Matrix Multiplication: Verifying Strong Uniquely Solvable Puzzles*

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Abstract. Cohn and Umans proposed a framework for developing fast matrix multiplication algorithms based on the embedding computation in certain groups algebras [12]. In subsequent work with Kleinberg and Szegedy, they connected this to the search for combinatorial objects called strong uniquely solvable puzzles (strong USPs) [11]. We begin a systematic computer-aided search for these objects. We develop and implement constraint-based algorithms build on reductions to SAT and IP to verify that puzzles are strong USPs, and to search for large strong USPs. We produce tight bounds on the maximum size of a strong USP for width $k \leq 5$, construct puzzles of small width that are larger than previous work, and improve the upper bounds on strong USP size for $k \leq 12$. Although our work only deals with puzzles of small-constant width, the strong USPs we find imply matrix multiplication algorithms that run in $O(n^\omega)$ time with exponent $\omega \leq 2.66$. While our algorithms do not beat the fastest algorithms, our work provides evidence and, perhaps, a path to finding families of strong USPs that imply matrix multiplication algorithms that are more efficient than those currently known.

Keywords: matrix multiplication · strong uniquely solvable puzzle · arithmetic complexity · integer programming · satisfiability · satisfiability benchmark · upper bounds · reduction · application

1 Introduction

An optimal algorithm for matrix multiplication remains elusive despite substantial effort. We focus on the square variant of the matrix multiplication problem, i.e., given two $n$-by-$n$ matrices $A$ and $B$ over a field $\mathcal{F}$, the goal is to compute the matrix product $C = A \times B$. The outstanding open question is: How many field operations are required to compute $C$? The long thought-optimal naïve algorithm based on the definition of matrix product is $O(n^3)$ time. The groundbreaking work of Strassen showed that it can be done in time $O(n^{2.808})$ [30] using a divide-and-conquer approach. A long sequence of work concluding with Coppersmith and Winograd’s algorithm (CW) reduced the running time

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Fig. 1: The leftmost diagram is a width-4 size-5 puzzle $P$. The middle three diagrams are the three sets of subrows of $P$. The rightmost diagram is the puzzle $P'$ resulting from reordering the subrows of $P$ as indicated by the arrows and then recombining them. Since $P$ can be rearranged as $P' \neq P$ without overlap, $P$ is not uniquely solvable.

Theorem 2. Any given width-$k$ puzzle can be rearranged as a distinct puzzle without cells with numbers overlapping in $O(n^{2.376})$ [26,28,31,13]. Recent computer-aided refinements of CW by others reduced the exponent to $\omega \leq 2.3728639$ [16,32,22].

**Approach** Cohn and Umans [12] introduced a framework for developing faster algorithms for matrix multiplication by reducing this to a search for groups with subsets that satisfy an algebraic property called the *triple-product property*, which allows matrix multiplication to be embedded in the group algebra. Their approach takes inspiration from the $O(n \log n)$ algorithm for multiplying degree-$n$ univariate polynomials by embedding into the group algebra of the fast Fourier transform, c.f., e.g., [14, Chapter 30]. Subsequent work [11] elaborated on this idea and developed the notion of combinatorial objects called *strong uniquely solvable puzzles* (strong USPs). These objects imply a group algebra embedding for matrix multiplication, and hence give a matrix multiplication algorithm as well.

A *width-$k$ puzzle* $P$ is a subset of $\{1, 2, 3\}^k$, and the cardinality of $P$ is the puzzle’s *size*. Each element of $P$ is called a *row* of $P$, and each row consists of three *subrows* that are elements of $\{1, *\}^k$, $\{2, *\}^k$, $\{3, *\}^k$ respectively. Informally, a puzzle $P$ is a *uniquely solvable puzzle* (USP) if there is no way to permute the subrows of $P$ to form a distinct puzzle $P'$ without cells with numbers overlapping. Figure 1 demonstrates a puzzle that is not a USP. A uniquely solvable puzzle is *strong* if a tighter condition for non-overlapping holds (see Definition 3). For a fixed width $k$, the larger the size of a strong USP, the faster matrix multiplication algorithm it gives [11]. In fact, Cohn et al. show that there exist an infinite family of strong USPs that achieves $\omega < 2.48$.

We follow Cohn et al.’s program by developing: (i) **verification algorithms** and heuristics to determine whether a puzzle is a strong USP, (ii) **search algorithms** to find large strong USPs, (iii) **practical implementations**

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1 Source code available here: [https://bitbucket.org/paraphase/matmult](https://bitbucket.org/paraphase/matmult)
algorithms, and (iv) new upper bounds on the size of strong USPs. The most successful of our verification algorithms work by reducing the problem through 3D matching to the satisfiability (SAT) and integer programming (IP) problems that are then solved with existing tools. The algorithms we develop are not efficient—they run in worst-case exponential time in the natural parameters. However, the goal is to find a sufficiently large strong USP that would provide a faster matrix multiplication algorithm, and the resulting algorithm’s running time is independent of the running time of our algorithms. The inefficiency of our algorithms limit the search space that we can feasibly examine.

Results Our theoretical results and implementation produces new bounds on the size of the largest strong USP for small-width puzzles. For small-constant width, \( k \leq 12 \), we beat the largest sizes of [11, Proposition 3.8]. Our lower bounds on maximum size are witnessed by strong USPs we found via search. For \( k \leq 5 \) we give tight upper bounds determined by exhaustively searching all puzzles after modding out common symmetries. For \( k \leq 12 \), we improve the upper bounds on the size of strong USPs. Although our current results do not beat [11] for unbounded \( k \), they give evidence that there may exist families of strong USPs that give matrix multiplication algorithms that are more efficient than those currently known. The best strong USP we can produce imply matrix multiplication algorithms with \( \omega \leq 2.66 \).

We also create a benchmark data set of SAT/UNSAT instances based on our reductions from strong-USP verification and examine the performance of solvers from the 2021 SAT Competition [6].

Related Work For background on algorithms matrix multiplication problem, c.f., e.g., [9]. There are also a number of negative results known. Naïvely, the dimensions of the output matrix \( C \) implies that the problem requires at least \( \Omega(n^2) \) time. Slightly better lower bounds are known in general and also for specialized models of computation, c.f., e.g., [29,20]. There are also lower bounds known for a variety of algorithmic approaches to matrix multiplication. Ambainis et al. showed that the laser method cannot alone achieve an algorithm with \( \omega \leq 2.3078 \) [4]. A recent breakthrough on arithmetic progressions in cap sets [15] combined with a conditional result on the Erdős-Szemerédi sunflower conjecture [3] imply that Cohn et al.’s strong USP approach cannot achieve \( \omega = 2 + \epsilon \) for some \( \epsilon > 0 \) [10]. Subsequent work has generalized this barrier [1,2] to a larger class of algorithmic techniques. Despite this, we are unaware of a concrete lower bound on \( \epsilon \) implied by these negative results. There remains a substantial gap in our understanding between what has been achieved by the positive refinements of LeGall, Williams, and Stothers, and the impossibility of showing \( \omega = 2 \) using the strong USP approach.

Recently Fawzi et al. showed how reinforcement learning techniques can be used to develop new matrix multiplication algorithms [17]. Their work produces matrix multiplication algorithms with \( \omega < 2.77 \), which is faster than Strassen’s
original algorithm ($\omega < 2.81$), but far from the refinements of Coppersmith-Winograd ($\omega < 2.372$) or the results achieved in this work.

**Organization** Section 2 begins with the formal definition of a strong USP and the Cohn-Umans framework. Sections 3 & 4, respectively, discuss our algorithms and heuristics for verifying that and searching for a puzzle that is a strong USP. Section 5 describes several upper bounds on the size of strong USPs. Sections 6 & 7 discuss our implementation and experimental results.

## 2 Preliminaries

For an integer $k$, we use $[k]$ to denote the set $\{1, 2, \ldots, k\}$. For a set $Q$, $\text{Sym}_Q$ denotes the symmetric group on the elements of $Q$, i.e., the group of permutations acting on $Q$. Cohn et al. introduced the idea of a puzzle [11].

**Definition 1 (Puzzle).** For $s, k \in \mathbb{N}$, an $(s, k)$-puzzle is a subset $P \subseteq [3]^k$ with $|P| = s$. We call $s$ the size of $P$, and $k$ the width of $P$.

We say that an $(s, k)$-puzzle has $s$ rows and $k$ columns. The columns of a puzzle are inherently ordered and indexed by $[k]$. The rows of a puzzle have no inherent ordering, however, it is often convenient to assume that they are ordered and indexed by the set of natural numbers $[s]$.

Cohn et al. establish a particular combinatorial property of puzzles that allows one to derive group algebras that matrix multiplication can be efficiently embedded into. Such puzzles are called strong uniquely solvable puzzles. However, to give some intuition we first explain a simpler version of the property called uniquely solvable puzzles.

**Definition 2 (Uniquely Solvable Puzzle (USP)).** An $(s, k)$-puzzle $P$ is uniquely solvable if for all $\pi_1, \pi_2, \pi_3 \in \text{Sym}_P$: Either (i) $\pi_1 = \pi_2 = \pi_3$, or (ii) there exists $r \in P$ and $c \in [k]$ such that at least two of the following hold: $(\pi_1(r))_c = 1$, $(\pi_2(r))_c = 2$, $(\pi_3(r))_c = 3$.

Informally, a puzzle is not uniquely solvable if each row of the puzzle can be broken into ones, twos, and threes pieces and then the rows can be reassembled in a different way so that each new row is a combination of a ones, a twos, and a threes piece where there is exactly one element of $[3]$ for each column. Observe that uniquely solvable puzzles can have at most $2^k$ rows because each ones piece, twos piece, and threes piece must be unique, as otherwise the duplicate pieces can be swapped making the puzzle not uniquely solvable.

The definition of strong uniquely solvable puzzle is below, it is nearly the same except that it requires that there be a collision on a column between exactly two pieces, not two or more pieces like in the original definition.

**Definition 3 (Strong USP (SUSP)).** An $(s, k)$-puzzle $P$ is strong uniquely solvable if for all $\pi_1, \pi_2, \pi_3 \in \text{Sym}_P$: Either (i) $\pi_1 = \pi_2 = \pi_3$, or (ii) there exists $r \in P$ and $c \in [k]$ such that exactly two of the following hold: $(\pi_1(r))_c = 1$, $(\pi_2(r))_c = 2$, $(\pi_3(r))_c = 3$. 

Finally, Cohn et al. defined a strengthening of SUSP which requires that every triple of rows witness the necessary overlap.

