

3-color bounded patterned self-assembly

Lila Kari · Steffen Kopecki · Shinnosuke Seki

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Abstract The problem of *patterned self-assembly tile set synthesis* (PATS) is to find a minimal tile set which uniquely self-assembles into a given pattern. Czeizler and Popa proved the NP-completeness of PATS and Seki showed that the PATS problem is already NP-complete for patterns with 60 colors. In search for the minimal number of colors such that PATS remains NP-complete, we introduce multiple bound PATS (MBPATS) where we allow bounds for the numbers of tile types of each color. We show that MBPATS is NP-complete for patterns with just three colors and, as a byproduct of this result, we also obtain a novel proof for the NP-completeness of PATS which is more concise than the previous proofs.

1 Introduction

Tile self-assembly is the autonomous formation of a structure from individual *tiles* controlled by local attachment rules. One application of self-assembly is the implementation of nanoscopic tiles by DNA strands forming double crossover tiles with four unbounded single strands Winfree et al. (1998). The unbounded single strands control the assembly of the structure as two, or more, tiles can attach to each other only if the bonding strength between these single strands is large enough. The general concept is to have many copies of the same tile types in a solution which then form a large crystal-like structure over time; often an initial structure, the *seed*, is present in the solution from which the assembly process starts.

A mathematical model describing self-assembly systems is the *abstract tile self-assembly model* (aTAM), introduced by Winfree (1998). Many variants of aTAMs have been studied: a main distinction between the variants is whether the *shape* or the *pattern* of a self-assembled structure is studied. In this paper we focus on the self-assembly of patterns, where a property, modeled as color, is assigned to each tile. Patterns in DNA crystals become visible by atomic force microscopy when the surface structures of the used tile types differ; for example when some of the tiles contain hairpin loops; see Liu et al. (1999). In Rothemund et al. (2004) this technique was used to visualize the self-assembly of Sierpinski triangles by DNA tiles. Further applications include the attachment of nanoparticles, like gold or silver, onto the surface of a self-assembled nanogrid, in order to produce materials with certain physical properties; see for example Zhang et al. (2006).

Formally, a pattern is a rectilinear grid where each vertex has a color: a k -colored $m \times n$ -pattern P can be seen as a function $P : [m] \times [n] \rightarrow [k]$, where $[i] = \{1, 2, \dots, i\}$. The optimization

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L. Kari · S. Kopecki (✉)
Department of Computer Science, The University of Western
Ontario, London, ON N6A 5B7, Canada
e-mail: steffen@csd.uwo.ca

L. Kari
e-mail: lila@csd.uwo.ca

S. Seki
Department of Information and Computer Science, Helsinki
Institute for Information Technology (HIIT), Aalto University,
P. O. Box 15400, 00076 Aalto, Finland
e-mail: shinnosuke.seki@aalto.fi

problem of *patterned self-assembly tile set synthesis* (PATS), introduced by Ma and Lombardi (2008), is to determine the minimal number of tile types needed to uniquely self-assemble a given pattern starting from an L -shaped seed. In this paper, we consider the decision variant of PATS, defined as follows:

Problem (k -PATS)

GIVEN: A k -colored pattern P and an integer m ;

OUTPUT: “Yes” if P can uniquely be self-assembled by using m tile types

Czeizler and Popa (2012) proved that PATS, where the number of colors on an input pattern is not bounded, is NP-hard, but the practical interest lies in k -PATS. Seki (2013) proved that k -PATS is NP-hard for the constant number of $k = 60$ colors. By the nature of the biological implementations, the number of distinct colors in a pattern can be considered small. In search for the minimal number k for which k -PATS remains NP-hard, we investigate a modification of PATS: *multiple bound PATS* (MBPATS) uses individual bounds for the number of tile types of each color.

Problem (k -MBPATS)

GIVEN: A pattern P with colors from $[k]$ and integers m_1 to m_k

OUTPUT: “Yes” if P can uniquely be self-assembled by using m_i tile types of color i , for $i \in [k]$

The main contribution of this paper is a polynomial-time reduction from PATS to 3-MBPATS which proves the NP-hardness of 3-MBPATS. However, our reduction does not take every pattern as input, we only consider a restricted subset of patterns for which PATS is known to remain NP-hard. The patterns we use as input are exactly those patterns that are generated by a polynomial-time reduction from 3-SAT to PATS. Using one of the reductions which were presented in Czeizler and Popa (2012), Seki (2013) as a foundation for our main result turned out to be unfeasible. Therefore, we present a novel proof for the NP-hardness of PATS which serves well as the foundation for our main result. Furthermore, our reduction from 3-SAT to PATS is more concise compared to previous reductions in the sense that in order to self-assemble a pattern P we only allow three more tile types than colors in P . In Czeizler and Popa’s approach the number of additional tile types is linear in the size of the input formula and Seki uses 84 tile types with 60 colors.

Let us note first that the decision variants of PATS and MBPATS can be solved in NP by simple “guess and check” algorithms.

Proposition 1 k -PATS and 3-MBPATS can be solved in NP.

Before we prove NP-hardness of k -PATS, in Sect. 3, and 3-MBPATS, in Sect. 4, we introduce the formal concepts of patterned tile assembly systems, in Sect. 2.

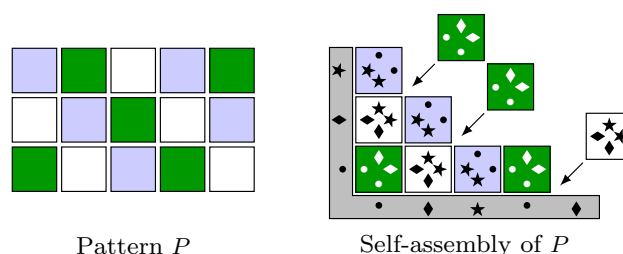


Fig. 1 Pattern P and how it can be self-assembled using three tile types

The results contained in this paper were presented at the DNA 19 conference in Tempe, Arizona, 2013. An extended abstract without full proofs was published in the conference proceedings Kari et al. (2013). Since the DNA 19 conference successive progress has been made in search for the minimal number k for which k -PATS, the original problem, remains NP-hard. It was proven that k -PATS is NP-hard for $k = 29$ Johnsen et al. (2013) and later for $k = 11$ Johnsen et al. Finally, to close this line of research, we want to report that Kari et al. (2014) proved the original conjecture that PATS is NP-hard for binary patterns ($k = 2$); at the time of submission only an arXiv version of the latter result was available. A difference in the proof of the latter result to previous proofs is that it utilizes a highly parallel computerized search in order to prove one crucial lemma and the proof is not entirely checkable by a human — a modern desktop computer would need about one year to do the computation. From Kari et al. (2014) we can also obtain that 2-MBPATS is NP-complete. A major difference of our approach to the approaches in Seki (2013), Johnsen et al. (2013), Johnsen et al., Kari et al. (2014) and its implications are stated in Remark 2.

2 Rectilinear tile assembly systems

In this section we formally introduce patterns and rectilinear tile assembly systems. An excellent introduction to the fundamental model aTAM is given in Rothmund and Winfree (2000).

Let C be a finite *alphabet of colors*. An $m \times n$ -pattern P , for $m, n \in \mathbb{N}$, with colors from C is a mapping $P : [m] \times [n] \rightarrow C$. By $C(P) \subseteq C$ we denote the colors in the pattern P , that is, the image or range of the function P . The pattern P is called k -colored if $|C(P)| \leq k$. The width and height of P are denoted by $w(P) = m$ and $h(P) = n$, respectively. The pattern is arranged such that position $(1, 1)$ is on the bottom left, $(m, 1)$ is on the bottom right, $(1, n)$ is on the top left, and (m, n) is on the top right of the pattern P . Figure 1 (left side) shows an example pattern.

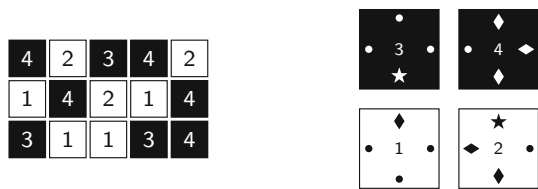


Fig. 2 The black/white pattern on the left can be assembled by using the four tile types on the right, which form a DRTAS; the pattern cannot be assembled by using only three tile types. The tile types and the positions in the pattern are labeled in order to illustrate which type is used in which position

Let Σ be a finite alphabet of glues. A colored Wang tile, or simply tile, $t \in C \times \Sigma^4$ is a unit square with a color from C and four glues from Σ , one on each of its edges. $\chi(t) \in C$ denotes the color of t and $t(N), t(E), t(W)$, and $t(S)$ denote the glues on the north, east, west, and south edges of t , respectively. We also call the south and west glues the *inputs* of t while the north and east glues are called *outputs* of t .

