better or more correction subsets, thereby having better collections of sets-to-hit. This induces a trade-off between the *efficiency* of the Grow strategy, the *quality* of the produced *satisfiable subset* as well as the corresponding *sets-to-hit* generated by the CorrSubsets procedure. In this section, we evaluate whether an efficient Grow-call is able to balance the efficiency and the quality of the produced satisfiable subset. Second, we analyze whether the enumeration of multiple, ideally p-disjoint, correction subsets reduces the time spent in the hitting set solver.

Thus, to answer **Q4**, we compare the incremental variants of OCUS, *bounded* OCUS, *split* OCUS, and only change the CorrSubsets strategy they use.

Efficient Correction Subset Enumeration Extending the observation of Section 5.3.1 that a call to an efficient MaxSAT solver helps in finding maximally satisfiable subsets, we propose three additional variants of Algorithm 7:

1. The first variant, *Multi-SAT*, repeatedly grows with SAT and blocks the corresponding correction subset until no more correction subsets can be extracted.

2. The second variant is *Multi-MaxSAT*. This correction subset enumerator repeatedly grows using the domain-specific MaxSAT introduced in Section 5.3.1 until the updated subset $\mathcal{S}'$ is no longer satisfiable.

3. The last variant *Multi-SubsetMax-SAT* repeatedly grows using the *SubsetMax-SAT* to balance the trade-off between efficiency and quality.

Figure 4 depicts for each incremental OCUS algorithm, the number of instances solved across time for varying correction subset approaches. For OCUS+Incr., all MaxSAT-based methods for enumerating correction subsets provide similar results and are able to explain more instances than the rest. The story for OCUS_Split+Incr. and OCUS_Bound+Incr. is

CorrSubsets	**Description**
SAT	*Extract a satisfiable model computed by the* ***SAT*** *solver.*
SubsetMax-SAT	*Extends the satisfiable subset computed by* ***SAT*** *by adding every remaining clause $c \in \mathcal{F} \setminus \mathcal{S}$ if $\mathcal{S} \cup \{c\}$ is satisfiable.*
Dom.-spec. MaxSAT	*Grow using an unweighted* ***MaxSAT*** *solver with domain-specific information, i.e. only previously derived facts and the original constraints (see Section 7.1).*
MaxSAT Full	*Grow with an unweighted* ***MaxSAT*** *solver using the full unsatisfiable formula $\mathcal{F}$.*
Multi SAT	*Repeatedly grow with* ***SAT*** *and block the corresponding correction subset until no more correction subsets can be extracted.*
Multi Dom.-spec. MaxSAT	*Repeatedly with* Dom.-spec. MaxSAT *and block the corresponding correction subset until no more correction subsets can be extracted.*
Multi SubsetMax-SAT	*Repeatedly grow with* SubsetMax-SAT *and block the corresponding correction subset until no more correction subsets can be extracted.*