**Definition 4 (Local SUSP).** A local strong uniquely solvable puzzle is an \((s,k)\)-puzzle where for each triple of rows \(u,v,w \in P\) with \(u,v,w\) not all equal, there exists \(c \in [k]\) such that \((u_c,v_c,w_c)\) is an element of

\[
L = \{(1,2,1), (1,2,2), (1,1,3), (1,3,3), (2,2,3), (3,2,3)\}.
\]

Every SUSP \(P\) corresponds to a much larger local SUSP \(P'\), which, informally, is the result of concatenating and duplicating the rows of \(P\) to explicitly demonstrate the \(\forall \pi_1, \pi_2, \pi_3\) part of Definition 3.

**Proposition 1 ([11, Proposition 6.3]).** Let \(P\) be a \((s,k)\)-SUSP, then there is a local \((\epsilon s!, \epsilon s \cdot k)\)-SUSP \(P'\).

Note that in all of the definitions, local, strong, uniquely solvability is invariant to the ordering of the rows of the puzzle, because \(P\) is a set—we use this fact implicitly.

Cohn et al. show the following connection between the existence of strong USPs and upper bounds on the exponent of matrix multiplication \(\omega\).

**Lemma 1 ([11, Corollary 3.6]).** Let \(\epsilon > 0\), if there is a strong uniquely solvable \((s,k)\)-puzzle, there is an algorithm for multiplying \(n\)-by-\(n\) matrices in time \(O(n^{\omega+\epsilon})\) where

\[
\omega \leq \min_{m \in \mathbb{N}} \left( \frac{3 \log m}{\log(m-1)} - \frac{3 \log s!}{s \cdot k \log(m-1)} \right).
\]

This result motivates the search for large strong USPs that would result in faster algorithms for matrix multiplication. In the same article, the authors also demonstrate the existence of an infinite family of strong uniquely solvable puzzles, for width \(k\) divisible by three, that achieves a non-trivial bound on \(\omega\).

**Lemma 2 ([11, Proposition 3.8]).** There is an infinite family of strong uniquely solvable puzzles that achieves \(\omega < 2.48\).

Finally, they conjecture that strong uniquely solvable puzzles provide a route to achieving quadratic-time matrix multiplication. Unfortunately, as mentioned in the introduction, this conjecture was shown to be false.

**Lemma 3 ([10]).** Strong uniquely solvable puzzles cannot show \(\omega < 2 + \epsilon\), for some \(\epsilon > 0\).

That said, there remains hope that the uniquely solvable puzzle approach could beat the refinements of Coppersmith-Winograd even if it cannot reach \(\omega = 2\).
Algorithm 1: Brute Force Verification

Input: An \((s,k)\)-puzzle \(P\).
Output: YES, if \(P\) is a strong USP and NO otherwise.

1: function VerifyBruteForce\((P)\) 
2:   for \(\pi_2 \in \text{Sym}_P\) do 
3:     for \(\pi_3 \in \text{Sym}_P\) do 
4:       if \(\pi_2 \neq 1 \lor \pi_3 \neq 1\) then 
5:         found = false. 
6:       for \(r \in P\) do 
7:         for \(i \in [k]\) do 
8:           if \(\delta_{r,1} + \delta_{(\pi_2(r)),2} + \delta_{(\pi_3(r)),3} = 2\) then found = true. 
9:           if not found then return NO. 
10:          return YES.

3 Verifying Strong USPs

The core focus of this article is the problem of verifying strong USPs, i.e., given an \((s,k)\)-puzzle \(P\), output YES if \(P\) is a strong USP, and NO otherwise. In this section we discuss the design of algorithms to solve this computational problem as a function of the natural parameters \(s\) and \(k\).

All of the exact algorithms we develop in this section have worst-case exponential running time. However, asymptotic worst-case running time is not the metric we are truly interested in. Rather we are interested in the practical performance of our algorithms and their capability for locating new large strong USPs. The algorithm that we ultimately develop is a hybrid of a number of simpler algorithms and heuristics.

We begin by discussing a naïve brute force algorithm based on the definition of strong USP (Subsection 3.1), see how it motivations a reduction to the 3D matching problem (Subsection 3.2), and then how we might formulate a reduction to the satisfiability and integer programming problems (Subsections 3.4 & 3.5). We then describe several verification heuristics based on properties of strong USP (Subsection 3.6) and combine them with the verification algorithms to produce a hybrid algorithm Verify (Subsection 3.7). As we discuss in Subsection 7.2, our hybrid algorithm is quickly able to check whether a given puzzle is a strong USP and aid in the search for strong USP.

3.1 Brute Force

The obvious algorithm for verification comes directly from the definition of a strong USP. Informally, we consider all ways of permuting the twos and threes pieces relative to the ones pieces and check whether the non-overlapping condition of Definition 3 is met. A formal description of the algorithm is found in Algorithm 1.
The ones in Line 4 of Algorithm 1 denote the identity in Sym$_P$, and $\delta_{a,b}$ is the Kronecker delta function which is one if $a = b$ and zero otherwise. Observe that Algorithm 1 does not refer to the $\pi_1$ of Definition 3. This is because the strong USP property is invariant to permutations of the rows and so $\pi_1$ can be thought of as an arbitrary phase. Hence, we fix $\pi_1 = 1$ to simplify the algorithm.

Seeing that $|\text{Sym}_P| = s!$, we conclude that the algorithm runs in time $O((s!)^2 \cdot s \cdot k \cdot \text{poly}(s))$ where the last factor accounts for the operations on permutations of $s$ elements. The dominant term in the running time is the contribution from iterating over all pairs of permutations. Finally, notice that if $P$ is a strong USP, then the algorithm runs in time $\Theta((s!)^2 \cdot s \cdot k \cdot \text{poly}(s))$, and that if $P$ is not a strong USP the algorithm terminates early. The algorithm’s poor performance made it unusable in our implementation, however, its simplicity and direct connection to the definition made its implementation a valuable sanity check against later more elaborate algorithms (and it served as effective onboarding to the undergraduate students collaborating on this project).

Although Algorithm 1 performs poorly, examining the structure of a seemingly trivial optimization leads to substantially more effective algorithms. Consider the following function on triples of rows $a,b,c \in P$: $f(a,b,c) = \bigvee_{i \in [k]} (\delta_{a_i,0} + \delta_{b_i,1} + \delta_{c_i,2} = 2)$. We can replace the innermost loop in Lines 7 & 8 of Algorithm 1 with the statement $\text{found} = \text{found} \lor f(r,\pi_1(r),\pi_2(r))$. Observe that $f$ neither depends on $P$, $r$, nor the permutations, and that Algorithm 1 no longer depends directly on $k$. To slightly speed up Algorithm 1 we can precompute and cache $f$ before the algorithm starts and then look up values as the algorithm runs. We precompute $f$ specialized to the rows in the puzzle $P$, and call it $f_P$.

### 3.2 Strong USP Verification to 3D Matching

It turns out to be more useful to work with $f_P$ than with $P$. It is convenient to think of $f_P$ as a function $f_P : P \times P \times P \to \{0,1\}$ that is the complement of the characteristic function of the relations of a tripartite hypergraph $H_P = \langle P \sqcup P \sqcup P, E \subseteq P^3 \rangle$ where the vertex set is the disjoint union of three copies of $P$ and $f_P$ indicates the edges that are not present in $H_P$.

Let $H = \langle P \sqcup P \sqcup P, E \subseteq P^3 \rangle$ be a tripartite 3-hypergraph. We say $H$ has a 3D matching (3DM) iff there exists a subset $M \subseteq E$ with $|M| = |P|$ and for all distinct edges $e_1, e_2 \in M$, $e_1$ and $e_2$ are vertex disjoint, i.e., $e_1 \cap e_2 = \emptyset$. Determining whether a hypergraph has a 3D matching is a well-known NP-complete problem (c.f., e.g., [18]). We say that a 3D matching is non-trivial if it is not the set $\{(r,r,r) \mid r \in P\}$. Figure 2 demonstrates a 3-hypergraph with a non-trivial 3D matching.

The existence of non-trivial 3D matchings in $H_P$ is directly tied to whether $P$ is a strong USP.

**Lemma 4.** A puzzle $P$ is a strong USP iff $H_P$ has no non-trivial 3D matching.

**Proof.** We first argue the reverse. Suppose that $H_P$ has a non-trivial 3D matching $M$. We show that $P$ is not a strong USP by using $M$ to construct $\pi_1, \pi_2, \pi_3 \in$
Fig. 2: An example hypergraph $G$ with edges $E = \{(r_1, r_1, r_2), (r_1, r_3, r_3), (r_2, r_2, r_1), (r_2, r_3, r_1), (r_3, r_2, r_3)\}$. The highlighted edges are a non-trivial 3D matching $M = \{(r_1, r_1, r_2), (r_2, r_3, r_1), (r_3, r_2, r_3)\}$ of $G$.

Sym$_P$ that witness this. Let $\pi_1$ be the identity permutation. For each $r \in P$, define $\pi_2(r) = q$ where $(r, q, *) \in M$. Note that $q$ is well defined and unique because $M$ is a 3D matching and so has vertex disjoint edges. Similarly define $\pi_3(r) = q$ where $(r, *, q) \in M$. Observe that by construction

$$M = \{(\pi_1(r), \pi_2(r), \pi_3(r)) \mid r \in P\}.$$

Since $M$ is a matching of $H_P$, $M \subseteq f_P$. Because $M$ is a non-trivial matching at least one edge in $(a, b, c) \in M$ has either $a \neq b$, $a \neq c$, or $b \neq c$. This implies, respectively, that as constructed $\pi_1 \neq \pi_2$, $\pi_1 \neq \pi_3$, or $\pi_2 \neq \pi_3$. In each case we have determined that $\pi_1$, $\pi_2$, and $\pi_3$ are not all identical. Thus we determined permutations such that for all $r \in P$, $f(\pi_1(r), \pi_2(r), \pi_3(r)) = 0$. This violates Condition (ii) of Definition 3, hence $P$ is not a strong USP.