A rectilinear tile self-assembly system (RTAS) (T, σ) over C and Σ consists of a set of colored Wang tiles $T \subseteq C \times \Sigma^4$ and an L-shaped seed σ . The seed σ covers positions $(0, 0)$ to $(m, 0)$ and $(0, 1)$ to $(0, n)$ of a two-dimensional Cartesian grid and it has north glues from Σ on the positions $(1, 0)$ to $(m, 0)$ and east glues from Σ on positions $(0, 1)$ to $(0, n)$. We will frequently call T an RTAS without explicitly mentioning the seed. The RTAS T describes the self-assembly of a structure: starting with the seed, a tile t from T can attach to the structure at position $(x, y) \in [m] \times [n]$, if its west neighbor at position $(x - 1, y)$ and south neighbor at position $(x, y - 1)$ are present and the inputs of t match the adjacent outputs of its south and west neighbors; the self-assembly stops when no more tiles from T can be attached by this rule. Arbitrarily many copies of each tile type in T are considered to be present while the structure is self-assembled, thus, one tile type can appear in multiple positions. Figure 1 shows the process of self-assembling a pattern by an RTAS with three tile types. A *tile assignment* in T is a function $f : [m] \times [n] \rightarrow T$ such that $f(x, y)(W) = f(x - 1, y)(E)$ and $f(x, y)(S) = f(x, y - 1)(N)$ for $(x, y) \in [m] \times [n]$. The RTAS *self-assembles* a pattern P if there is a tile assignment f in T such that the color of each tile in the assignment f is the color of the corresponding position in P , that is, $\chi \circ f = P$. A terminological convention is to call the elements in T *tile types* while the elements in a tile assignment are called *tiles*.

A *directed RTAS* (DRTAS) T is an RTAS where any two distinct tile types $t_1, t_2 \in T$ have different inputs, that is, $t_1(S) \neq t_2(S)$ or $t_1(W) \neq t_2(W)$. A DRTAS has at most one tile assignment and can self-assemble at most one pattern. If T self-assembles an $m \times n$ -pattern P , it defines

the function $P_T : [m] \times [n] \rightarrow T$ such that $P_T(x, y)$ is the tile in position (x, y) of the tile assignment given by T . In this paper, we investigate minimal RTASs which uniquely self-assemble one given pattern P ; an example shown in Fig. 2. An observation from Göös and Orponen (2011) allows us to focus on DRTAS only when searching for minimal RTAS that uniquely self-assemble a given pattern:

Proposition 2 *If a pattern P can uniquely be self-assembled by an RTAS T with m tile types, then there is also a DRTAS T' with m tile types which (uniquely) self-assembles P .*

Remark 1 In the following proofs, a central concept is to show that the design of a pattern P enforces that any DRTAS T which self-assembles P (and maybe respects some tile type bounds) contains *tile types of a certain form*. As we are flexible with choosing the set of glues, we can always obtain a DRTAS with different tile types by applying some bijection on the set of glues. A subtler point is that glues used on horizontal edges and glues used on vertical edges can be seen as separate sets of glues as these edges can never glue to each other. For the ease of notation, we will use the same glue labels for horizontal and vertical glues, but keep in mind that we may apply one bijection to all horizontal glues and another bijection to all vertical glues in order to obtain an *isomorphic* DRTAS.

3 NP-hardness of PATS

In this section, we prove the NP-hardness of PATS. The proof we present uses many techniques that have already been employed in Czeizler and Popa (2012), Seki (2013). Let us also point out that we do not intend to minimize the number of colors used in our patterns or the size of our patterns. Our motivation is to give a proof that is easy to understand and serves well as a foundation for the results in Sect. 4.

A boolean formula F over variables V in *conjunctive normal form with three literals per clause*, 3-CNF for short, is a boolean formula such that

$$F = (c_{1,1} \vee c_{1,2} \vee c_{1,3}) \wedge (c_{2,1} \vee c_{2,2} \vee c_{2,3}) \wedge \dots \wedge (c_{\ell,1} \vee c_{\ell,2} \vee c_{\ell,3})$$

where $c_{i,j} \in \{v, \neg v \mid v \in V\}$ for $i \in [\ell]$ and $j = 1, 2, 3$. It is well known that the problem 3-SAT, to decide whether or not a given formula F in 3-CNF is satisfiable, is NP-complete; see for example Papadimitriou (2003). The NP-hardness of PATS follows by the polynomial-time reduction from 3-SAT to PATS, stated in Theorem 1.

Theorem 1 *For every formula F in 3-CNF there exists a pattern P_F such that F is satisfiable if and only if P_F can*

be self-assembled by a DRTAS with at most $|C(P_F)| + 3$ tile types. Moreover, P_F can be computed from F in polynomial time.

Theorem 1 follows by Lemmas 3 and 5, which are presented in the following.

Corollary 1 PATS is NP-hard.

The pattern P_F consists of several rectangular subpatterns which we will describe in the following. None of the subpatterns will be adjacent to another subpattern. The remainder of the pattern P_F is filled with unique colors; a color c is unique in a pattern P if it appears only in one position in P , that is, $|P^{-1}(c)| = 1$. As a technicality that will become useful only in the proof of Theorem 2 in Sect. 4, we require that each position adjacent to the L-shaped seed or to the north or east border of pattern P_F has a unique color. Clearly, for each unique color in P_F we require exactly one tile in any DRTAS which self-assembles P_F . Since each subpattern is surrounded by a frame of unique colors, the subpatterns can be treated as if each of them would be adjacent to an L-shaped seed and we do not have to care about the glues on the north border or east border of a subpattern.

As stated earlier, the number of tile types m that is required to self-assemble P_F , if F is satisfiable, is $m = |C(P_F)| + 3$. Actually, every color in $C(P_F)$ will require one tile type only except for one color which is meant to implement an OR-gate; see Fig. 3. Each of the tile types with color \square_{or} is supposed to have west input $w \in \{0, 1\}$, south input $s \in \{0, 1\}$, east output $w \vee s$, and an independent north output.

Our first subpattern p , shown in Fig. 4, ensures that every DRTAS which self-assembles the subpattern p contains at least three tile types with color \square_{or} . Throughout this section, two tiles with distinct labels are considered to have distinct colors. For the upcoming proof of Theorem 2 we need a more precise observation which draws a connection

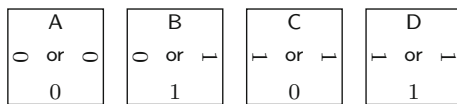


Fig. 3 The four tile types used to implement the OR-gate

between the number of distinct output glues and the

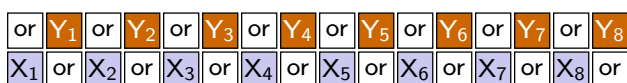


Fig. 4 The subpattern p

number of distinct tile types with color \square_{or}

Lemma 1 A DRTAS T which self-assembles a pattern including the subpattern p contains either

- (i) three distinct tile types $o_1, o_2, o_3 \in T$ with color \square_{or} all having distinct north and east glues,
- (ii) four distinct tile types $o_1, o_2, o_3, o_4 \in T$ with color \square_{or} all having distinct north glues and together having two distinct east glues,
- (iii) four distinct tile types $o_1, o_2, o_3, o_4 \in T$ with color \square_{or} all having distinct east glues and together having two north glues, or
- (iv) eight distinct tile types $o_1, \dots, o_8 \in T$ with color \square_{or} all having distinct east or north glues.

Proof In the subpattern p , each of the eight tiles t_1 to t_8 with colors \square_{Y_1} to \square_{Y_8} has south and west neighbors colored by \square_{or} . Since these tiles have mutually distinct colors they are all of different types as their inputs (south and west edges) have to differ. Therefore, the combination of outputs (north and east edges) of the tile types with color \square_{or} cannot be less than eight.