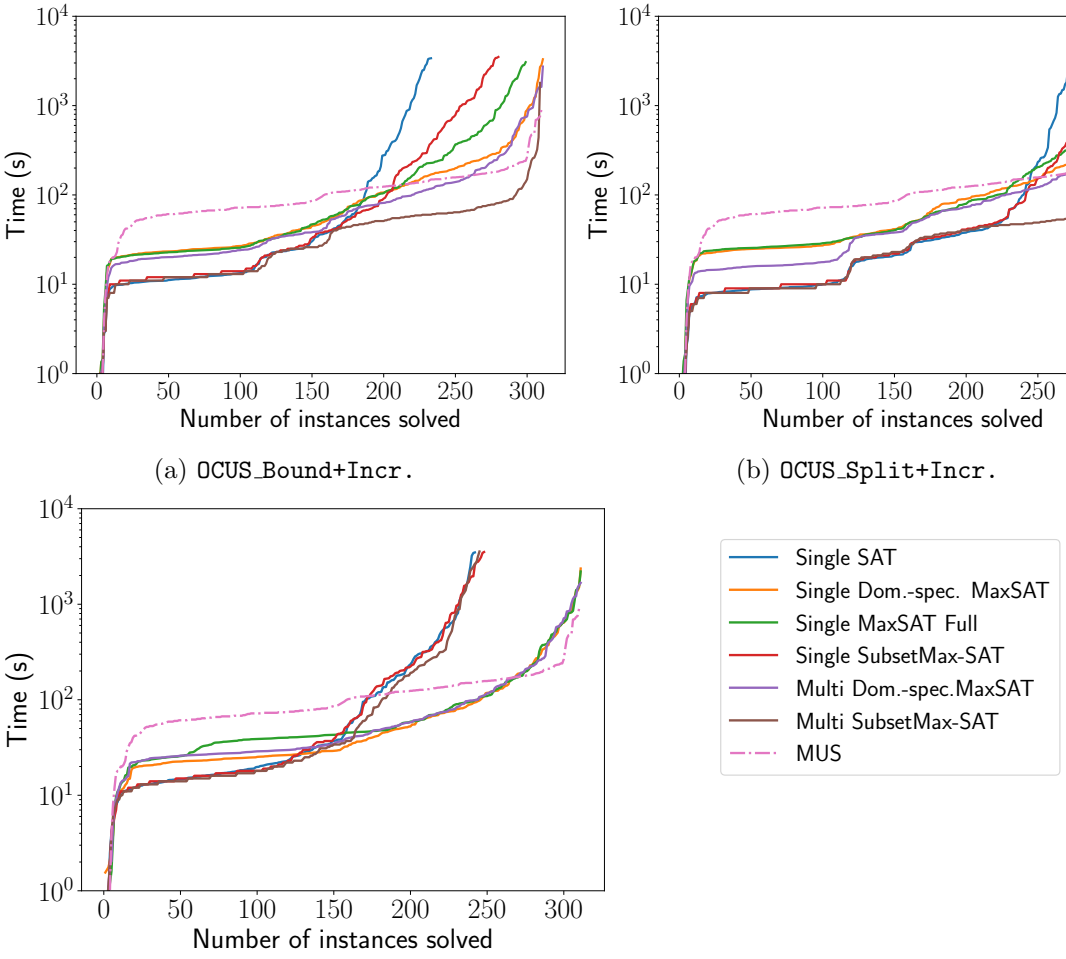
Table 7: Description of the correction subset procedures.

different. The best method for enumerating correction subsets with OCUS_Split+Incr. and OCUS_Bound+Incr. is *Multi*-SubsetMax-SAT. *Multi*-SubsetMax-SAT is able to consistently beat all other correction subset enumeration methods and is substantially faster than the naive MUS approach. To summarize, the best explanation sequence configuration corresponds to the iterated MIP-incremental approach of OCUS_Split+Incr. combined with *Multi*-SubsetMax-SAT.

Runtime Decomposition We now look at the runtime decomposition in Table 8 for the best performing CorrSubsets configuration, i.e. *Multi*-SubsetMax-SAT, also for the non-incremental OCUS variants. For the non-incremental variants, we observe that the shift in computation from the hitting set solver to correction subset enumeration clearly reaps its benefits.

	***Multi*-SubsetMax-SAT**				
config	**explained**	%OPT	%SAT	%CorrSS	$\mathbf{N_{sth}}$
OCUS	[291 / 403]	68.15%	2.78%	29.07%	3649
OCUS_Bound	[311 / 403]	39.87%	6.53%	53.6%	29747
OCUS_Split	[311 / 403]	45.24%	3.62%	51.14%	28320
OCUS+Incr.	[245 / 403]	87.38%	1.03%	11.59%	402
OCUS_Bound+Incr.	[309 / 403]	81.57%	5.68%	12.76%	1251
OCUS_Split+Incr.	[311 / 403]	79.64%	1.77%	18.58%	1274
MUS	[311 / 403]	—	—	—	—

Table 8: Runtime decomposition of core parts of OCUS. On the left, most of the computation time is spent in computing more optimal (constrained) hitting sets, while on the right, the runtime is shifted toward higher-quality correction subsets.