The forward direction is symmetric. Suppose that $P$ is not a strong USP. We show that $H_P$ has a 3D matching. For $P$ not to be a strong USP there must exist $\pi_1, \pi_2, \pi_3 \in \text{Sym}_P$ not all identical such that Condition (ii) of Definition 3 fails. Define $e(r) = (\pi_1(r), \pi_2(r), \pi_3(r))$ and $M = \{e(r) \mid r \in P\}$. Since Condition (ii) fails, we have that $f_P(e(r)) = \text{false}$ for all $r \in P$. This means that for all $r \in P$, $e(r) \in f_P$ and hence $M \subseteq f_P$. Since $\pi_1$ is a permutation, $|M| = |P|$. Observe that $M$ is non-trivial because not all of the permutations are identical and there must be some $r \in P$ with $e(r)$ having non-identical coordinates. Thus $M$ is a non-trivial 3D matching.

As a consequence of Definition 3, strong-USP verification is in coNP. Note that although 3D matching is an NP-complete problem, Lemma 4 does not immediately imply that verification of strong USPs is coNP-complete because $H_P$ is not an arbitrary hypergraph. It remains open whether strong-USP verification is coNP-complete. Lemma 4 implies that to verify $P$ is a strong USP it suffices to determine whether $H_P$ has a non-trivial 3D matching. In the subsequent subsections we examine algorithms for the later problem. We can, in retrospect, view Algorithm 1 as an algorithm for solving 3D matching.

We note that the parameters $s$ and $k$ are not fully independent. First, $s \leq 3^k$ because the maximum number of rows in a puzzle of width $k$ is $|3|^k = 3^k$. Second, we eliminate the dependence on $k$ entirely by transforming an $(s, k)$-puzzle
Algorithm 2: Bidirectional Dynamic Programming Verification

Input: An \((s,k)\)-puzzle \(P\).

Output: YES, if \(P\) is a strong USP and NO otherwise.

1: function VERIFY_DYNAMIC_PROGRAMMING\((P)\)
2: Let \(T = \emptyset\).
3: Construct 3D matching instance \(H_P\).
4: function SEARCH_HALF\((\ell, Q, \ell_Q, R, \ell_R, \delta, t)\)
5: if \(\ell = t\) then
6: if \(\delta = 1\) then \(\triangleright\) Forward Base Case
7: \(\text{Insert } (Q, R) \text{ into } T\).
8: return false.
9: else \(\triangleright\) Reverse Base Case
10: if \((P - Q, P - R) \in T\) then
11: return true.
12: else return false.
13: \(\text{res} = false.\) \(\triangleright\) Recursive Case
14: for \(\ell'_Q = \ell_Q + 1\) to \(s\) do
15: for \(\ell'_R = \ell_R + 1\) to \(s\) do
16: if \((p_\ell, p_\ell'_Q, p_\ell'_R) \in H_P \land \neg res\) then
17: \(\text{res} = \text{SEARCH_HALF}((\ell + \delta, Q \cup \{p_\ell'_Q\}, \ell'_Q, R \cup \{p_\ell'_R\}, \ell'_R, \delta, t)).\)
18: return res.
19: SearchHalf\((1, \emptyset, 0, \emptyset, 0, 1, [s/2] + 1)\).
20: return SearchHalf\((s, \emptyset, 0, \emptyset, 0, -1, [s/2])\).

into a 3D matching instance on the vertex set \([s]^3\). However, this transformation is not without cost, because the size of \(H_P\) is a function of the cube of \(s\) rather than linear in the size of the puzzle \(s \cdot k\).

3.3 Dynamic Programming

The realization that the verification of strong USPs is a specialization of 3D matching leads to a dynamic programming algorithm for verification that runs in linear-exponential time \(O(2^{2s}\text{poly}(s) + \text{poly}(s,k))\). The reduction allows us to replace the permutations from \(\text{Sym}_P\) with subsets of \(P\) and effectively reduce the cost of the outer loops of Algorithm 1 from \(s! = \Theta(2^{s \log s})\) to \(2^s\).

Algorithm 2 describes a recursive bidirectional dynamic programming algorithm for strong-USP verification that uses the 3D matching instance. The algorithm consists of two phases. Let \(t = \lfloor s/2 \rfloor\). The first phase determines all possible sets \(Q, R \subseteq P\) with \(|Q| = |R| = t\) such that there is 3D matching \(M_1\) of \(H_P\) when restricted to the vertices \(\{p_1, p_2, \ldots, p_t\} \cup Q \cup R\). The sets \(Q, R\) satisfying the requirement are stored in a table \(T\) during the first phase on Line 7. The second phase determines all possible sets \(Q, R \subseteq P\) with \(|Q| = |R| = s - t\)
such that there is a 3D matching $M_2$ of $H_P$ when restricted to the vertices \(\{p_{t+1}, p_{t+2}, \ldots, p_s\} \cup Q \cup R\). For each pair $(Q, R)$ the algorithm considers in the second phase, it checks whether $(P - Q, P - R)$ was inserted into $T$ during the first phase. If the pair is present, it means that there is a 3D matching of $H_P$ which is \(M = M_1 \cup M_2\). This works because, by Line 10, $M_1$ and $M_2$ are partial 3D matchings on \(\{p_1, \ldots, p_t\} \cup (P - R) \cup (P - Q)\), respectively, which implies that $M_1$ and $M_2$ are vertex disjoint. The first phase always returns \textit{false}, which is ignored, and the second phase returns whether a complete matching could be found, and, hence, by Lemma 4, whether $P$ is a strong USP.

The running time of this algorithm is dominated by the number of pairs of sets $(Q, R)$ it examines. Observe that rows of $P$ are considered in order in Lines 15 & 16. Further, the algorithm tracks the index of the last elements added to $Q$ and $R$ in $\ell_Q$ and $\ell_R$, respectively. The algorithm only adds new elements to $Q$ or $R$ that have higher indexes than ones previously added. Altogether this implies that each pair of sets $(Q, R)$ is only considered at most once during a phase. Since $Q, R \subseteq P$, there are at most \(\sum_{i=0}^{t} \binom{n}{i} \cdot \binom{s}{i} \leq (\sum_{i=0}^{t} \binom{i}{i})^2 \leq (2^s)^2 = 4^s\) pairs $(Q, R)$. This means that \text{SEARCHHALF} is called at most $4^s$ times during each phase. Hence the running time of the algorithm is $O(4^s \cdot s^2 \cdot \text{poly}(s) + T_{3DM}(s,k))$ where $s^2$ factor comes from the inner loops, \text{poly}(s) time to manipulate the sets and track the contents of $T$ as a hash table, and $T_{3DM}(s, k)$ accounts for the time to construct $H_P$. The memory requirements of Algorithm 2 are similarly high—the first phase uses $O(4^s \cdot s)$ bits to store $T$.

Note that Algorithm 2 does not early terminate on $P$ that are strong USP, because it must search through all pairs before determining that none can be found. The algorithm could be modified to allow early termination when $P$ is not a strong USP by causing the second phase of search to immediately return in Line 18 once the first 3D matching witness has been located. However, this still requires the first phase to run to completion. A remedy for this would be to run both phases in parallel and have them check against each other. We chose not to because it would substantially complicate the implementation and would be unlikely to ultimately improve the performance of our combined algorithms.

For comparison, more advanced techniques like those of Björklund et al. can achieve a better asymptotic time of $O(2^s \cdot \text{poly}(s))$ [8]. We chose not to implement their algorithm, because we judged that it would not substantially increase the domain for which verification was possible.

### 3.4 3D Matching to Satisfiability

By Lemma 4, one can determine whether a puzzle $P$ is a strong USP by constructing the graph $H_P$ and deciding whether it has a non-trivial 3D matching. Here we reduce our 3D matching problem to the satisfiability (SAT) problem on conjunctive normal form (CNF) formulas and then use a state-of-the-art SAT solver to resolve the reduced problem. To perform the reduction, we convert the graph $H_P$ into a CNF formula $\Psi_P$, a depth-2 formula that is the AND of
ORs of Boolean literals. We construct $\Psi_P$ so that $\Psi_P$ is satisfiable iff $H_P$ has a non-trivial 3D matching.

Let $H_P = (V = P \cup P \cup P, E \subseteq P^3)$ be the 3D matching instance associated with the puzzle $P$. Our goal is to determine whether there is a non-trivial 3D matching $M \subseteq E$. A naïve reduction would be to have variables $M_{u,v,w}$ indicating inclusion of each edge $(u, v, w) \in P^3$ in the matching. This results in a formula $\Psi_P$ with $s^3$ variables and size $\Theta(s^3)$ because including an edge $e \in P^3$ excludes the $\Theta(s^2)$ edges $e'$ with $e \cap e' \neq \emptyset$. To decrease the size of $\Psi_P$ we instead use sets of variables to indicate which vertices in the second and third part of $V$ are matched with each vertex in the first part. In particular we have Boolean variables $M^1_{1,u,v}$ and $M^2_{2,u,w}$ for all $u, v, w \in P$, and these variable map to assignments in the naïve scheme in the following way: $M^1_{1,u,v} \land M^2_{2,u,w} \iff M_{u,v,w}$.

We now write our CNF formula for 3D matching. First, we have clauses that prevents non-edges from being in the matching:

$$\Psi^\text{non-edge}_P = \bigwedge_{(u,v,w) \in E} (\neg M^1_{1,u,v} \lor \neg M^2_{2,u,w}).$$

Second, we add clauses require that every vertex in $H_P$ is matched with some edge:

$$\Psi^{\geq 1}_P = \left( \bigwedge_{u \in P} (\forall v \in P \ M^1_{1,u,v}) \land (\forall w \in P \ M^2_{2,u,w}) \right) \land \left( \bigwedge_{v \in P} (\forall u \in P \ M^1_{1,u,v}) \right) \land \left( \bigwedge_{w \in P} (\forall u \in P \ M^2_{2,u,w}) \right).$$

Third, we require that each vertex be matched with at most one edge and so have clauses that exclude matching edges that overlap on one or two coordinates.

$$\Psi^{\leq 1}_P = \bigwedge_{i \in \{1,2\}} \bigwedge_{(u,v),(u',v') \in P^2} (u = u' \lor v = v') \land (u, v \neq u', v') \Rightarrow \neg M^i_{1,u,v} \lor \neg M^i_{1,u',v'}.$$ 

Fourth, we exclude the trivial 3D matching by requiring that at least one of the diagonal edges not be used: $\Psi^\text{non-trivial}_P = \bigvee_{u \in P} \neg M^1_{1,u,u} \lor \neg M^2_{2,u,u}$. Finally, we AND these into the overall CNF formula: $\Psi_P = \Psi^\text{non-edge}_P \land \Psi^{\leq 1}_P \land \Psi^{\geq 1}_P \land \Psi^\text{non-trivial}_P$. The size of the CNF formula $\Psi_P$ is $\Theta(s^3)$, has $2s^2$ variables, and is a factor of $s^2$ smaller than the naïve approach. Thus we reduce 3D matching to satisfiability by converting the instance $H_P$ into the CNF formula $\Psi_P$.

