

# A New Practical Cube Attack via Recovering Numerous Superpolys

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**Abstract.** Cube attack is one of the most powerful approaches for recovering keys of stream ciphers. Practical cube attacks generate several superpolys first and solve the system constructed by these superpolys afterward. Unlike previous practical attacks, we propose a new cube attack that transfers the difficulty of generating easy-solving superpolys to solving the system built by numerous nonlinear ones. In the offline phase, we recovered lots of nonlinear superpolys by improving the approach proposed by Delaune et al. at SAC 2022 in theory. In the online phase, taking advantage of the sparsity and asymmetry of these numerous superpolys, we present a new testing method to solve the constructed system efficiently. As applications, the latest attack could practically recover the keys for 820- and 832-round TRIVIUM with the time complexity no more extensive than  $2^{46}$  and  $2^{50}$ , while the previous highest number of rounds of TRIVIUM that can be attacked practically is 830. We believe the proposed approach can be used to attack more rounds of TRIVIUM and other stream ciphers.

**Keywords:** Practical cube attack · Stream ciphers · Trivium · Solving nonlinear polynomial systems

## 1 Introduction

**Cube Attack:** Since Dinur and Shamir proposed the cube attack at EUROCRYPT 2009 [DS09], the cube attack has been effectively employed to attack various stream ciphers [ADMS09, DS11, FV14, DMP<sup>+</sup>15, SBD<sup>+</sup>16]. Todo et al. proposed the division property in [Tod15, TM16], and its integration with the cube attack significantly improved the attacks on TRIVIUM, Grain128a, ACORN in [TIHM17] by leveraging the Mixed Integer Linear Programming (MILP) model. Specifically, let  $\mathbf{k}$  and  $\mathbf{v}$  be secret and public variables. The output bit of a stream cipher can be expressed as a Boolean polynomial  $f(\mathbf{k}, \mathbf{v})$ . A cube is composed of many values of  $\mathbf{v}$ 's. Some bits of  $\mathbf{v}$  take all possible combinations of values, while the other bits of  $\mathbf{v}$  remain unchanged. One can obtain a relatively simple relation in secret variables by taking the sum of the values of  $f(\mathbf{k}, \mathbf{v})$  over all values in the cube. This relation is called the superpoly of the cube, and it is much simpler than  $f(\mathbf{k}, \mathbf{v})$ . By analyzing superpolys, some information about the secret variables can be achieved.

Due to the complex structure of  $f(\mathbf{k}, \mathbf{v})$ , recovering the superpoly from a given cube has traditionally been challenging. The original paper [DS09] proposed a linearity test to verify linear superpolys, allowing the algebraic normal form (ANF) of the superpoly to be recovered if the test confirmed linearity. Later, a quadraticity test was introduced [PJ12] and was used to mount the attacks against TRIVIUM in [FV14]. However, since all these attacks were experimental cryptanalysis, there is a probability that the linearity and quadraticity tests fail.

**Division Property:** A significant advancement of the cube attack is the proposal of the division property [Tod15, TM16]. Todo et al. revealed the relation between integral cryptanalysis [KW02] and the division property. At the same time, integral cryptanalysis was also assumed to be equivalent to square attacks [DKR97] or higher-order differential attacks [Lai94]. Division property is an effective tool for analyzing the monomials in  $f(\mathbf{k}, \mathbf{v})$ , but the computation is expensive. Consequently, the Mixed Integer Linear Programming (MILP) approach was introduced to model the propagations of the bit-based division property [XZBL16]. Thanks to the efficiency of MILP tools, the bit-based division property for six lightweight block ciphers was shown. Since then, more improvements have been given in [SWW17, TIHM17, WHT<sup>+</sup>18]. However, traditional division property often suffers from accuracy problems. Taking the method proposed in [TIHM17] for example, if there is no division trail such that the output is 1, one can confirm that some specific monomial must not appear in the superpoly with absolute confidence. But if such a division trail exists, the corresponding monomial may or may not appear. Hao et al. finally resolved this inaccuracy problem in [HLM<sup>+</sup>20], where the model for “three-subset division property without unknown subset” was proposed.