More formally, let $O \subseteq T$ be the set of tiles with color \square_{or} . Let i be the number of distinct north glues on tiles from O and let j be the number of distinct east glues

$$i = |\{t(N) \mid t \in O\}|, \quad j = |\{t(E) \mid t \in O\}|.$$

If $i \cdot j$ were less than 8, at least the inputs of two of the eight tiles t_1, \dots, t_8 would coincide as their placement solely depends on the outputs of tiles from O . There are four possibilities:

- (i) $i \geq 3$ and $j \geq 3$, therefore, $|O| \geq 3$,
- (ii) $i \geq 4$ and $j = 2$, therefore, $|O| \geq 4$,
- (iii) $i = 2$ and $j \geq 4$, therefore, $|O| \geq 4$, or
- (iv) $i \geq 8$ or $j \geq 8$, therefore, $|O| \geq 8$.

□

We aim to have statement (ii) of Lemma 1 satisfied, but so far all four statements are possible. The subpatterns q_1 to q_5 in Fig. 5 will enforce the functionality of the OR-gate tile types.

Lemma 2 Let P be a pattern that contains the subpatterns p and q_1 to q_5 , and let $m = |C(P)| + 3$. A DRTAS T with at most m tile types which self-assembles pattern P contains four tile types with color \square_{or} of the forms shown in Fig. 3. For every other color in $C(P)$ there exists exactly one tile type in T . Moreover, the tile type with color \square_{\rightarrow} has east output 0 and the tile type with color \square_{\leftarrow} has west input 1.

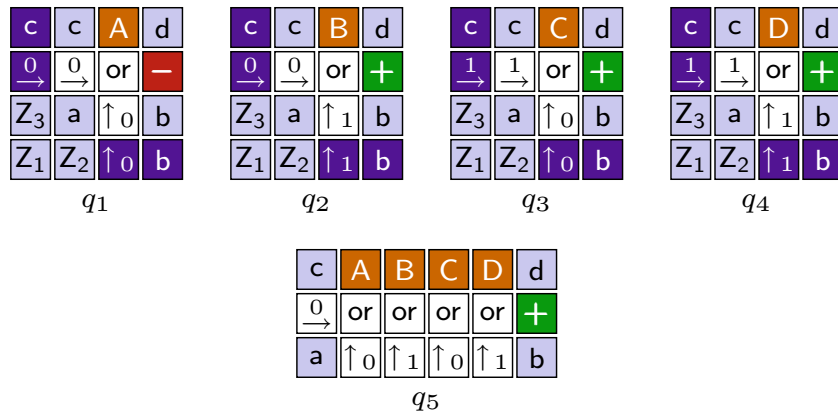


Fig. 5 The subpatterns q_1 to q_5

Proof By Lemma 1, the DRTAS T contains at least three tile types with color $\boxed{\text{or}}$. Since we need at least one tile type for each color in $C(P)$, there is one tile type left in T whose color is not determined yet. By $o_i \in T$ we denote the tile of color $\boxed{\text{or}}$ in subpattern q_i for $i = 1, 2, 3, 4$. We will show that all four tiles o_1, o_2, o_3, o_4 are of different types and are the tile types shown in Fig. 3, from left to right.

Suppose by contradiction, there were only three tile types with color $\boxed{\text{or}}$ and only one tile type with color \boxed{c} . Two of the tiles with colors \boxed{A} , \boxed{B} , \boxed{C} , and \boxed{D} in patterns q_1 to q_4 would have the same south and west neighbors and, hence, the inputs of the two corresponding tile types would coincide — a property which is forbidden for DRTAS s. Thus, either there are four tile types with color $\boxed{\text{or}}$ or two tile types with color \boxed{c} . For every other color there is exactly one tile type.

As there is only one tile type with color \boxed{b} the tiles o_1 and o_2 have to be of different types; otherwise, the tiles with colors $\boxed{-}$ and $\boxed{+}$ would have the same inputs in subpatterns q_1 and q_2 . Because tiles o_1 and o_2 have the same west neighbor, the tiles with colors $\boxed{\uparrow 0}$ and $\boxed{\uparrow 1}$ are responsible for the placement of o_1 and o_2 , respectively; this means the north glues of the tile types with colors $\boxed{\uparrow 0}$ and $\boxed{\uparrow 1}$ differ. Symmetrically, o_1 and o_3 are of different types and the east glues of the tile types with colors $\boxed{\xrightarrow{0}}$ and $\boxed{\xrightarrow{1}}$ differ. Next, we see that the four tiles o_1 to o_4 all have different inputs, thus, the types of o_1 to o_4 are mutually distinct and there is only one tile type with color \boxed{c} .

By the freedom of naming the used glues, see Remark 1, we assume that the tile type with color $\boxed{\xrightarrow{0}}$ has east output 0, and the tile type with $\boxed{\xrightarrow{1}}$ has east output 1, the tile type with color $\boxed{\uparrow 0}$ has north output 0, and the tile type with

color $\boxed{\uparrow 1}$ has north output 1. The two tiles with colors $\boxed{+}$ and $\boxed{-}$ have the same south input whence their west input differs and depends on the neighboring or-gate tile. We assume that the tile with color $\boxed{-}$ has west input $0'$ and the tile with color $\boxed{+}$ has west input $1'$. We have $o_1(E) = 0'$ and $o_2(E) = o_3(E) = o_4(E) = 1'$. By Lemma 1, the north outputs of the four tiles o_1 to o_4 have to be distinct.

Next, we take a look at subpattern q_5 . The tiles with colors \boxed{A} , \boxed{B} , \boxed{C} , and \boxed{D} , in the top row of subpattern q_5 enforce that the four or-gates below are of the same types as o_1, o_2, o_3 , and o_4 , from left to right; otherwise the south inputs of the top row cannot match the north outputs of the middle row. By the placement of the four or-gate tiles it is clear that $0 = 0'$ and $1 = 1'$ as desired. \square

The subpatterns that we defined so far did not depend on the formula F . Now, for each variable $v \in V$ we define three subpatterns $r_1(v), r_2(v), r_3(v)$ and for a clause C from F we define one more subpattern $s(C)$; these patterns are given by Fig. 6. For a formula F in 3-CNF we let P_F be the pattern that contains all the subpatterns p, q_1 to $q_5, r_1(v)$ to $r_3(v)$ for each variable $v \in V$, and $s(C)$ for each clause C from F , where each subpattern is placed to the right of the previous subpattern with one column of unique colors in between. Then, P_F has height 6, because the top and bottom rows contain only unique colors, and P_F has width $45 + 11 \cdot |V| + 6 \cdot \ell$. The next lemma follows from this observation.

Lemma 3 *Given a formula F in 3-CNF, the pattern P_F can be computed from F in polynomial time.*

Proof This is obvious by the design of the pattern. \square

The subpatterns $r_1(v)$ and $r_2(v)$ ensure that the two tile types with colors \boxed{v} and $\boxed{\neg v}$ have distinct north outputs.

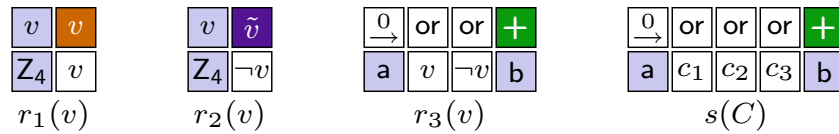


Fig. 6 The subpatterns $r_1(v)$ to $r_3(v)$ for a variable $v \in V$ and the subpattern $s(C)$ for a clause $C = (c_1 \vee c_2 \vee c_3)$ in F where $c_i = v$ or $c_i = \neg v$ for some variable $v \in V$ and $i = 1, 2, 3$

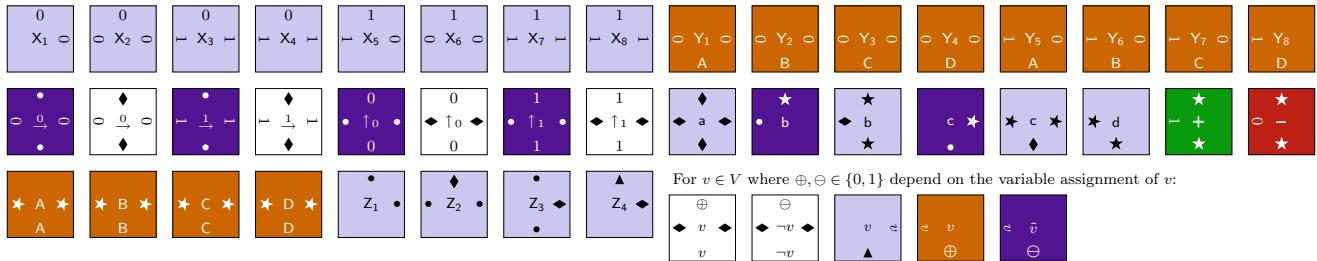


Fig. 7 All tile types, except for the or-gate, used to self-assemble the subpatterns in P_F . Unlabeled edges only appear on the outside borders of subpatterns; unique glues on these edges can be used to attach the subpatterns to the remaining structure

The subpattern $r_3(v)$ then implies that one of the north glues is 0 and the other one is 1.