### 3.5 3D Matching to Integer Programming

In parallel to the previous subsection, we use the connection between verification of strong USPs and 3D matching to reduce the former to integer programming, another well-known $\textbf{NP}$-complete problem (c.f., e.g., [21]) and then apply
a state-of-the-art solver to resolve it. Again, let \( H_P = \langle V, E \rangle \) be the 3D matching instance associated with \( P \). We construct an integer program \( Q_P \) over \( \{0,1\} \) that is infeasible iff \( P \) is a strong USP. Here the reduction is simpler than the previous one because linear constraints naturally capture matching.

We use \( M_{u,v,w} \) to denote a variable with values in \( \{0,1\} \) to indicate whether the edge \((u,v,w)\in P \) is present in the matching. To ensure that \( M \) is a subset of \( E \) we add the following edge constraints to \( Q_P \): \[ \forall u,v,w \in P, \sum_{u,v,w \in P} M_{u,v,w} = 0. \]

We also require that each vertex in each of the three parts of the graph is incident to exactly one edge in \( M \). This is captured by the following vertex constraints in \( Q_P \): \[ \forall w \in P, \sum_{u,v \in P} M_{w,u,v} = \sum_{u,v \in P} M_{w,v,u} = \sum_{u,v \in P} M_{u,w,v} = 1. \]

Lastly, since we need that the 3D matching be non-trivial we add the constraint: \[ \sum_{u \in P} M_{u,u,u} < |P|. \]

To check whether \( P \) is a strong USP we determine whether \( Q_P \) is not feasible, i.e., that no assignment to the variables \( M \) satisfy all constraints. We note that reduction from 3D matching to IP is polynomial time and that there are \( s^3 \) variables in \( Q_P \), and that the total size of the constraints is \( s^3 \cdot \Theta(1) + 3s \cdot \Theta(s^2) + 1 \cdot \Theta(s^3) = \Theta(s^3) \), similar to size of \( \Psi_P \) in the SAT reduction.

3.6 Heuristics

Although the exact algorithms presented in the previous sections make substantial improvements over the brute force approach, the resulting performance remains impractical. To resolve this, we also develop several fast verification heuristics that may produce the non-definitive answer MAYBE in place of YES or NO. Then, to verify a puzzle \( P \) we run this battery of fast heuristics and return early if any of the heuristics produce a definitive YES or NO. When all of the heuristics result in MAYBE, we then run one of the slower exact algorithms that were previously discussed. The heuristics have different forms, but all rely on the structural properties of strong uniquely solvable puzzles.

**Downward Closure** The simplest heuristics we consider is based on the fact that strong USPs are downward closed.

**Lemma 5.** If \( P \) is a strong USP, then so is every subpuzzle \( P' \subseteq P \).

**Proof.** Let \( P \) be a strong USP and \( P' \subseteq P \). By Definition 3, for every \((\pi_1,\pi_2,\pi_3) \in \text{Sym}_3^P\) not all identity, there exist \( r \in P \) and \( i \in [k] \) such that exactly two of the following hold: \((\pi_1(r))_i = 1, (\pi_2(r))_i = 2, (\pi_3(r))_i = 3\). Consider restricting the permutations to those that fix the elements of \( P \setminus P' \). For these permutations it must be the case that \( r \in P' \) because otherwise \( r \in P \setminus P' \) and there is exactly one \( j \in [3] \) for which \((\pi_j(r))_j = j\) holds. Thus we can drop the elements of \( P \setminus P' \) and conclude that for every tuple of permutations in \( \text{Sym}_{P'} \) the conditions of Definition 3 hold for \( P' \), and hence that \( P' \) is a strong USP.

This leads to a polynomial-time heuristic that can determine that a puzzle is not a strong USP. Informally, the algorithm takes an \((s,k)\)-puzzle \( P \) and \( s' \leq s \),
Algorithm 3: Downward-Closure Heuristic

Input: An \((s, k)\)-puzzle \(P\), and size \(s' \leq s\).
Output: NO, if \(P\) has a set of \(s'\) rows that do not form a strong USP, and MAYBE otherwise.

1: function \textsc{HeuristicDownwardClosed}(\(P, s'\))
2: for \(P' \subseteq P, |P'| = s'\) do
3: if \(P'\) is not a strong USP then return NO.
4: return MAYBE.

and verifies that all subsets \(P' \subseteq P\) with size \(|P'| = s'\) are strong USPs. If any subset \(P'\) is not a strong USP, the heuristic returns NO, and otherwise it returns MAYBE. For completeness, this algorithm is described in Algorithm 3.

This algorithm runs in time \(O(\binom{s}{s'} \cdot T(s', k))\) where \(T(s', k)\) is the runtime for verifying an \((s', k)\)-puzzle. In practice we did not apply this heuristic for \(s'\) larger than 3. When \(s'\) is some constant \(d\), the running time becomes \(O(s^d \cdot T(d, k)) = O(s^d k)\) using the brute force algorithm (Algorithm 1) for verification of the puzzle \(P'\).

**Unique Pieces** Every strong uniquely solvable puzzle is a uniquely solvable puzzle. A necessary condition for a puzzle to be a USP is that for each element in \([3]\), the collection of subrows contains no duplicates.

**Lemma 6 (Implicit in [11]).** If \(P\) is a USP, then for all \(e \in [3]\), and distinct rows \(r_1, r_2 \in P\), there is a column \(c \in [k]\) were one of the rows \(r_1\) or \(r_2\) has an \(e\) and the other one does not.

**Proof.** Suppose, for the sake of contradiction, that this is not the case, and distinct rows \(r_1, r_2 \in P\) have \(e\) in exactly the same columns for some \(e \in [3]\). We show that \(P\) is not a USP. Choose \(\pi_e = (r_1 r_2)\), i.e., the permutations that transposes the subrows for \(e\) in rows \(r_1\) and \(r_2\). Choose the other two permutations for the elements of \([3]\) \(\setminus\{e\}\) to be the identity. Since the permutations are not all the identity, the second half of Definition 2 applies. However, the puzzle that results from the permutations is identical to \(P\) and for all \(e \in [k]\) and each row \(r \in P\) there exists exactly on \(i \in [3]\) where \((\pi_e)(r))_c = i\). Hence the definition of uniquely solvable is not satisfied and we have a contradiction. \(\square\)

Note that the reverse direction of Lemma 6 does not hold. The puzzle in Figure 1 is an example of this: It is not uniquely solvable, but the subrows for each element are distinct.

We can make Lemma 6 effective as via a linear-time heuristic capable of ruling out puzzles that are not (strong) USPs. Although straightforward, for completeness we formalize our approach in Algorithm 4. When the sets are implemented as hash tables, the expected running time of this algorithm is \(O(s \cdot k)\) time, which is linear in the size of the puzzle \(P\). An alternative worst-case \(O(s \cdot k)\) time implementation uses radix sort to sort the characteristic sequences
Algorithm 4: Unique Pieces Heuristic

**Input:** An \((s,k)\)-puzzle \(P\).

**Output:** NO, if a witness is found for \(P\) not being a (strong) USP, and MAYBE otherwise.

1. **function** HeuristicUniquePieces\((P)\)
2. Initialize empty sets \(S_1, S_2, S_3\).
3. for \(r \in P\) do
4.   for \(e \in [3]\) do
5.     Let \(h = \{c \in [k] \mid r_c = e\}\).
6.     if \(h \in S_e\) then return NO.
7.     \(S_e = S_e \cup \{h\}\).
8. return MAYBE.

of the subrows as binary numbers and then scans adjacent rows to to detect duplication.

The unique pieces heuristic is equivalent to the downward-closure heuristic for subpuzzles of size two.

**Lemma 7.** Let \(P\) be an \((s,k)\)-puzzle, then \(\text{HeuristicUniquePieces}(P) = \text{HeuristicDownwardClosed}(P,2)\).

**Proof.** We show both directions.

Suppose that \(P\) fails the unique pieces heuristic for, w.l.o.g., \(e = 1\), then there are distinct rows \(r_1, r_2 \in P\) where the cells that contain 1 are all in the same columns. This means we can swap those 1’s subrows without causing overlap or changing the puzzle. This implies that \(P' = \{r_1, r_2\}\) is not a (strong) USP. Since \(|P'| = 2\) and \(P' \subseteq P\), the downward closure heuristic for \(s' = 2\) will also conclude that \(P\) is not a (strong) USP.

Suppose that \(P\) fails the downward-closure heuristic for \(s' = 2\). Then there is a pair of distinct rows \(r_1, r_2 \in P\) for which \(P' = \{r_1, r_2\}\) is not a strong USP. Suppose there is no columns were \(r_1\) and \(r_2\) differ, then the subrows of \(r_1, r_2\) are the same for all elements, and so \(P\) fails the unique pieces heuristic.

For the other case, suppose there is at least one column \(c \in [k]\) where \(r_1\) and \(r_2\) differ. W.l.o.g., let that column be \((r_1)_c, (r_2)_c\) = (1,2). Because \(P'\) is not an SUSP and this column is (1,2), there can be other no columns that are in from the set \{(1, 3), (2, 3), (3, 2), (3, 1)\} otherwise they would form an SUSP with the column (1,2). This means the only columns that \(P'\) contains are from the set \{(1, 2), (2, 1), (1, 1), (2, 2), (3, 3)\}. Therefore, the columns which contain 2 must match and the subrows for 2 in \(r_1\) and \(r_2\) are identical. Thus, \(P'\), and so \(P\), fails the unique pieces heuristic. \(\square\)

A corollary of this proof is that for size-two puzzles, every USP is also a strong USP.

**Corollary 1.** Let \(P\) be a \((2,k)\)-puzzle, if \(P\) is a uniquely solvable puzzle, then \(P\) is a strong uniquely solvable puzzle.
Since the unique pieces heuristic is equivalent to the downward-closure heuristic for \( s' = 2 \) and the running time of unique pieces is linear in the puzzle size, \( O(s \cdot k) \), and the running time of downward closed is \( O(s^2 \cdot k) \), we use the unique pieces heuristic in place of downward closed for \( s' = 2 \).