**TRIVIUM:** TRIVIUM is a bit-oriented synchronous stream cipher based on NLSFR [DCP08]. It is one of the eSTREAM hardware-oriented finalists and an International Standard under ISO/IEC 29192-3:2012. TRIVIUM has attracted much attention due to its simple structure and high level of security. TRIVIUM uses an 80-bit key and an 80-bit IV, so the complexity of the exhaustive search for the key is  $2^{80}$  evaluations, and any attack of TRIVIUM must have a lower complexity than  $2^{80}$ .

**Practical cube attacks against TRIVIUM:** a key-recovery attack on 784-round TRIVIUM was given in [FV14]. In 2021, a practical attack against 805-round TRIVIUM was proposed in [YT21], and many linear superpolys were found in practical time. In the online phase of the attack, the linear superpolys make it relatively easy to solve for the secret variables. Furthermore, superpolys involving balanced secret variables are also utilized in the attack, which reduces the difficulty of searching for cubes. In [Sun21], practical attacks on 806 and 808-round TRIVIUM were realized. By improving the method for searching for valuable cubes whose superpolys each have an independent secret variable, full key-recovery attacks on 815 and 820-round TRIVIUM were completed in [CT23]. Based on the variable substitution technique and the combination of superpolys, [LHHW24] further increased the number of TRIVIUM practical attack rounds to 825 rounds, currently the highest number of rounds of TRIVIUM vulnerable to a practical attack. It is worth mentioning that [WQW23] claims to have achieved a practical attack on 830-round TRIVIUM using the correlation cube attack. This method has two significant limitations: the attack does not apply to the entire key space, and the attack complexity reaches  $2^{60}$ , which we believe is still some distance from the truly practical attack.

**Models for recovering superpolys:** A vital step of the cube attack is to recover the superpoly for a given cube. The first precise MILP-based model was given by Hao et al. [HLM<sup>+</sup>20]. Hu et al. improved this model in their consequent works, including [HST<sup>+</sup>21]. A new graph-based model for describing TRIVIUM was proposed in [DDGP22]. This graph-based approach uses fewer MILP variables and many new techniques for speed-up. Thus, the speed of recovering superpolys has been improved significantly. Since our work is based on the graph-based model, we will introduce Delaune et al.’s work in more detail in Sec. 2.4. Later, Cheng and Qiao slightly improved the graph-based model by finding more “patterns” [CQ23], but the efficiency of recovering superpolys is not improved.

**Contributions:** Practical cube attacks generate several superpolys first and solve the system constructed by these superpolys afterward. To make the systems easy to solve, previous practical attacks require generating “good” superpolys, whereas “good” superpolys usually are linear superpolys or superpolys with balanced bits. However, these good superpolys are challenging to obtain for a high number of rounds of stream ciphers.

Thus, the critical insight of our attack is to transfer the difficulty of generating superpolys to solving them. That is, instead of solving the system constructed by “good” superpolys, we prefer solving the system built by numerous nonlinear ones that are “not-so-good”. We have three contributions in this paper.

1. To obtain numerous superpolys efficiently, we improved the graph-based model and obtained significant improvement in the efficiency. Delaune et al. proposed the concept of “pattern” to reject useless trails (meaning the solutions) in the graph-based mode. We found that there are still many useless trails in the models after using Delaune et al.’s 3CBP pattern. The natural idea is to use more patterns when building the model, but more patterns tend to lead to errors, as mentioned in [DDGP22]. So, we studied the properties of the patterns in theory and proposed new theories to ensure different patterns could work correctly. A few new techniques were also applied, e.g., dividing the model into sub-models and solving the sub-models in parallel. As a result, more useless trails can be rejected effectively; hence, the efficiency of recovering superpolys has improved significantly. Besides, our new algorithm can find and exploit new patterns during the computation. We believe the improved graph-based model can be applied to most stream ciphers, not limited to TRIVIUM.
2. We propose a new practical cube attack against stream ciphers using numerous superpolys. Specifically, we proposed a new method of solving a system constructed by numerous nonlinear superpolys. We noticed that the superpolys of stream ciphers are usually asymmetric in variables, and if the system is over-defined, it is possible to determine the values of some variables efficiently. Thus, in the new attack, we first find a mother cube such that its superpolys are relatively sparse, and then we recover numerous superpolys of its sub-cubes to construct an over-defined system. In the online phase of the cube attack, we test the values of each unknown to check whether a contradiction appears. For example, if  $x = 0$  leads to a contradiction, we can confirm that  $x = 1$  is correct. This test will be very efficient if the number of superpolys in the system is large and the superpolys are sparse. This test can be finished in a few hours in our experiments, and the values of about 95% keys can be determined after this test. At last, we enumerate the values of the undetermined variables to find out the complete keys, which can also be done practically.
3. We applied the new attack to round-reduced TRIVIUM, and can practically recover the keys of 820- and 832-round TRIVIUM. We admit that there is a main drawback to our new attack. That is, we cannot prove our attack is practical for all keys in theory, which is also the drawback of the correlation cube attacks. However, from the experiments, we think the new attack is able to recover almost all keys practically. We summarize related practical attacks against TRIVIUM in Tab. 1.