(a) `OCUS_Bound+Incr.`

(b) `OCUS_Split+Incr.`

(c) `OCUS+Incr.`

Figure 4: Average cumulative explanation time of correction subset configurations for the incremental O(C)US variants. The legends for each graph are ordered from the least instances explained (top) to the most instances explained (bottom).

Compared to Table 6, more instances are explained, and the computation is more balanced both for incremental and non-incremental `OCUS` algorithms. The non-incremental `OCUS` variants require considerably more correction subsets to be extracted and somewhat fewer in the incremental case. However, the number of instances explained is substantially higher for all `OCUS` configurations.

8.5 Efficiency of Single Step O(C)US, Instantaneous and Step-wise

In this section, we analyze whether the algorithms we developed could be fit for an interactive context. By an interactive context, we consider two types of settings. First, a user may want an *immediate explanation step* for the given CSP, and second, a user is asking for the next step, and the next, and so forth.

Table 9 depicts *Multi*-SubsetMax-SAT the best performing CorrSubsets procedure of Fig. 4. For each OCUS algorithm, we compute the average time to produce the first explanation step $\overline{t_1}$ (instantaneous), the average time to generate one step-wise explanation $\overline{t_{step}}$, and the explanation time quantiles 25 up to 100, where quantile 100 q_{100} symbols the most expensive step to generate over all the problem instances.

	***Multi*-SubsetMax-SAT**							
config	$\overline{\mathbf{t_1}}$	$\overline{\mathbf{t_{step}}}$	$\mathbf{q_{25}}$	$\mathbf{q_{50}}$	$\mathbf{q_{75}}$	$\mathbf{q_{95}}$	$\mathbf{q_{98}}$	$\mathbf{q_{100}}$
OCUS	3.41	2.54	0.51	0.77	1.39	8.37	18.50	523.67
OCUS_Bound	1.70	1.35	0.58	0.92	1.88	3.67	4.45	7.34
OCUS_Split	0.92	1.31	0.54	0.90	1.84	3.58	4.24	6.11
OCUS+Incr.	4.33	3.66	0.27	0.42	0.72	8.69	21.46	3452.20
OCUS_Bound+Incr.	3.22	0.58	0.39	0.51	0.67	1.07	1.57	17.58
OCUS_Split+Incr.	2.58	0.45	0.32	0.43	0.54	0.70	1.04	18.05

Table 9: **Non-timed out instances:** Decomposition of runtime for individual explanations into time to generate the first explanation step (t_1), the average time to produce an additional explanation step $\overline{t_{expl}}$ and q_{xx} the quantiles of the explanation times.

For the non-incremental variants, in the upper part of Table 9, OCUS is able to compute part of the explanations faster than the other OCUS configurations. We see, however, that both incremental and non-incremental OCUS still take a lot of time for some explanations compared to the other OCUS-based algorithms.

In the case of *OCUS_Bound*, the time to the first explanation reflects how important the ordering of literals to explain is for quickly finding a good bound on the cost of the next best explanation.

Logic Grid Puzzles In Table 10, we detail the runtime for explaining the logic grid puzzles of Bogaerts et al. (2020). In that work, due to the use of heuristics for finding low-cost explanations, the full explanation of a puzzle took between '15 minutes and a few hours'. Explaining the pasta puzzle takes less than 5 minutes using OCUS_Split+Incr. with *Multi*-SubsetMax-SAT as CorrSubsets procedure. Not only can we generate optimal explanations with respect to a given cost function, but we can also quickly provide an initial explanation and additional explanations. This suggests that our methods can be integrated into an interactive setting.