**Greedy** This heuristic attempts take advantage of Lemma 4 and greedily search for a 3D matching for the instance \( H_P \). The heuristic proceeds iteratively, determining the vertex of the first part of the 3D matching instance with the least edges and randomly selecting an edge of that vertex to put into the 3D matching. If the heuristic successfully constructs a 3D matching it returns NO indicating that the input puzzle \( P \) is not a strong USP. If the heuristic reaches a point were prior commitments have made the matching infeasible, the heuristic starts again from scratch. This process is repeated some number of times before it gives up and returns MAYBE. In our implementation we use \( s^2 \) attempts because it is similar to the running time of the reductions and it empirically reduced the number of instances requiring full verification in the domain of puzzles with \( k = 6, 7, 8 \) while not increasing the running time by too much. The greedy heuristic is formalized in Algorithm 5.

The array \( cts \) is used to store the number of edges \( cts[u] \) that remain associated with vertex \( u \) along the first coordinate. Much of the algorithm is devoted to maintaining this invariant. The sets \( U, V, W \) store the vertices along the three coordinates, respectively, that have already been incorporated into the partial 3D matching. Like in Algorithm 2 we do not store the matching itself, only the vertices involved. The break at Line 10 triggers when the partial 3D matching is a dead end and cannot be extended into a full 3D matching. The condition of Line 23 is true when a full 3D matching has been constructed and causes the algorithm to return that \( P \) is not a strong USP.

The running time of this algorithm is \( O(s^3t + T_{3DM}(s, k)) \), where \( T_{3DM}(s, k) \) is the time required to construct 3D matching instances from \( (s, k) \)-puzzles. This algorithm has the potential to be considerably slower than the downward-closure heuristic, and in practice we set \( t = s^2 \). However, the main loop can terminate early at Line 10 when it fails to extend the 3D matching, this permits the expected time to much less than the worst case. For a puzzle \( P \) that is a strong USP, the heuristic takes the full \( \Omega(s^3t + T_{3DM}(s, k)) \) time.

Compared to the downward-closure and unique pieces heuristics this heuristic is much less efficient. As a result we only run it when when the other heuristics have failed. See Subsection 7.2 for a comparison of effectiveness these heuristics in our experiments.

### 3.7 Hybrid Algorithm

Our final verification algorithm (Algorithm 6) is a hybrid of several exact algorithms and heuristics. The size thresholds for which algorithm and heuristic to apply were determined experimentally for small \( k \) and are focused on the values where our strong USP search algorithms are tractable \( k \leq 6 \) (or nearly
Algorithm 5: Greedy Heuristic

Input: An \((s,k)\)-puzzle \(P\), and iteration bound \(t\).
Output: NO, if a witness is found for \(P\) not being a strong USP, and MAYBE otherwise.

1: function HeuristicGreedy(\(P\))
2: Construct 3D matching instance \(H_P\).
3: for \(i = 1\) to \(t\) do
4:   for \(u \in P\) do
5:      \(cts[u] = \sum_{v,w \in P} H_P(u,v,w)\). \(\triangleright\) Number of edges incident vertex \(u\).
6:   Let \(U,V,W = \emptyset\).
7:   Let \(m = 0\). \(\triangleright\) Number of edges in matching.
8: while \(m < s\) do
9:   Select \(u \in \{w \in \bar{U} \mid cts[w] = \max_{v \in \bar{U}} cts[v]\}\) uniformly at random.
10:   if \(cts[u] = 0\) then break.
11:   Let \(D = \{(v,w) \in \bar{V} \times \bar{W} \mid H_P(u,v,w) = 1\}\).
12:   Select \((v,w) \in D\) uniformly at random.
13:   for \(v' \in P\) do \(\triangleright\) Update edge counts.
14:      for \(w' \in P\) do
15:         if \((v', w') \in \bar{V} \times \bar{W}\) and \(H_P(u,v',w') = 1\) then
16:            \(cts[u]--\).
17:         if \((v', w') \in \bar{U} \times \bar{W}\) and \(H_P(v',v,w') = 1\) and \(v' \neq u\) then
18:            \(cts[v']--\).
19:         if \((v', w') \in \bar{U} \times \bar{V}\) and \(H_P(v',w',w) = 1\) and \(v' \notin \{u,v\}\) then
20:            \(cts[v']--\).
21:      \(U,V,W = U \cup \{u\}, V \cup \{v\}, W \cup \{w\}\). \(\triangleright\) Add edge to matching.
22:      \(m = m + 1\).
23:   if \(m \geq s\) then return NO. \(\triangleright\) 3D matching found so not SUSP, halt.
24: return MAYBE.

tractable \(k \leq 8\)). We decide to run both of the reductions to SAT and IP in parallel because it is not clear which algorithm performs better in general. Since verification halts when either algorithm completes, the wasted effort is within a factor of two of what the better algorithm could have done alone. We also chose to do this because we experimentally observed that there were many instances that one of the algorithms struggled with that the other did not—this resulted in a hybrid algorithm that out performed the individual exact algorithms on average. We show in Subsection 7.2 that our hybrid algorithm and heuristics perform well in practice at quickly verifying strong USPs for small width \(k\). Further, Subsection 7.3 contains a discussion of the relative performance of the SAT and IP approaches on different instance types from our benchmark experiments.
Algorithm 6: Hybrid Verification

Input: An \((s,k)\)-puzzle \(P\).

Output: YES, if \(P\) is a strong USP, and NO otherwise.

1: function Verify\((P)\)
2: if \(s \leq 2\) then return Verify\text{BruteForce}\((P)\).
3: Return result if Heuristic\text{UniquePieces}\((P)\) is not MAYBE.
4: if \(s \leq 7\) then return Verify\text{DynamicProgramming}\((P)\).
5: Return result if Heuristic\text{DownwardClosed}\((P,3)\) is not MAYBE.
6: Return result if Heuristic\text{Greedy}\((P)\) is not MAYBE.
7: Run Verify\text{SAT}(P) and Verify\text{IP}(P) in parallel and return first result.

4 Searching for Strong USPs

With a practical verification algorithm in hand, we consider the problem of searching for large strong USPs. Because the set of strong USPs is downward closed, a natural search strategy is: Start with the empty set and repeatedly consider adding rows while maintaining the strong-USP property. However, while this strategy will lead to a maximal-size strong USP, it is not guaranteed to produce a maximum-size strong USP. This is because the set of strong USPs does not form a matroid, rather it is only an independence system (c.f., e.g., [25]).

In particular, (i) the empty puzzle is a strong USP and (ii) the set of strong USP are downward closed by Lemma 5. The final property required to be a matroid, the augmentation property, requires that for every pair of strong USPs \(P_1, P_2\) with \(|P_1| \leq |P_2|\) there is a row of \(r \in P_2 \setminus P_1\) such that \(P_1 \cup \{r\}\) is also a strong USP. For a simple counterexample consider the strong USPs \(P_1 = \{32\}\) and \(P_2 = \{12, 23\}\). Using Lemma 6, we see that neither \(P_1 \cup \{12\} = \{12, 32\}\) nor \(P_1 \cup \{23\} = \{23, 32\}\) are strong USPs, and hence the augmentation property fails. One consequence is that naïve greedy algorithms will likely be ineffective for finding maximum-size strong USPs. Furthermore, we do not currently know of an efficient algorithm that can take a strong USP \(P\) and determine a row \(r\) such that \(P \cup \{r\}\) is a strong USP.

Despite that, we have had some success in applying general-purpose tree-search techniques with pruning based on the symmetries of strong USPs together with our practical verification algorithm to construct maximum-size strong USPs for small \(k\).

4.1 Puzzle Symmetry

Since puzzles are defined as sets of rows, the ordering of the rows of a puzzle \(P\) does not affect the SUSP property. Similarly, but slightly less obviously, the SUSP property is invariant to reordering the columns of the puzzle, because the required existential condition \(\exists c \in [k]\) st. (...) from Definition 3 is independent
of the ordering of the columns. Lastly, the alphabet $[3]$ typically used to represent the elements of a puzzle is completely arbitrary, any set of three distinct values would suffice. These values are not interpreted mathematically, aside from their convenience in expressing the SUSP definition concisely. This logic can be formalized into the following lemma.

**Lemma 8.** Let $\rho \in \text{Sym}_{[k]}$, $\delta \in \text{Sym}_{[3]}$. A $(s, k)$-puzzle $P$ is a strong USP iff \[\{(\delta(r(c)))_{c \in [k]} \mid r \in P\}\] is a strong USP.

**Proof.** Follows immediately from Definition 1 and Definition 3. $\square$

This lemma implies that the SUSP property is invariant with respect to these kinds of puzzle transformations. We call two puzzles $P, P'$ that are related in this way isomorphic, and use the notation $P \cong P'$ to denote this. The relation $\cong$ is an equivalence relation, because permutations are invertable, and so it partitions the set of puzzles into equivalence classes.

This notion of isomorphism is naturally related to the same notion in graphs. For each $(s, k)$-puzzle $P$ we can define a colored, undirected graph $G_P$. This graph consists of vertices that are partitioned into four sets of different colors: $V = \{\text{row}_r\}_{r \in [s]} \cup \{\text{col}_c\}_{c \in [k]} \cup \{e_i\}_{i \in [3]} \cup \{v_{r,c}\}_{(r,c) \in [s] \times [k]}$. There are $s+k+3+s \cdot k$ vertices in $G_P$. The first three parts are vertices representing the rows and columns of $P$, and the elements of $[3]$, respectively, and the fourth part are vertices for each of the $s \cdot k$ cells in the $P$. The edge relation of $G_P$ is straightforward: Each vertex $v_{r,c}$ is connected to three vertices corresponding to the row, columns and element that the cell indexed $(r,c)$ contains in $P$. In particular, the three edges attached to $v_{r,c}$ are $(v_{r,c}, \text{row}_r), (v_{r,c}, \text{col}_c), (v_{r,c}, e_{\text{H}_{P(r,c)}})$. In total, $G_P$ has $3 \cdot s \cdot k$ edges. Because the vertex sets for rows, columns, and elements are each uniquely colored and each cell of $P$ is connected to vertices representing its row, column, and element, the automorphisms of $G_P$ are in 1-1 correspondence to the automorphisms of $P$ under permutations of rows, columns, and elements. This implies that for two $(s, k)$-puzzles $P, P'$, if $G_P \cong G_{P'}$ then there exists permutations of the rows, columns, and elements of $P$ which results in $P'$. Further by Lemma 8, if $G_P \cong G_{P'}$, then $P \cong P'$, and $P$ is an SUSP iff $P'$ is an SUSP.