Lemma 4 *Let P_F be the pattern for a formula F over variables V in 3-CNF and let T be a DRTAS with at most $m = |C(P_F)| + 3$ tile types which self-assembles pattern P_F . For all variables $v \in V$, there is a unique tile type $t_v^\oplus \in T$ with color \boxed{v} and a unique tile type $t_v^\ominus \in T$ with color $\boxed{\neg v}$ such that either $t_v^\oplus(N) = 1$ and $t_v^\ominus(N) = 0$ or $t_v^\oplus(N) = 0$ and $t_v^\ominus(N) = 1$.*

Proof Let $v \in V$, $t_v^\oplus \in T$ be the tile type with color \boxed{v} , and $t_v^\ominus \in T$ be the tile type with color $\boxed{\neg v}$. The fact that t_v^\oplus and t_v^\ominus are unique is stated Lemma 2 and, furthermore, for every color in $C(P_F)$ except for $\boxed{\text{or}}$ there exists just one tile type in T with that color. In particular, there is only one tile type with color \boxed{v} . Since the north neighbors of the tile of type t_v^\oplus in subpattern $r_1(v)$ and the tile of type t_v^\ominus in subpattern $r_2(v)$ differ while their north neighbors have the same west input, we conclude that $t_v^\oplus(N) \neq t_v^\ominus(N)$. Moreover, both of the tile types are a south neighbor of an or-gate tile in subpattern $r_3(v)$, hence, $t_v^\oplus(N), t_v^\ominus(N) \in \{0, 1\}$. \square

Now, these glues serve as input for the or-gates in the subpatterns $s(C)$. The following lemma concludes the proof of Theorem 1.

Lemma 5 *Let P_F be the pattern for a formula F over variables V in 3-CNF and let $m = |C(P_F)| + 3$. The formula F is satisfiable if and only if P_F can be self-assembled by a DRTAS T with at most m tile types.*

Proof The formula F is satisfiable if and only if there is a variable assignment $f : V \rightarrow \{0, 1\}$ which satisfies every clause in F . Suppose such a variable assignment f exists. For every variable $v \in V$ we let $t_v^\oplus \in T$ be the tile type with color \boxed{v} and $t_v^\ominus \in T$ be the tile type with color $\boxed{+}$. We let $t_v^\oplus(N) = f(v)$ and $t_v^\ominus(N) = 1 - f(v)$. The remaining glues on t_v^\oplus and t_v^\ominus and the other tile types are given in Fig. 7 plus the four or-gate tile types in Fig. 3. By design, it is clear that these tile types can self-assemble all the subpatterns p , q_1 to q_5 , and $r_1(v)$ to $r_3(v)$ for $v \in V$; see also Fig. 8. Now, consider the subpattern $s(C)$ for a clause $C = (c_1 \vee c_2 \vee c_3)$ in F . It is not difficult to observe that, since the clause C is satisfied by the assignment f , at least one of the north glues of the tiles in $s(C)$ with colors $\boxed{c_1}$, $\boxed{c_2}$, and $\boxed{c_3}$ is 1. The design of the or-gate tile types ensures that the right or-gate tile in $s(C)$ has east output 1 and the tile with color $\boxed{+}$ can be placed — concluding that P_F can be self-assembled by the given DRTAS having m tile types.

Conversely, suppose P_F can be self-assembled by a DRTAS with m tile types. By Lemma 4, for each variable $v \in V$ the tile type t_v^\oplus with color \boxed{v} has either north output 0 or 1. We define a variable assignment $f : V \rightarrow \{0, 1\}$ by $v \mapsto t_v^\oplus(N)$. Recall from Lemma 2 that the four or-gate tile types in T actually implement an or-gate. Furthermore, in a subpattern $s(C)$ where $C = (c_1 \vee c_2 \vee c_3)$ is a clause from F , the west input of the left or-gate tile is 0, and if the east output of the right or-gate tile were 0, then the tile type with color $\boxed{+}$ could not be placed in $s(C)$ (instead the tile type with color $\boxed{-}$ would be placed). Hence, at least one of

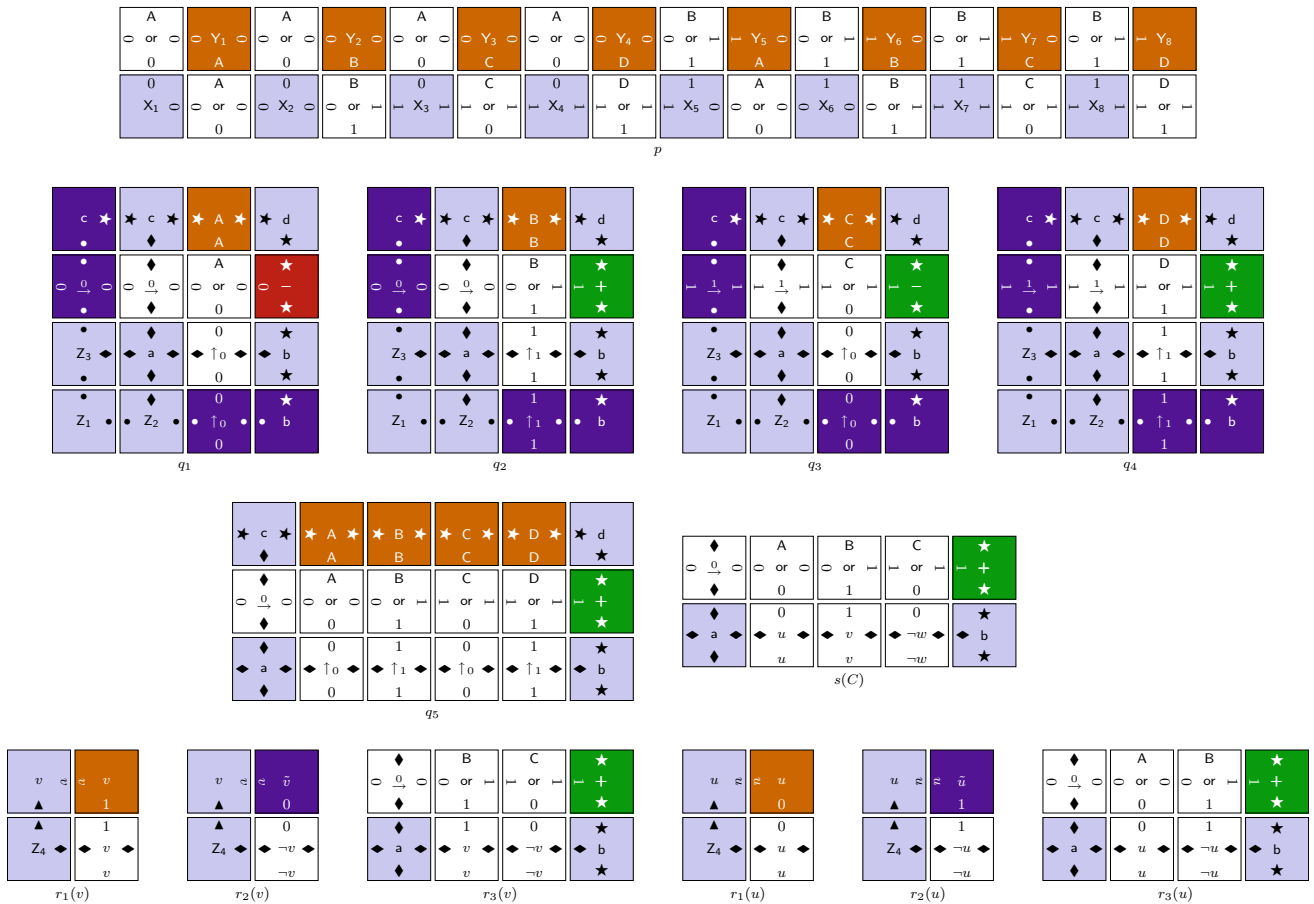


Fig. 8 The subpatterns p , q_1 to q_5 , $s(C)$, $r_1(v)$ to $r_3(v)$, and $r_1(u)$ to $r_3(u)$ in P_F with tile assignments, where $C = (u \vee v \vee \neg w)$ and $u, v, w \in V$ with the variable assignment $u \mapsto 0$, $v \mapsto 1$, and $w \mapsto 1$. The

used tiles are described in Fig. 3 and 7. The other subpatterns in P_F can be tiled analogously

the north glues of the tiles with colors c_1 , c_2 , and c_3 is 1. Using the fact that for $v \in V$ the north output of the tile type with color $\neg v$ is 1 if and only if the north output of the tile type with color v is 0, stated in Lemma 4, we infer that f is a variable assignment that satisfies every clause in F . Therefore, F is satisfiable. \square