The next step is to find out what causes instances to timeout before the full explanation sequence has been generated with *Multi*-SubsetMax-SAT for all OCUS configurations.

Timed out Instances Most of the instances that timed out had on average more literals to explain than those that did not. Table 11 provides more context about the timed out instances:

- *#timed out* is the number of instances that have timed out.
- *#none* is to the number of instances where no explanation step was generated.
- $\overline{\%\text{ expl}}$ is the average percentage of literals that were explained before the instance timed out.

puzzle	$\mathbf{t_1}$	$\overline{\mathbf{t_{expl}}}$	$\mathbf{t_{tot}}$
origin	1.07s	0.29s	43.05s
p12	1.25s	0.43s	63.85s
p13	1.20s	0.37s	56.22s
p16	1.04s	0.27s	40.98s
p18	1.14s	0.16s	23.32s
p19	3.76s	0.55s	137.08s
p20	1.14s	0.16s	23.38s
p25	1.12s	0.26s	38.32s
p93	1.13s	0.32s	47.83s
pasta	0.60s	2.98s	286.03s

Table 10: Runtime decomposition of **Logic Grid Puzzles** of Bogaerts et al. (2020) into time to generate the first explanation step (t_1), the average time to produce an additional explanation step $\overline{t_{expl}}$, and time to generate a full explanation sequence t_{tot}.

config	#none	#timed out	$\overline{\%\text{ expl}}$
`OCUS`	3	112	44.57
`OCUS_Bound`	32	92	35.21
`OCUS_Split`	15	92	43.43
`OCUS+Incr.`	4	158	52.94
`OCUS_Bound+Incr.`	44	94	31.98
`OCUS_Split+Incr.`	15	92	49.45

Table 11: **Timed out instances:** *#none* is the number of instances where no explanations step was found before the time out, *#timed out* is the number of instances that timed out, % expl is the average percentage of literals explained.

In Fig. 5 we specifically report the average time taken to generate a first explaining step ($\overline{\mathbf{t_1}}$) for all configurations.

Note from Table 11 that `OCUS`(+Incr.) has the smallest number of instances where no explanation was found. Unlike `OCUS_Bound`(+Incr.) and `OCUS_Split`(+Incr.), `OCUS`(+Incr.) does not need to iterate over the many literals to explain in order to find a good bound on the cost of the next best explanation step. Furthermore, we observe that `OCUS`(+Incr.) is the fastest at generating a first explanation step with many outliers close to the .

Similar to the observations in Section 8.2.2, incrementality has a high impact on the time to explain an instance for all `OCUS` configurations. Adding incrementality to all `OCUS` configurations results in more instances with no explanation found than without incrementality. However, incrementality helps to explain more literals, except for `OCUS_Bound`, which first requires computing many OUSs before the best one is found. A similar trend can be seen in Fig. 5, where the introduction of incrementality increases the time to generate a first explanation step. Second, `OCUS_Bound` depends on a good ordering of the literals, which can change at any explanation step in the sequence.

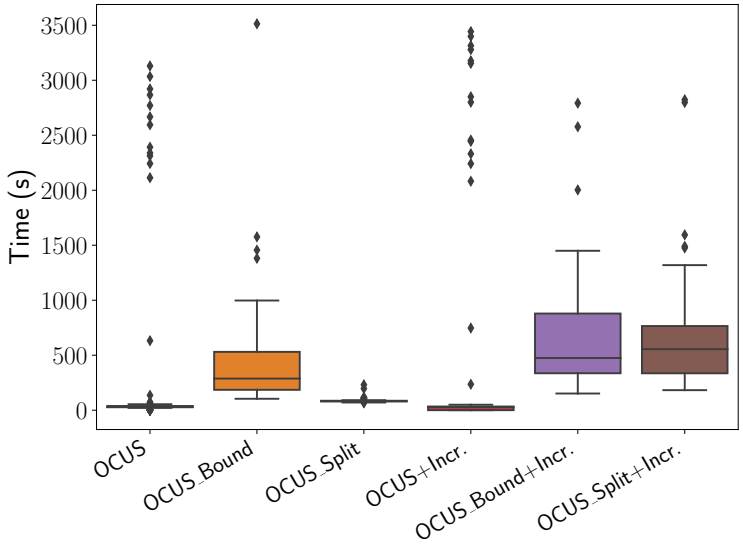


Figure 5: Average time to a first explanation step $\overline{\mathbf{t_1}}$.