### 4.2 Symmetry-Pruned Tree Search

A natural way to search for strong USPs is based on breadth-first search and uses the fact that strong USP are downward closed (Lemma 5): To find the largest possible width-$k$ strong USP, (i) start with all possible first rows – the $3^k$ $(1, k)$-puzzles, (ii) attempt to extend the resulting puzzles with all possible rows keeping only the puzzles that are strong USPs and which are not isomorphic to the strong USPs that have been seen before to form the new search frontier, and (iii) repeat Step (ii) until the search frontier is empty.

To ensure the algorithm does not revisit isomorphic puzzles, we use canonical graph representations $[G_P]$ of the puzzle graphs $G_P$. A canonical graph representation is a binary encoding of a graph with the property that for any two graphs $G_1, G_2, [G_1] = [G_2]$ iff $G_1 \cong G_2$ (c.f., e.g., [24]). As the search algorithm runs we
Algorithm 7: Symmetry-Pruned Breadth-First Search

**Input:** An integer $k \geq 0$.

**Output:** The number $b$, which is the size of the largest width-$k$ strong USP.

```algebra
1: function SP-BFS($k$)
2: Let $Q$ be an empty queue.
3: Let $I$ be an empty set.
4: Let $b = 0$.
5: enqueue($Q$, $\emptyset$).
6: while $Q$ is not empty do
7:     $P = \text{dequeue}(Q)$.
8:     for $r \in [3]^k \setminus P$ do
9:         Let $P' = P \cup \{r\}$.
10:        if Verify($P'$) and $[G_{P'}] \not\in I$ then
11:            enqueue($Q$, $P'$).
12:           $I = I \cup \{[G_{P'}]\}$.
13:          $b = |P'|$.
14:      return $b$.
```

record the set $I$ of canonical graph representations $[G_P]$ of each distinct puzzle $P$ that has been added to the search frontier. Each time a puzzle $P'$ is considered for being added to the search frontier we first check whether its canonical graph representation $[G_{P'}] \in I$, if it is, we do not add $P'$ to the frontier. The use of canonical representations of puzzles dramatically shrinks the search space by searching from $[P]$ rather than every $P' \cong P$ and by not allowing duplicates of $[P]$ to be enqueued. This algorithm SP-BFS is formalized in Algorithm 7.

We argue the correctness of this algorithm.

**Lemma 9.** For $k \in \mathbb{N}$, SP-BFS($k$) returns the maximum integer $s$ for which there exists an $(s,k)$-SUSP.

**Proof.** Ignoring the pruning that $I$ performs for a moment, it is routine to argue that SP-BFS behaves like a generic breadth-first search algorithm over the tree of all strong USPs. This is because of the downward-closure property of strong USP (Lemma 5), which makes any strong USP $P$ reachable from the trivial strong USP $\emptyset$ using a series of row inclusions. SP-BFS($k$) results in an exhaustive search of all strong USPs of width $k$ and return the maximum size $b$ of such SUSPs.

We argue that when considering the pruning that $I$ contributes to, SP-BFS($k$) enqueues exactly one element of each equivalence class of puzzles that are SUSPs. Then, as a consequence of Lemma 8, the algorithm must explore every equivalence class of width-$k$ SUSPs. Hence, it explores an equivalence class with SUSPs of maximum size and subsequently returns that size, which is the expected output.

To complete the argument and show that the symmetry pruned search covers the entire search space of equivalence classes, suppose, for the sake of contradic-
tion, that there is some smallest $s$ such that there is an $(s, k)$-puzzle $P$ that does not have its equivalence class $[P]$ searched. We know that $s > 1$, because the algorithm starts by considering all possible $(1, k)$-puzzles. Let $P'$ be the $(s-1, k)$-puzzle created from $P$ by removing one of its rows $r$, $P'$ has as least one row because $s > 1$. By hypothesis, the equivalence class of $[P']$ has been visited by SP-BFS because $P'$'s size is $s - 1 < s$. Consider $[P]$ and remove the row that corresponded to $r$ to form $[P]''$. It must be the case that $[P]'' \cong [P]'$. This isomorphism extends to $[P]$ in that there must be a row $r'$ such that $([P]' \cup \{r'\}) \cong [P]$, where $r'$ replaces the row removed from $[P]$. Therefore, since $[P']$ is searched, the algorithm must consider all possible rows to extend by, including $r'$. This is means that the equivalence class of $[P]$ is searched, contradicting our assumption. Therefore every equivalence class of SUSPs is searched by SP-BFS.

This approach reduces the size of the search space, improving both the running time of the search and the space required to keep track of the frontier puzzles. The worst case running time of SP-BFS is $O(3^k \cdot \#EQUIV(k) \cdot T_{\text{Verify}}(s_k + 1, k) + T_{\text{Canonize}}(s_k, k))$, where $\#EQUIV(k)$ is the number equivalence classes of strong USP of width $k$, $T_{\text{Verify}}(s_k + 1, k)$ is the time to verify the maximum size $(s_k + 1, k)$-puzzles examined by the algorithm, and $T_{\text{Canonize}}(s_k, k)$ is the time to compute the canonical graph representation of each puzzle $P$ considered by the algorithm (assuming $T_{\text{Verify}}$ and $T_{\text{Canonize}}$ are monotone in their parameters).

See Subsection 7.1 for the experimental results of running SP-BFS and a discussion of implementation issues.

\section{Upper Bounds}

Although the main focus of this research line is to construct sufficiently large strong USP that would imply faster matrix multiplication algorithms, our techniques and approach can also be applied to search for tighter upper bounds on the size of strong USP. We describe several SUSP-size upper bounds in this section.

\textbf{$\omega$ Bound.} Prior work explicitly discusses bounds on the capacity of infinite families of USP (c.f., [11, Lemma 3.2, Theorem 3.3]). Since every SUSP is a USP, these bounds also apply to SUSP and can be restated to apply to individual puzzles. The first bound, which we denote as the \textit{"{o} bound\textquotedblright}, results from (i) Lemma 1, which is monotone non-increasing for fixed $k$, and (ii) the fact that $\omega \geq 2$. To compute this bound we evaluate the inequality of Lemma 1 on increasingly large $s$ until just before the consequence implies $\omega < 2$ which is in contradiction with $\omega \geq 2$.

\textbf{Unique Pieces Bound.} The second bound, which we denote as the \textit{unique pieces bound\textquotedblright}, following directly from Lemma 6. Since that lemma requires that each row of a (strong) USP have a unique ones, twos, and threes piece, the total number of rows in a strong USP cannot be more than $2^k$. 
**USP Bound.** The third bound, which we denote as the “USP bound”, results from the proof of [11, Lemma 3.2]. Although not spelled out in that article, the proof relies on the following subclaim that directly bounds $s$ as a function of $k$.

**Proposition 2.** Let $P$ be a $(s,k)$-USP, then

$$s \leq \sum_{c_1=0}^{k-c_1} \sum_{c_2=0}^{k-c_2} \min \left( \binom{k}{c_1}, \binom{k}{c_2}, \binom{k}{k-(c_1+c_2)} \right) = O \left( k^2 \cdot \left( \frac{3}{2^{2/3}} \right)^k \right).$$

Note that the USP bound is asymptotically tighter than the unique pieces bound as $\frac{3}{2^{2/3}} \approx 1.8899 < 2$.

**Clique Bound.** The fourth bound, which we denote as the “clique bound”, results from the fact that SUSPs are downward closed (Lemma 5). In particular if $P$ is an SUSP, then for every $P' \subseteq P$ with 2 rows must also be an SUSP. Fix $k \in \mathbb{N}$ and consider a graph $G_k$ whose vertices correspond to the possible rows of a width-$k$ puzzle, i.e., strings in $[3]^k$, and where there is an edge between $r_1, r_2 \in [3]^k$ if $\{r_1, r_2\}$ is an SUSP. Observe that by downward closure, each $(s,k)$-SUSP corresponds to a clique of size $s$ in $G_k$. This approach naturally generalizes from the Clique problem to $h$-HypergraphClique problem where the graph $G_k^h$ consists the same $3^k$ vertices as $G_k = G_k^2$, but instead has the arity-$h$ edges $\{r_1, r_2, \ldots, r_h\}$ which are $(h,k)$-SUSPs.

**Proposition 3.** Let $P$ be an $(s,k)$-SUSP and $2 \leq h \leq s$. Then for

$$G_k^h = \langle V = [3]^k, E = \{P' \subseteq V | P' \text{ is a strong USP and } |P'| = h\} \rangle,$$

$(G_k^h, s) \in h$-HypergraphClique.

Therefore, the size of a maximum hypergraph clique in $G_k^h$ is an upper bound of size of width-$k$ SUSP. We use “clique bound” to denote the specific instantiation of this bound for $h = 2$.

**Exhaustive Bound.** For fifth bound, which we denote as the “exhaustive bound”, we consider the results of Algorithm 7 when run in the domain of $k$ where the full search space can be feasibly explored. Because these bounds are based on exhaustive search they are inherently tight.

**Downward-Closure Bound.** The final bound we consider follows from the downward-closure property of SUSPs.

**Proposition 4.** Let $P$ be an $(s,k)$-SUSP with $k > 1$, then there exists an $(\lceil \frac{s}{2} \rceil, k-1)$-SUSP.

**Proof.** Fix any $c \in [k]$ and consider the $c^{th}$ column of $P$, then, by averaging, there must be an element of $e \in [3]$ that appears at least $\lceil \frac{s}{2} \rceil$ times in that column. Let $P' \subset P$ be the subpuzzle of $P$ whose rows have $e$ in the $c^{th}$ column. $P'$ is a strong USP, because $P$ is a strong USP and strong USPs are downward
closed (Lemma 5). Form $P''$ by removing the $\ell$th column of $P'$. $P''$ is a strong USP, because $P'$ is a strong USP and the strong-USP property is invariant to addition or removal of constant columns. By construction, $P''$ is a $\left(\left\lceil \frac{s}{3} \right\rceil, k - 1\right)$-SUSP.

This bound is not as independently applicable like the others, but it can lift upper bounds of $s \leq u$ at $k$ to $s \leq 3u$ at $k + 1$.

See Subsection 7.1 for the results of evaluating the above bounds for small width and a discussion of issues involved in concretely calculating them.

6 Implementation

We implemented our verification algorithms, heuristics, and search algorithms, along with various utilities and appropriate datastructures to represent underlying information such as puzzles in C++. The source code for our implementation is available under a MIT License at https://bitbucket.org/paraphase/matmult.