Remark 2 Note that, because we place unique colors next to the seed structure, the glue encoding on the seed structure is not important for our construction. Indeed a seed which has the same glue label in all positions can be used to assemble the pattern P_F ; we just have to adjust the glues on the unique tile types which border the seed structure. Therefore, the problem remains NP-hard if we consider the seed structure to be part of the input. Our construction in Sect. 4 allows the seed to be part of the input as well; however, it cannot consist of only one glue label.

This poses a major difference to all proofs of the NP-hardness of k -PATS with constant k in Seki (2013), Johnsen

et al. (2013), Johnsen et al., Kari et al. (2014). In these proofs the main strategy is to define gadget patterns which can only be self-assembled by a unique tile set T (and tile sets which are isomorphic to T). Every pattern P_α which is generated in the reduction $f : \alpha \mapsto P_\alpha$ from an instance α of another NP-complete problem (usually, a variant of the SAT problem) to k -PATS contains this gadget pattern and, therefore, uniquely identifies the tile set which has to be used to self-assemble the pattern P_α . Then, it is shown that the problem instance α has a solution if and only if a seed for P_α exists which is compatible with the tile set T . In other words, in these proofs T can also be part of the input, but the seed is the crucial unknown component in k -PATS.

4 NP-hardness of 3-MBPATS

The purpose of this section is to prove the NP-hardness of 3-MBPATS. Let us define a set of restricted input pairs \mathcal{I} for PATS. The set \mathcal{I} contains all pairs (P, m) where $P = P_F$ is

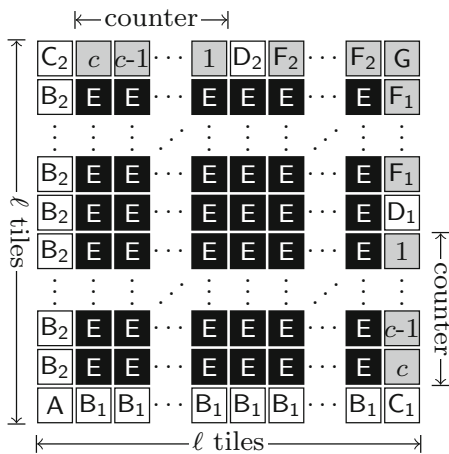


Fig. 9 Black/white/gray supertile which portrays a color $c \in C$

the pattern for a formula F in 3-CNF as defined in Sect. 3 and $m = |C(P)| + 3$. Consider the following restriction of PATS.

Problem (MODIFIED PATS)

GIVEN: A pair (P, m) from \mathcal{I}

OUTPUT: “Yes” if P can uniquely be self-assembled by using m tile types

As we choose exactly those pairs (P, m) as input for the problem that are generated by the reduction, stated in Theorem 1, we obtain the following corollary which forms the foundation for the result in this section.

Corollary 2 MODIFIED PATS is NP-hard.

Theorem 2 states a polynomial-time reduction from MODIFIED PATS to 3-MBPATS which implies that 3-MBPATS is NP-hard.

Theorem 2 For every input pair $(P, m) \in \mathcal{I}$ there exist a black/white/gray-colored pattern Q and integers m_b, m_w, m_g such that: P can be self-assembled by a DRTAS with at most m tile types if and only if Q can be self-assembled by a DRTAS with at most m_b black tile types, m_w white tile types, and m_g gray tile types. Moreover, the tuple (Q, m_b, m_w, m_g) can be computed from P in polynomial time.

Lemma 12 states the “if part” and Lemma 8 states the “only if part” of Theorem 2. Lemma 6 states that (Q, m_b, m_w, m_g) can be computed from P in polynomial time.

Corollary 3 3-MBPATS is NP-hard.

For the remainder of this section, let $(P, m) \in \mathcal{I}$ be one fixed pair, let $C = C(P)$ and $k = |C|$. We may assume that $C = [k]$ is a subset of the positive integers. The tile bounds are $m_b = 1$ for black tile types, $m_w = 5k - 3(w(P) +$

$h(P)) + 14$ for white tile types, and $m_g = 2k + 3$ for gray tile types. Note that, due to the pattern design in Sect. 3, $h(P) = 6$ is constant.

Let $\ell = 5k + 8$. For a color $c \in C$, we define an $\ell \times \ell$ square pattern as shown in Fig. 9. The blowup of such a supertile with a possible tile assignment is shown in Fig. 10. We refer to this pattern as well as to its underlying tile assignment as *supertile*. In contrast to the previous section, the positions in the supertile are labeled which does not mean that the colors or the tiles used to self-assemble the pattern are labeled; the colors are black, white, or gray. The horizontal and vertical *color counters* are the c gray positions in the top row, respectively right column, which are succeeded by a white tile in position D_2 , respectively D_1 . The color counters illustrate the color c that is portrayed by the supertile. The patterns of two supertiles which portray two distinct colors differ only in the place where the white tile is positioned in its top row and right column.

For colors in the bottom row and left column of the pattern P we use *incomplete supertiles*: a supertile portraying a color c in the bottom row of pattern P lacks the white row with positions A, B_1 , and C_1 ; a supertile representing a color c in the left column of pattern P lacks the white column with positions A, B_2 , and C_2 . In particular, the supertile portraying color $P(1, 1)$ does not contain any of the positions A, B_1, B_2, C_1 , and C_2 . Recall that all incomplete supertiles portray a color c that is unique in P .

The pattern Q is shown in Fig. 11. By $Q\langle x, y \rangle$ we denote the pattern of the supertile covering the square area spanned by positions $((x - 1) \cdot \ell, (y - 1) \cdot \ell)$ and $(x \cdot \ell - 1, y \cdot \ell - 1)$ in Q ; the incomplete supertiles cover one row and/or column less. The pattern is designed such that supertile $Q\langle x, y \rangle$ portrays the color $P(x, y)$ for all $x \in [w(P)]$ and $y \in [h(P)]$. Additionally, Q contains three *gadget rows* and three *gadget columns* which are explained in Fig. 12. The purpose of these gadget rows and columns is to ensure that the color counters can only be implemented in one way when using no more than m_g gray tile types. All together Q is of dimensions $w(Q) = \ell \cdot w(P) + 2$ times $h(Q) = \ell \cdot h(P) + 2$. Obviously, the pattern Q can be computed from P in polynomial time.

Lemma 6 (Q, m_b, m_w, m_g) can be computed from P in polynomial time.

Proof This is obvious by the design of the pattern. \square

For a DRTAS Θ which self-assembles Q , we extend our previous notion such that $Q_\Theta\langle x, y \rangle$ denotes the tile assignment of supertile $Q\langle x, y \rangle$ given by Θ . In the following, we will prove properties of such a DRTAS Θ . Our first observation is about the black and gray tile types plus two of the white tile types.