To conclude, for an interactive context where the user asks for *an immediate explanation*, `OCUS_Split` will be the fastest to compute an explanation step. If the user *explores the sequence of explanations* and repeatedly *asks for additional explanations*, `OCUS_Split+Incr.` will be able to capitalise on incrementality to bring the average time close to real time.

9. Conclusion and Future Work

In this paper, we tackled the problem of efficiently generating explanations that are optimal with respect to a cost function. For that, we introduced algorithms that replace the many calls to an unsatisfiable core extractor of Bogaerts et al. (2021), with a single call to an optimal constrained unsatisfiable subset (`OCUS`). Our algorithm for computing `OCUS`s uses the implicit hitting set duality between Minimum Correction Subsets and Minimal Unsatisfiable Subsets. We propose two additional variants for the 'exactly one of' constraint used in step-wise explanation generation. The main bottleneck of these approaches is having to repeatedly compute *optimal* hitting sets. To compensate, we have developed methods for enumerating correction subsets that explore the trade-off between efficiency and quality of the subsets generated. An open question in an interactive setting is whether there are other methods of enumerating correction subsets that are better suited to reducing the time to first explanation and the average explanation time.

To efficiently generate the *whole* explanation sequence, we introduced *incrementality*, which allows the reuse of computed information, i.e. satisfiable subsets remain valid from one explanation call to another. In the case of `OCUS` for explanation sequence generation, where the underlying hitting set solver is MIP-based, we instantiate the MIP solver once for all explanation steps and keep track of computed sets-to-hit. However, MIP solvers do not natively support non-linear cost functions. Therefore, the current implementation of `OCUS` may not be able to fully capture the complexity of what constitutes a good explanation due

to the limitations of the cost functions we can encode. Furthermore, the question of which interpretability metric to use to characterise understandable explanations remains open.

The concept of (incremental) `OCUS` is not limited to explaining satisfaction problems. We are also interested in exploring other applications, such as configuration and machine learning, where it is necessary to compute not only minimal but also optimal unsatisfiable subsets. For example, a potential avenue for future work is how these explanation generation methods map to a constraint optimisation setting where branching or searching is required to solve the problem at hand. The synergies of our approach with the more general problem of QMaxSAT (Ignatiev et al., 2016) is another open question.

Finally, for interactive settings such as interactive tutoring systems, we are able to generate explanations in near real time (less than a second) using `OCUS_Split`. Another question is how to distribute the computation across multiple cores to parallelize the computation to further speed up the generation of explanations.

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Appendix A. Puzzle Data

		Properties of instances		
		n	avg. # clauses	avg. # lits-to-explain
puzzle type	**instance**			
logic	pasta	1	4572	96
	150	8	7535	150
	250	1	17577	250
sudoku	9x9-easy	25	14904	497
	9x9-simple	25	14904	497
	9x9-intermediate	25	14904	501
	9x9-expert	25	14904	505
demystify	binairo	156	16759	99
	garam	10	14486	756
	kakurasu	1	226	16
	kakuro	6	6961	240
	killersudoku	13	3609685	729
	miracle	1	59331	729
	nonogram	1	9813	36
	skyscrapers	16	17991	159
	star-battle	5	7533	82
	sudoku	76	34143	729
	tents	4	18644	476
	thermometer	1	1227	36
	x-sums	1	109717	729

Table 12: Characteristics of puzzle instances

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