We use a number of external libraries with subroutines that are key to the functioning of our algorithms. Our IP-based verifier and Clique bound calculator both use the commercial, closed-source mixed-integer programming solver Gurobi to solve the integer programs produced by our reductions [19]. Our SAT-based verifier uses, by default, the kissat-sc2021-sat solver from the 2021 SAT Competition by A. Biere, M. Fleury, and M. Heisinger [6, page 10]. Note that the conference version of this article used the MapleCOMSPS solver—see Subsection 7.3 for a discussion of solver benchmarks, comparisons, and choice. We implemented Algorithm 7 using our hybrid verifier, and the graph automorphism library Nauty [24] as a subroutine to perform the required graph canonization on $G_P$. The original versions of our SP-BFS implementation targeted a high-performance computing cluster environment, because our brute force and dynamic programming implementations were not efficient enough. Subsequent improvements to our verification algorithms made this unnecessary. Despite this, our SP-BFS implementation is still in MPI and uses a MapReduce framework [27] to maintain a distributed search frontier.

Our code base also contains multiple implementations of depth-first-search-inspired algorithms for locating strong USPs. These algorithms use our hybrid verification implementation and puzzle symmetry pruning technique discussed in Section 4. For brevity and to keep this article focused on strong-USP verification, we elect not to discuss these algorithms and defer them to a subsequent article. That said, some of the concrete puzzles we found and report in the next section were generated by such algorithms. These puzzles once found were experimentally verified as strong USPs using the techniques discussed in detail in Section 3.
Matrix Multiplication: Verifying Strong Uniquely Solvable Puzzles

7 Experimental Results

Our experimental results come in several flavors for small-constant width \( k \): (i) constructive lower bounds on the maximum size of width-\( k \) strong USPs witnessed by found puzzles, (ii) upper bounds on the maximum size of width-\( k \) strong USPs, (iii) the number of SUSPs and SUSP equivalence classes for width \( k \), (iv) experimental data comparing the run times of our verification algorithms and distinguishing likelihood of our heuristics, and (v) a benchmark data set of SAT/UNSAT instances that we use to compare the effectiveness of competitive SAT solvers as subroutines for the SAT-based part of our verifier.

All of the results in this section were produced by running our algorithm implementations on the same Ubuntu 20.04 PC with a 3.00 GHz Intel Core i9-10980XE CPU and 128 GB of RAM.

7.1 New Upper and Lower Bounds on the Size of Strong USPs

New Lower Bounds. Table 1 summarizes new lower bounds for maximum SUSP size in comparison with [11]. The lower bounds of [11] are from the constructions in their Propositions 3.1 and 3.8, which give families of strong USPs for even \( k \) or \( k \) divisible by three. For \( k \)'s which are not divisible by two or three, we extrapolate their construction by adding a new column, this preserves the SUSP property. The upper bounds on \( \omega \) in this table are computed by plugging \( s \) and \( k \) into Lemma 1 and optimizing over \( m \). For clarity we omit \( \omega \)'s that would be larger than previous columns. Our results in this table we produced by running SP-BFS and other search algorithms which verify that the final result is a strong USP. Our bounds are tight for all \( k \leq 5 \), because of the exhaustive nature of SP-BFS, and constructively improve the known lower bounds for 4 \( \leq k \leq 12 \).

Figure 3 contains representative examples of maximal-size strong USPs we found for \( k \leq 6 \). The strong uniquely solvable (14,6)-puzzles we found represent the greatest improvement in \( \omega \) versus the construction of [11] for small \( k \). Further, our puzzle for \( k = 12 \) is the result of taking the Cartesian product of two copies of a strong uniquely solvable (14,6)-puzzles. Note that Proposition 3.8 of [11]...
gives an infinite family of strong USPs that achieves $\omega < 2.48$ as $k$ goes to infinity, which is stronger than our results are directly able to achieve.

**New Upper Bounds.** Table 2 summarizes the results of evaluating the bounds from Section 5 for puzzles of width $k \leq 12$. The calculations were routine except for the clique bound that required constructing $G_k$, converting it into a mixed integer program, and solving that program using Gurobi [19]. This was feasible on our test system up to $k = 11$. We also experimented with calculating the upper bounds for the 3-HypergraphClique bound, but found it infeasible to compute for $k \geq 5$ and so have omitted the results. The final row of the table contains the best upper bounds we achieved, including applying the downward-closure bound to lift adjacent bounds at $k = 6$ and $k = 12$. These upper bounds are stronger than those immediately implied by [11].

Observe that exhaustive search produced the best and tightest bounds, and that the clique bound is considerably stronger than the unique pieces, USP, and $\omega$ bounds. The unique pieces bounds appears to be stronger than the USP bound, but we know that that is an artifact of the small value of $k$. As $k$ increase, the USP bound will become tighter than the unique pieces bound. Based on the processing time we spent on $k = 6$, we conjecture that $s = 14$ is tight for $k = 6$ and that our lower bounds for $k > 6$ are not. Our results suggests there is considerable room for improvement in the construction of strong USPs, and that it is possible that there exist large puzzles for $k = 7, 8, 9$ that would beat [11]'s constructions and perhaps come close to the Coppersmith-Winograd refinements. That said, it seems that new insights into the SUSP search problem are required to proceed for $k > 6$.

**Counting Strong USP.** Table 3 shows the number of strong USPs and equivalence classes of SUSP exhaustively calculated using SP-BFS with and without symmetric pruning. Observe that the number of strong USPs is many orders of magnitude more than the number of equivalence classes of strong USPs, even for (3,3)-SUSPs. Exhaustive search became infeasible even with puzzle symmetry.
Table 2: Upper bounds on the size of SUSPs for widths $k \leq 12$. Bold font indicates the bound is tight, and blanks indicate the calculation for this puzzle width was infeasible.

7.2 Algorithm Performance

To measure the performance of our verification algorithms and heuristics we ran them on 10,000 random puzzles at each point on a sweep through parameter space for widths $k = 5 \ldots 12$ and sizes $s = 1 \ldots 60$. We chose to test performance via random sampling because we do not have access to a large set of solved instances. This domain coincides with the frontier of our search space, and we tuned the parameters of the heuristics and algorithms in the hybrid algorithm to perform well in this domain. We did not deeply investigate performance characteristics outside of this domain. In Figures 4, 5, & 6 we plot results, for brevity, that are representative of the parameter space only for $k \in \{6, 9\}$.

**Running Time.** Figure 4 shows the average running times of our verification algorithms in seconds. The brute force and dynamic programming algorithms perform poorly except for very small size, $s \leq 8$, and their curves loosely match the exponential-time bounds we expect. The plots for the two reduction-based algorithms (SAT and IP) behave similarly to each other. They are slower than brute force and dynamic programming for small values of $s$, and their behavior for large $s$ is quite a bit faster. We speculate that the former is due to the cost of constructing the reduced instance and overhead of the third party tools. Further observe that the SAT reduction handily beats the IP reduction on large size for $k = 6$, but as $k$ increases, the gap decreases. We also note that across the settings of $k$ the IP reduction has effectively the same running time and is independent of $k$. This is likely because the size of the IP instance depends only on $s$. The hybrid algorithm generally performs best or close to best at small values of $s$ and is clearly faster for large values of $s$. Notice that it matches the dynamic programming algorithm closely for small values of $s$ and then diverges when the
reduction-based algorithms and heuristics are activated at larger \( s \). Observe that the hybrid algorithm is effectively constant time for large \( s \), though the size for which this happens increases as a function of \( k \). We expect this is because the density of strong USPs decreases rapidly with \( s \), and that the randomly selected puzzles are likely far from satisfying Definition 3 and, hence, they are quickly rejected by the unique pieces heuristics. Further evidence of this is that running time of the hybrid algorithm converges to the running time of the unique pieces heuristic for large \( k \).

**Heuristic Effectiveness.** Figure 5 shows the probability that each individual heuristic distinguishes a random puzzle in our benchmark. Observe that the distinguishing power of the downward closure heuristic for \( s' = 2 \) and unique pieces heuristics coincide, demonstrating experiment consistency with Lemma 7. Further, and for the same reason, the downward closure heuristic for \( s' = 3 \) has at least as high a distinguishing likelihood as the unique pieces heuristic. In the plots, these three heuristics achieve almost 100% probability of distinguishing random puzzles by size \( s = 30 \). The greedy heuristic perform less well than the others and get substantially worse as \( k \) increases. We do not plot the running times of the heuristics here, but they behave as expected by the earlier analysis. As we noted earlier, unique pieces is linear time in the size of the puzzle and the fastest of the heuristics. Figure 4 shows how the running time of the hybrid algorithm and unique pieces converges as essentially all random puzzles of large size, which the benchmark examined, are verified as non-SUSPs by this heuristic.

**Variation in Running Time.** Finally, we look at the variation in the running times of the hybrid algorithm in Figure 6. For small \( s \), the running time distribution is far from a normal distribution—the average is far above the median.

---

### Table 3: Number of equivalence classes (bold face, left) versus total number of encoded SUSPs (normal face, right) by \((s,k)\)-puzzle dimensions. Computed using Algorithm 7.

| \( s \) | \( 1 \) | \( 2 \) | \( 3 \) | \( 4 \) | \( 5 \) | \( 6 \) |
|---|---|---|---|---|---|---|
| 1 | 1 | 3 | 29 | 327 | 481 | 729 |
| 2 | 2 | 24 | 9 | 408 | 33 | 4,848 | 91 | 50,160 | 229 | 486,024 |
| 3 | 9 | 1,800 | 240 | 182,304 | 2,429 | 8,361,000 | 16,971 | 291,347,280 |
| 4 | 728 | 2,445,120 | 59,149 | 992,377,400 | 1,611,648 | ? |
| 5 | 190 | 3,248,640 | 707,029 | ? | ? | ? |
| 6 | ? | ? | ? |
| 7 | ? | ? |
| 8 | 89,196 | ? | ? | ? |
| 9 | ? | ? |

Empty cells indicate that the number of SUSPs and equivalence classes is zero. '?'s indicate unknown values that were infeasible to compute.
and middle 50\% of running times. This effect becomes even more pronounced as \( k \) increases. However, we find that as \( s \) increases, the median running time converges with the median running time of the unique pieces heuristic, and then for larger \( s \), the average running time converges as well. This is a consequence of the hybrid algorithm having to run the orders of magnitude slower reduction-based algorithms when the fast heuristics fail to resolve the instance. Although not plotted here, we found that the range of the distribution of running times for the SAT-based verifier was larger than for the IP-based verifier, even though the IP-based verifier was slower on average.

Overall, our hybrid verification algorithm performs reasonably well in practice on random instances, despite reductions through \textit{NP}-complete problems.