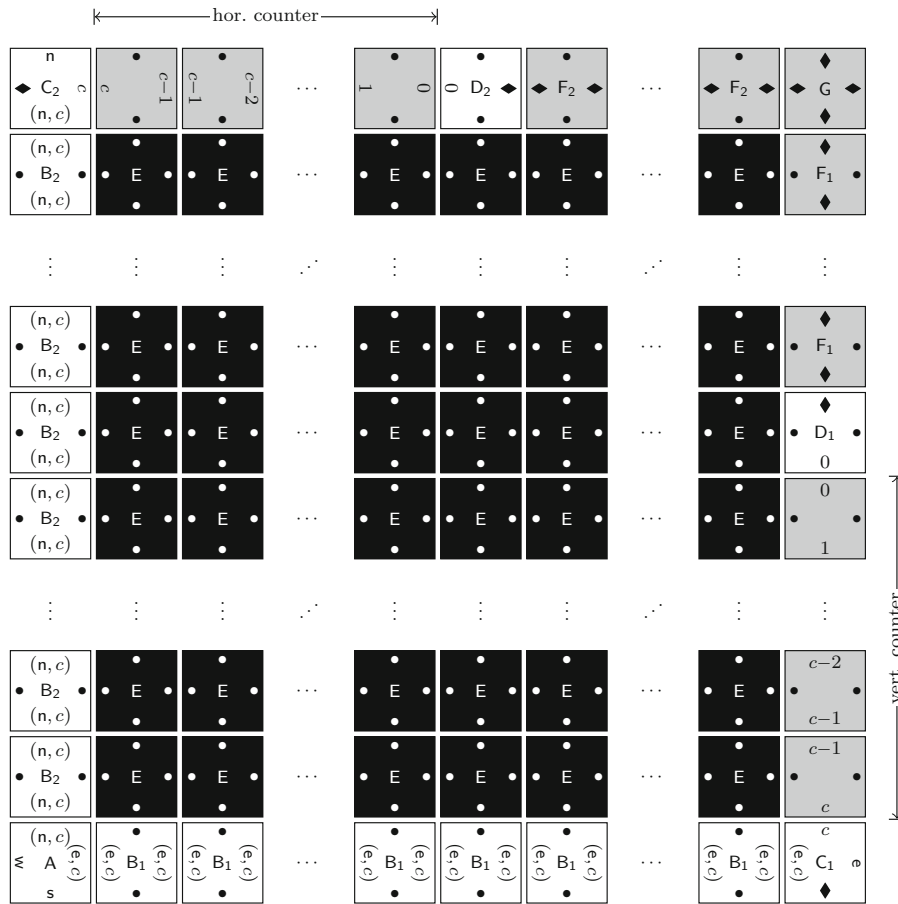


Fig. 10 Blowup of one supertile with a possible tile assignment, representing a tile with color c and glues n , e , s , and w on its north, east, south, and west edges, respectively

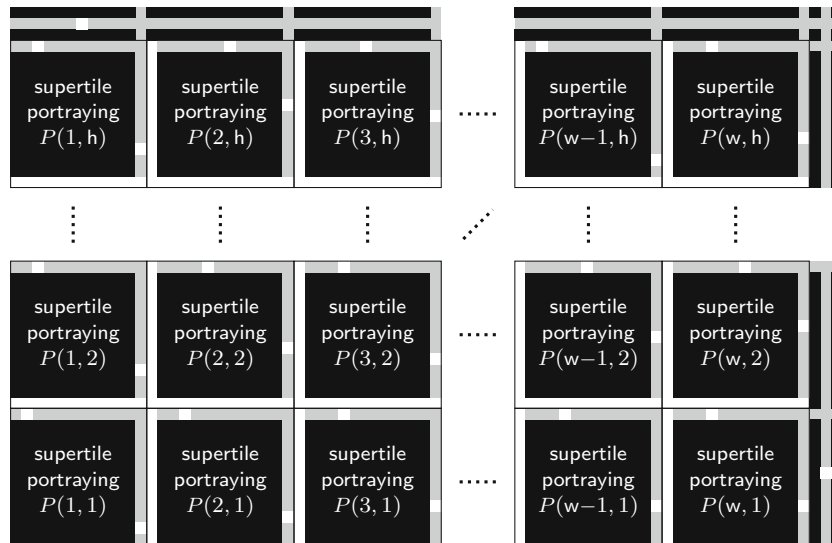


Fig. 11 Black/white/gray pattern Q defined by the k -color pattern P with $w = w(P)$ and $h = h(P)$

Lemma 7 Let Θ be a DRTAS which self-assembles the pattern Q using at most $m_b = 1$ black tile types and $m_g = 2k + 3$ gray tile types. The black and gray tile types in Θ are of the form shown in Fig. 13 and Θ contains two white

tiles of the form shown in the figure. In every supertile, the horizontal and vertical color counters are implemented by a subset of the counter tile types and for a position E, D_1, D_2, F_1, F_2 , or G the correspondingly labeled tile

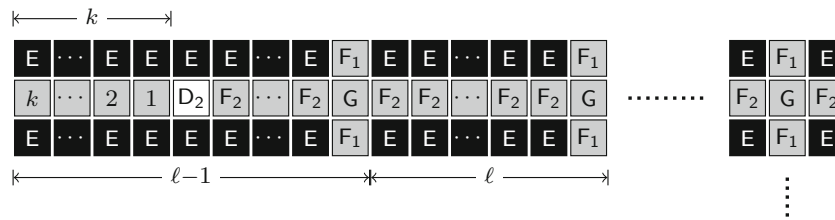


Fig. 12 The gadget rows on the north border of the pattern Q , the gadget columns are symmetrical: the middle row (resp., column) contains gray tiles except for one white tile in position $k + 1$; the

upper and lower rows (resp., left and right columns) contain gray tiles in positions above the gray column (resp., right of the gray row) of a supertile, the other tiles are black

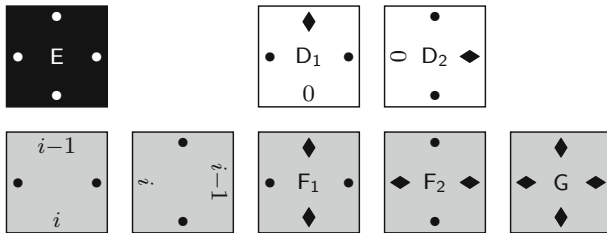


Fig. 13 The black tile type, two of the white tile types, and all gray tile types: the labeled tile types are used in the corresponding positions of each supertile and the gadget pattern; the unlabeled tile types, called counter tiles for $i \in [k]$, implement the vertical and horizontal color counters

type is used. Furthermore, the glues $\bullet, \blacklozenge, 0, 1, \dots, k$ are all distinct.

Proof In every supertile we find a black square that consists of more than just one tile, therefore, the sole black tile type must have the same north and south glues, respectively east and west glues. We may assume that \bullet is the glue on all four edges of the black tile type.

Now, we have a look at the tile assignment of the three gadget rows; see Fig. 12. In the middle row, the first k gray tiles are succeeded by a white tile. As the south input of all k tiles is the north glue \bullet of the black tiles, if the same tile type would be used in two of these k positions, there were a cycle in the gray tile types used which would be repeated over and over and no white tile could occur after k gray tiles; furthermore, all the east outputs (resp., west inputs) of these tiles are distinct. Thus, these tiles implement a horizontal counter which is capable of counting to k , or more intuitively, counting from k down to 1. Next a white tile is used whose west input is distinct from its east output; otherwise, the same white tile type would be used again. As the white tile is succeeded by $4k + 6$ gray tiles with south input \bullet , all gray tiles used in this row have to occur at least twice, therefore, all tiles, used in these positions, have to be distinct from the tiles implementing the horizontal counter; we use the label \blacklozenge for the east output of the white tile in position D_2 and the west input of the gray tile in left-most position F_2 . Finally, observe that all tiles described so far have south and north glue \bullet and that their east and west glues are distinct from \bullet .

From the three gadget columns we obtain analogous results for the vertical counter, the white tile in position D_1 , and the gray tiles in the first $4k + 6$ positions F_1 . None of the tiles in the middle column can coincide with a tile in the middle row since they have the glue \bullet on different inputs.

Since we need at least one tile for each of the positions F_1 and F_2 , there is only one gray tile type left in Θ . Any tile at position G has north and east outputs from $\blacklozenge, 0, 1, \dots, k$ as these edges are adjacent to gray tiles. We cannot use a tile which we have described so far for any of the positions G . Therefore, all tiles in positions F_1 (resp., F_2) in the gadget are of the same type whose north and south (resp., east and west) glues equal. All positions G share the same tile type τ whose south and west inputs are \blacklozenge . If the east output of τ were one of $0, 1, \dots, k$, then a white tile were among the $k + 1$ tiles succeeding the left-most position G in the middle gadget row; hence, $\tau(E) = \blacklozenge$ and, symmetrically, $\tau(N) = \blacklozenge$.

All supertiles have to share the same black and gray tile types as there are no other black and gray tile types in Θ . The color counters have to be implemented by the counter tile types. As the south and west inputs of the tiles in positions D_1 and D_2 are determined by its gray and black neighbors, it is also clear that only the described white tiles can be used in these positions. Now, the types of the tiles in positions F_1, F_2 , and G are also determined by their inputs. \square

Remark 3 Consider a DRTAS Θ that self-assembles the pattern Q using most m_b black tile types and m_g gray tile types. If we have a look at the tile assignment of the black square plus the gray column and row in a supertile, we see that this block has inputs \bullet on all edges except for edges where the color counters are initialized and it has outputs \bullet on all edges, except for its right-most and top-most output edges which are \blacklozenge . This means that all information on how to initialize the color counters has to be carried through the white lines and rows, that are, the tiles in positions A, B_1, B_2, C_1, C_2 . Moreover, the tile in position A is the only one with non-generic input from other supertiles. This tile fully determines the tile assignment of the supertile and can be seen as the control tile or seed of the supertile.

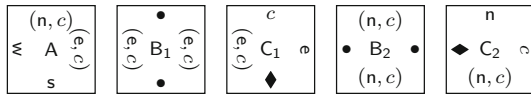


Fig. 14 White tile types for the supertile portraying a color $c \in C$, except for the or-gate, where $t \in T$ with $c = \chi(t)$, $n = t(N)$, $e = t(E)$, $s = t(S)$, and $w = t(W)$

Henceforth, for a supertile $s = Q_\theta(x, y)$ we extend our notion of glues such that $s(S)$ and $s(W)$ denote the south and west input of the tile in position **A**, respectively, $s(N)$ and $s(E)$ denote the north and east output of the tiles in positions **C₂** and **C₁**, respectively. For incomplete supertiles only one of $s(N)$ or $s(E)$ is defined.

Two supertiles in Q_θ are considered distinct if their tile assignment differs in at least one position. By the observations above, two complete supertiles are distinct if and only if their control tiles are of distinct types; this is equivalent to require that the inputs of the two supertiles differ. Since incomplete supertiles portray unique colors in P , they are distinct from any supertile in Q_θ but itself.

There is some flexibility in how the white tile types are implemented in a DRTAS Θ which self-assembles Q . Let us present one possibility which proves the “only if part” of Theorem 2.

Lemma 8 *If P can be self-assembled by a DRTAS T with m tile types, then Q can be self-assembled by a DRTAS Θ using m_b black tile types, m_w white tile types, and m_g gray tile types.*

Proof Let the DRTAS Θ contain the tile types given in Fig. 13. By Lemma 7, the tiles of these types can self-assemble the gadget pattern and the black square plus color counters in every supertile. Recall from Lemma 2 that T contains four tile types for the or-gate and only one tile type for every other color in C .

First, consider $c \in C \setminus \{\text{or}\}$ and let $t \in T$ be the tile type with color c . We use the tile types in Fig. 14 for the supertile portraying c . Note that none of the five tile types share the same inputs. The labels on them depict the positions in the supertile where each tile is used. We do not need any of these white tile types for the incomplete supertile representing the color $P(1, 1)$. For the other incomplete supertiles we only need two of these tile types. Recall that, by design, a color which is portrayed by an incomplete supertile in Q is unique in P . This amounts to $5 \cdot (|C| - 1) - 3 \cdot (h(P) + w(P)) + 1$ white tile types in Θ for all the supertiles portraying colors in $C \setminus \{\text{or}\}$. We have one remark for the colors in the top row and right column of P : since these colors do not occur in any other

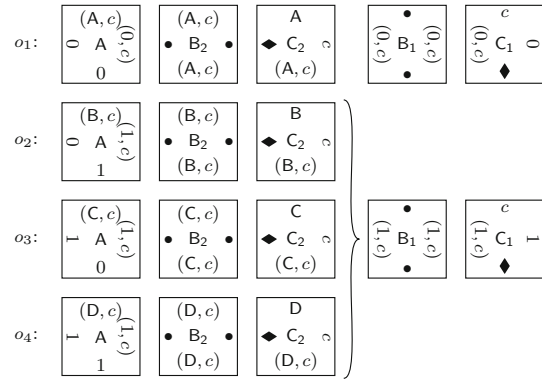


Fig. 15 White tile types for supertiles portraying the or-gate where $o_1, o_2, o_3, o_4 \in T$ are defined in Fig. 3

position of the pattern and the north and/or east glues of the respective tiles are not used in P , we may assume that all these glues are \bullet ; this allows for the proper attachment of the gadget pattern.

Now, consider $c = \text{or}$. Recall from Lemma 2 that there are $o_1, o_2, o_3, o_4 \in T$ with color c as depicted in Fig. 3. We use the 16 white tile types in Fig. 15 for the four supertiles portraying c . The supertiles for o_2, o_3 , and o_4 share tile types in positions **B₁** and **C₁**, as labelled. Note that the inputs of the 16 tile types are mutually distinct.

Let Θ contain all the white tile types we have defined plus the two white tile types from Fig. 13 and note that the white tile types add up to

$$m_w = 5 \cdot |C| - 3 \cdot (h(P) + w(P)) + 14$$

as desired. If two distinct tile types in Θ had the same inputs, it had to be two tile types for position **A** which implies that two distinct tile types in T would have same inputs as well; thus, Θ is a properly defined DRTAS. The L -shaped seed of Θ is defined such that the incomplete supertiles for the bottom row and left column, as well as the gadgets, can properly attach.

By Remark 3, it is clear that, starting from its control tile (or the L -shaped seed), every supertile properly self-assembles as long as its west and south neighboring supertiles are present. Let Q' be the pattern that is self-assembled by Θ . Using induction over x and y , the supertile $s = Q'_\theta(x, y)$ represents the tile $t = P_T(x, y)$ because the respective glues of s and t coincide, for all $x \in [w(P)]$ and $y \in [h(P)]$. Furthermore, by design of the supertiles in the top row and right column of Q' , the gadget rows and columns can self-assemble. We conclude that Θ self-assembles $Q = Q'$. \square

For the converse implication of Theorem 2, let us show how to obtain a DRTAS that self-assembles P from the supertiles in Q_θ . The following lemma follows from the bijection between supertiles in Q_θ and tiles in P_T .

Lemma 9 *Let Θ be a DRTAS which self-assembles Q using at most m_b black tile types and m_g gray tile types, and let*

$$S = \{Q_\Theta\langle x, y \rangle \mid x \in [w(P)], y \in [h(P)]\}$$

be the set of all distinct supertiles in Q_Θ . There exists a

DRTAS T with $|S|$ tile types which self-assembles P such that for each supertile $s \in S$ there exists a tile type $t_s \in T$ with the same glues on the respective edges and s portrays the color of t_s . For an incomplete supertile the statement holds for the defined glue.

Proof Note that, except for the tiles with colors in the first row and column of P , the tiles in T are fully defined. For the undefined glues on tile types, representing incomplete supertiles, we introduce unique matching glues; the L -shaped seed of T is defined to match these glues. Clearly, the first column and row of P can be self-assembled by T . Recall from Remark 3 that the control tile in position A of a complete supertile s fully determines the supertile and its outputs. The placement of the control tile is determined by the east output of the west neighbor and the north output of the south neighbor of s . Let P' be the pattern which is self-assembled by T . Using induction over x and y , we see that if $s = Q_\Theta\langle x, y \rangle$, then $t_s = P'_T\langle x, y \rangle$ for all $x \in [w(P)]$ and $y \in [h(P)]$; thus, T self-assembles $P = P'$. \square

We continue with the investigation of the white tile types that are used to self-assemble the pattern Q . We will show that, if one white tile type were used in any two distinct positions, we would obtain that Θ is not a DRTAS.