### 7.3 Choice of SAT Solver

In the conference version of this article we examined only one SAT solver for use in our implementation, MapleCOMSPS, a conflict-driven solver that uses a learning rate branching heuristic, and that was a top performer at the 2016 SAT Competition [7,23,5]. In this article we create a set of benchmark satisfiability instances, using the SUSP verification reduction on a variety of puzzles (recall
Fig. 5: Plots of the likelihood that each of the heuristics produces a definitive results on 10,000 random \((s,k)\)-puzzles for each size \(s \in \{50\}\) and width \(k \in \{6,9\}\). Here “row pairs” is HeuristicDownwardClosed\((P,2)\) and “row triples” is HeuristicDownwardClosed\((P,3)\). The row pairs points are plotted, but are hard to see, because the unique pieces points coincides with them.

Subsection 3.4), and examined the performance of 35 solvers submitted to the main track of the 2021 SAT Competition [6]. We select benchmark instances consisting of \((s,k)\)-puzzle with sizes from the set

\[
\{(2,2), (3,3), (5,4), (8,5), (14,6), (21,7), (30,8), (42,9)\}
\]

We choose these sizes, because we want positive and negative instances and these sizes represent the largest strong USPs of each width we have been able to locate through search. For each size we created ten puzzles that are strong USPs and ten puzzles that are not. To create the ten non-USPs we randomly generated a puzzle of that size and verified it was not a strong USP. To create the ten strong USPs we for each size we used the results of our search algorithms. Then we ran all of the puzzles through our SAT reduction to create .dimacs files for each instance. Note that the SUSPs correspond to UNSAT instances and non-SUSPs correspond to SAT instances. In total there are 160 instances in this benchmark. We then ran each of the 35 solvers on each the 160 instance files and check the output of each run against the expected result. For each trial, we record the user CPU time reported by the Linux \texttt{time} command, or a timeout if the program runs more than 5000 seconds without halting (mimicking the rules of the real SAT competition). For comparison, we also run the MapleCOMSPS solver (from

\[2 \text{ There were 39 SAT solvers submitted to the main track. We use the default build configuration for each submission. We were unable to build three of them, and one that builds repeatedly crashed on all benchmarks without producing a result. We tested the remaining 35.} \]
Fig. 6: Log box plots of the distribution of the running times of the hybrid verification algorithm on 10,000 random \((s,k)\)-puzzles for each \(s \in [50], k \in \{6,9\}\). The blue circles denote the average running times of the hybrid algorithm. The dark blue blocks indicates the median times. The thick vertical lines indicate the middle 50% of times, and the thin vertical lines indicate the full range of running times at each \(s\).

earlier version of this article), our MIP-based verifier (recall Subsection 3.5) and our final hybrid verification algorithm on the same set of benchmark puzzles.

To compare the results of each solver we calculate the maximum time to complete each instance across all of the runs, which is 5000 seconds if a run timed out, and then divide by that maximum time to normalize all of the running times to the interval \([0,1]\). We calculate a benchmark score for each solver by summing their relative running times across all instances. Table 4 contains the benchmark scores for each solver.

MapleCOMSPS, the solver we used in the conference version of this article, performs similarly to the best scoring solvers from the 2021 competition. The recorded timeouts across all solvers come almost exclusively from the UNSAT instances derived from \((30,8)\)-SUSPs and \((42,9)\)-SUSPs. The Gurobi-based verifier performs substantially worse than the best performing satisfiability solvers on SAT instances (non-SUSPs), but dramatically better on UNSAT instances (SUSPs).

Figure 7 shows the performance of the Gurobi-based verifier against the five solvers with the best SAT scores. In this plot the instance completion times for each solver are sorted in increasing order, so that curves further to the left are better. If this were not a log-plot, the area to the left of the curve would be proportional to the benchmark scores from Table 4. Observe that for SAT instances, the SAT solvers, including MapleCOMSPS, follow similar trajectories. Gurobi performs an order of magnitude worse across all SAT instances. The hybrid algorithm, although plotted, is not visible because of how effective the heuristics are at identifying random SAT (non-SUSP) instances. For UNSAT
instances, the situation is different. Gurobi performs relatively more slowly for small, easier instances, but substantially better than the SAT solvers for larger, harder instances. The performance of the solvers on easier UNSAT instances is more varied than the corresponding case for SAT instances, but this does not translate into much of a difference in benchmark score because the magnitude of the relative completion time is low.

For UNSAT instances, the benchmark score is dominated by the number of timeouts, each of which effectively adds one to the score. Indeed, the plots for the SAT solver cut off between instance numbers 60 to 70, because the remaining instances cause timeouts. Finally, notice that hybrid algorithm out performs the others for small UNSAT instances – these are instances of the sort where the brute force and bi-directional search algorithms are applied. For larger instances the hybrid algorithm tracks an order of magnitude worse than the Gurobi-based verifier. This is because our algorithm is tuned to encounter many more SAT instances (non-SUSPs) than UNSAT instances (SUSPs). Further, because the one-sided heuristics rule out SAT instances quickly in practice, on UNSAT instances the hybrid algorithm runs these heuristics first, but then has to fall back on the Gurobi-based verifier causing some overhead.

Ultimately, the results of these benchmarking experiments suggest that there is not a substantial difference between using the 2016 MapleCOMSPS and the best solvers from the 2021 competition. Even so, we choose kissat-sc20221-sat as the default solver in our implementation, because it performed the best on our benchmark of SAT instances. Using our current approach, Gurobi is essential to the feasible verification of SUSPs.

The benchmark instances and puzzles, and the entirety of the raw timing data can be found in our repository.

8 Conclusions

We initiated the first study of the verification of strong USPs and developed practical software for both verifying and searching for them. We give tight results on the maximum size of width-$k$ strong USPs for $k \leq 5$ and improved upper and lower bounds on maximum strong-USP size for $k \leq 12$. We prove a number of properties of strong USPs related the verification and search. We also produce a new set of benchmark instances for SAT solvers.

Although our results do not produce a new upper bound on the running time of matrix multiplication, they demonstrate there is promise in this approach. There are a number of open questions. Is strong-USP verification coNP-complete? What is the maximum strong-USP capacity? Is there a way to bridge the apparent gap between the values of $\omega$ implied by single SUSPs and the values implied by infinite families of SUSPs? What are tight bounds on maximum-size strong USPs for $k \geq 6$ and do these bound lead to asymptotically faster algorithms for matrix multiplication?

3 https://bitbucket.org/paraphase/matmult/src/main/data_set/
The main bottleneck in our work is the size of the search space—new insights seem to be required to substantially reduce it. Are there subclasses of strong USPs that can be more effectively searched? Are there search strategies that would be more effective on this space?

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| Solver                  | SAT  | UNSAT | Total  | Timeouts |
|-------------------------|------|-------|--------|----------|
| cadical-hack-gb         | 17.51| 15.97 | 33.48  | 15       |
| cadical-less-UP         | 19.81| 16.14 | 35.95  | 15       |
| cadical-PriPro          | 19.49| 15.62 | 35.11  | 15       |
| cadical-PriPro_no_bin   | 16.55| 15.73 | 32.28  | 15       |
| cadical-rp              | 19.08| 15.78 | 34.85  | 15       |
| cadical-sc2021          | 18.82| 16.80 | 35.62  | 16       |
| Cadical_SCAVEL01        | 33.49| 16.73 | 50.23  | 15       |
| Cadical_SCAVEL02        | 40.97| 27.28 | 68.26  | 15       |
| cleanmaple              | 30.44| 18.93 | 49.37  | 17       |
| CleanMaple_PriPro       | 30.70| 20.18 | 50.87  | 18       |
| hCaD                    | 19.70| 16.52 | 36.22  | 16       |
| hKis                    | 13.15| 17.30 | 30.45  | 16       |
| kissat_bonus            | 13.04| 16.59 | 29.63  | 15       |
| kissat_cf               | 12.06| 16.19 | 28.26  | 14       |
| kissat_gb               | 12.52| 17.27 | 29.79  | 17       |
| kissat-MAB              | 15.28| 16.07 | 31.36  | 15       |
| kissat-sat_crvr_gb      | 13.37| 16.64 | 30.01  | 16       |
| kissat-sc2021           | 12.32| 16.08 | 28.40  | 14       |
| kissat-sc2021-sat       | **12.02**| 16.06| **28.08**| 14       |
| kissat-sc2021-sweep     | 12.82| 16.24 | 29.07  | 16       |
| lstech_maple            | 15.13| 14.83 | 29.96  | 12       |
| Maple_MBDR_BJL6_Tier2   | 19.46| 16.02 | 35.47  | 14       |
| Maple_MBDR_BJL7_Local   | 19.98| 15.49 | 35.47  | 13       |
| Maple_MBDR_Cent_PERM_10K| 25.20| 15.96 | 41.16  | **12**   |
| Maple_MBDR_Cent_PERM_75K| 25.07| 16.00 | 41.06  | **12**   |
| Maple_simp21            | 12.53| 16.72 | 29.26  | 15       |
| MapleSSV                | 15.56| 16.68 | 32.24  | 16       |
| parafrost-nomdn-sc2021  | 18.11| 15.56 | 33.67  | 14       |
| parafrost-sc2021        | 24.15| 15.61 | 39.76  | 14       |
| Relaxed_LCFTP           | 12.80| 17.55 | 30.35  | 16       |
| Relaxed_LCFTP_V2        | 13.97| 16.17 | 30.14  | **12**   |
| Relaxed_LCMDCBDL_BLB    | 15.38| 15.95 | 31.33  | 14       |
| Relaxed_LCMDCBDL_SCAVEL01| 13.95| 16.08 | 30.03  | 15       |
| Relaxed_LCMDCBDL_SCAVEL02| 25.45| 79.43 | 104.88 | 17       |
| slime                   | 17.26| 14.73 | 31.99  | 13       |
| MapleCOMSPS             | 12.98| 17.42 | 30.40  | 16       |
| Gurobi                  | 30.20| 0.00  | 30.20  | 0        |
| Hybrid                  | 0.00 | 0.01  | 0.01   | 0        |

Table 4: Scores for solvers on our SUSP verification benchmark. The SAT and UNSAT score are out of 80, the total score and timeouts are out of 160. Lower scores are better and minimum values for each SAT solver are bold in each column. The top part of the table includes the SAT solvers we tested from the 2021 SAT Competition [6].
Fig. 7: Plots of the sorted relative completion times for SAT and UNSAT instances on the five best-scoring solvers for that instance type.