Lemma 10 *Let Θ be a DRTAS which self-assembles the pattern Q using at most m_b black tile types and m_g gray tile types. A white tile type from Θ which is used in one of the positions $A, B_1, B_2, C_1, C_2, D_1$, or D_2 cannot be used in another position in any supertile.*

Proof Clearly, we do not have to argue about positions which are gray or black. By Lemma 7 and the design of supertiles, a tile type used in a position

- (1) B_1 has south and north glue \bullet ;
- (2) B_2 has west and east glue \bullet ,
- (3) C_1 has south glue \blacklozenge and north glue in $[k]$;
- (4) C_2 has west glue \blacklozenge and east glue in $[k]$;
- (5) D_1 has east and west glue \bullet , south glue 0 , and north glue \blacklozenge ;
- (6) D_2 has south and north glue \bullet , west glue 0 , and east glue \blacklozenge .

First, suppose the same tile type would be used in position A and one of the positions B_1, B_2, C_1, C_2, D_1 , or D_2 . The tile type had north or east output from $\bullet, \blacklozenge, 1, \dots, k$; therefore, the north or east neighbor of the tile of this type in position A would be black or gray — a contradiction.

Due to the distinction in their inputs, the same tile type cannot be used in the following pairs of positions: $(B_1, C_1), (B_1, D_1), (B_2, C_2), (B_2, D_2), (C_1, D_1), (C_1, D_2), (C_2, D_1), (C_2, D_2), (D_1, D_2)$.

If a tile type were used in any pair of positions $(B_1, B_2), (B_1, C_2), (B_2, C_1)$, or (C_1, C_2) it would have the same inputs as one of the gray or black tiles.

If a tile type were used in position B_1 and D_2 , then the east neighbor of the tile of this type in position B_1 would be the gray tile labelled F_2 or G from Fig. 13. Symmetrically, no tile type can be used in both positions B_2 and D_1 . \square

Let B_1^* be the right-most position B_1 in a supertile, adjacent to position C_1 , and let B_2^* be the top-most position B_2 in a supertile, adjacent to position C_2 . The following argument is about tiles in the five positions $K = \{A, B_1^*, B_2^*, C_1, C_2\}$ of each supertile. Following Remark 3 it is clear that a tile in position A fully determines the supertile, tiles in positions B_1^* and C_1 carry the color and the east glue of a supertile, whereas tiles in positions B_2^* and C_2 carry the color and the north glue.

Lemma 11 *Let Θ be a DRTAS which self-assembles Q using at most m_b black tile types and m_g gray tile types. Let s_1 and s_2 be supertiles in Q_Θ .*

- (1) If s_1 and s_2 portray different colors, they cannot share any tile types in positions from K .
- (2) If $s_1(E) \neq s_2(E)$, they cannot share any tile types in A, B_1^* , or C_1 .
- (3) If $s_1(N) \neq s_2(N)$, they cannot share any tile types in A, B_2^* , or C_2 .

The three statements hold for all available positions in incomplete supertiles.

Proof By Lemma 10, we do not have to consider mixups of positions. Firstly, recall from Remark 3 that the tile in position A determines the supertile and its outputs. Two supertiles portraying different colors or having different outputs cannot share the same tile type in positions A .

Now, consider a supertile s_1 representing the color c . The type γ of the tile in position C_1 defines the east output $s_1(E) = \gamma(E)$ and initializes the vertical color counter. If γ is used in another supertile s_2 in position C_1 , then s_2 portrays the same color c and $s_1(E) = s_2(E)$. As the south input of every tile in a position C_1 is \blacklozenge , the type β of the tile in position B_1^* of s_1 determines the placement of γ in position C_1 . Thus, if β is used in another supertile s_2 in position B_1^* , then s_2 portrays the same color c and $s_1(E) = s_2(E)$. This concludes the proof of statement (ii). Statements (i) and i(ii) follow by symmetric arguments on the tile types in positions C_2 and B_2^* . \square

Remark 4 We do not claim that two supertiles could not share any tile types in positions B_1 or B_2 while portraying

different colors or having different output. Indeed, consider two supertiles s_1 and s_2 portraying different colors and let β and β' be tile types for positions \mathbf{B}_1 with $\beta(E) = \beta'(W) = x$ and $\beta(W) = \beta'(E) = y$. If the control tile of s_1 has east glue x while the control tile of s_2 has east glue y , these supertiles have different tile types in positions \mathbf{C}_1 but share the tile types β and β' in their positions \mathbf{B}_1 .

Let us conclude the proof of Theorem 2.

Lemma 12 *The pattern P can be self-assembled by a DRTAS T with m tile types if Q can be self-assembled by a DRTAS Θ with m_b black tile types, m_w white tile types, and m_g gray tile types.*

Proof We will prove that Q_Θ cannot contain more than m distinct supertiles while Θ respects the given tile bounds. Then, the claim follows from Lemma 9. The black, gray, and two white tile types in Θ are defined by Lemma 7. We are now counting the minimal number of white tile types that we need to self-assemble the pattern Q . The number of distinct tile types used as control tiles, in positions \mathbf{A} , is equal to the number of distinct complete supertiles of Q_Θ .

Consider a color $c \in C$. There is at least one supertile in Q_Θ which portrays color c and, assuming the supertile is complete, we need five white tile types in positions from K of the supertile, by Lemma 10, and these five tile types cannot be used for any of positions from K of a supertile portraying another color, by Lemma 11. If the supertile is incomplete but $c \neq P(1, 1)$, hence c is unique in P , we only need two white tile types which cannot be used in any of the positions from K of another supertile. We do not need any additional white tile types for the supertile portraying $P(1, 1)$. For the supertiles portraying colors in $C \setminus \{\text{or}\}$ we need $5 \cdot (|C| - 1) - 3 \cdot (w(P) + h(P)) + 1$ white tiles which cannot be used in a position from K in a supertile representing the or-gate; furthermore, the two white tile types for positions \mathbf{D}_1 and \mathbf{D}_2 also cannot be used in a position from K . Among these white tile types we find only $|C| - w(P) - h(P)$ types used as control tiles.

We only have 16 white tile types left for the or-gate supertiles. From Lemma 1 and Lemma 9 we infer that Q_Θ contains either

- (i) three distinct supertiles $s_1, s_2, s_3 \in T$ portraying $\boxed{\text{or}}$ all having distinct north and east glues,
- (ii) four distinct supertiles $s_1, s_2, s_3, s_4 \in T$ portraying $\boxed{\text{or}}$ all having distinct north glues and together having at least two distinct east glues,
- (iii) four distinct supertiles $s_1, s_2, s_3, s_4 \in T$ portraying $\boxed{\text{or}}$ all having distinct east glues and together having at least two north glues, or

- (iv) eight distinct supertiles $s_1, \dots, s_8 \in T$ portraying $\boxed{\text{or}}$ all having distinct east or north glues.

Indeed, if none of these conditions were true for Q_Θ , then, using the construction given in Lemma 9, we could generate a DRTAS T which self-assembled P and invalidated Lemma 1.

By Lemma 11, two distinct supertiles portraying $\boxed{\text{or}}$ cannot share tile types in positions \mathbf{A} , they can only share tile types in positions \mathbf{B}_1^* and \mathbf{C}_1 if their east outputs equal, and they can only share tile types in positions $\mathbf{B}_1^*, \mathbf{C}_1$ if their north outputs equal. For case (i) we need at least 15 white tile types of which three can be used as control tiles; the left over tile type might be used as another control tile. For cases (ii) and (iii) we need at least 16 white tile types of which four can be used as control tiles. Case (iv) is not possible because we would need at least 26 white tile types. A more involved analysis reveals that only case (ii) is possible, but for our purpose it is enough that the remaining 16 white tile types contain at most four types that can be used as control tiles.

The number of distinct supertiles in Q_Θ is limited by the number of tile types that can be used as control tiles plus the number incomplete supertiles. We obtain that Q_Θ contains $k + 3 = m$ distinct supertiles as desired. Using Lemma 9, the pattern P can be self-assembled by a DRTAS T with m tile types. \square

5 Conclusions

We prove that k -MBPATS, a natural variant of k -PATS, is NP-complete for $k = 3$. Furthermore, we present a novel proof for the NP-completeness of PATS and our proof is more concise than previous proofs. We introduce several original techniques for pattern design in our proofs, in particular in Sect. 4 which are different from those developed in other papers on NP-hardness of the k -PATS problem. Recall that no manually-checkable proof is known for k -PATS with $k \leq 10$ yet (the proof of 2-PATS in Kari et al. (2014) is computer-assisted). We anticipate that proof techniques reported in this paper can be of help for providing a manually-checkable proof for 2-PATS and in other studies regarding pattern tile set synthesis.

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