All superpolys and codes of related algorithms in this paper are available at [https://github.com/ysun0102/recovering\\_numerous\\_superpolys](https://github.com/ysun0102/recovering_numerous_superpolys).

This paper is organized as follows. Preliminaries come in Sec. 2. The theory and algorithm of the new graph-based algorithm is presented in Sec. 3. Sec. 4 introduces the new cube attack. We apply the new attack to TRIVIUM in Sec. 5. We conclude this paper in Sec. 6.

**Table 1:** Summary of the practical key recovery attacks on TRIVIUM. #S.polys: the number of superpolys used in the attack; Data: the number of oracle requests; Time: the total time complexity of the attack.

Round	#S.polys	Cube size	Attack type	Data	Time	Reference
672	63	12	Cube	$2^{18.58}$	$2^{19}$	[DS09]
767	35	28-31	Cube	$2^{31}$	$2^{45}$	[DS09]
784	42	30-33	Cube	$2^{33}$	$2^{39}$	[FV14]
805	42	33-38	Cube	$2^{38}$	$2^{41.40}$	[YT21]
806	29	34-37	Cube	$2^{39}$	$2^{39.88}$	[Sun21]
808	37	39-41	Cube	$2^{44}$	$2^{44.58}$	[Sun21]
810	39	40-42	Cube	$2^{44}$	$2^{44.17}$	[LHHW24]
815	35	44-46	Cube	$2^{47}$	$2^{47.32}$	[CT23]
820	30	48-51	Cube	$2^{53}$	$2^{53.17}$	[CT23]
820*	$2^{13}$	38	Correlation Cube	$2^{51}$	$2^{60}$	[WQW23]
<b>820</b>	<b>1912</b>	<b>38-45</b>	<b>Cube</b>	<b><math>2^{45}</math></b>	<b><math>&lt; 2^{46}</math></b>	Sec. 5.2
825	31	49-52	Cube	$2^{53}$	$2^{53.09}$	[LHHW24]
825*	$2^{12}$	41	Correlation Cube	$2^{53}$	$2^{60}$	[WQW23]
830*	$2^{13}$	41	Correlation Cube	$2^{54}$	$2^{60}$	[WQW23]
<b>832</b>	<b>1373</b>	<b>43-49</b>	<b>Cube</b>	<b><math>2^{49}</math></b>	<b><math>&lt; 2^{50}</math></b>	Sec. 5.2

\*: The 820-, 825- and 830-round attacks in [WQW23] work for only  $2^{79.8}$ ,  $2^{79.7}$  and  $2^{79.3}$  of the keys in the key space, respectively.

## 2 Preliminaries

### 2.1 Cube attack

Let  $\mathbb{F}_2[\mathbf{x}]$  be the polynomial ring over the field  $\mathbb{F}_2 = \{0, 1\}$  in the variables  $\mathbf{x} = (x_0, x_1, \dots, x_{n-1})$ . Given a bit-vector  $\mathbf{u} = (u_0, u_1, \dots, u_{n-1}) \in \mathbb{F}_2^n$ , the product  $\prod_{i=0}^{n-1} x_i^{u_i}$  is called a **monomial** in  $\mathbb{F}_2[\mathbf{x}]$ . A **polynomial** is a finite sum of monomials.

Cube attack was proposed at EUROCRYPT 2009 [DS09]. For a cipher with  $n$  secret variables and  $m$  public variables, each output bit of this cipher can be represented as a polynomial in these variables. Denote  $\mathbf{k} = (k_0, k_1, \dots, k_{n-1})$  and  $\mathbf{v} = (v_0, v_1, \dots, v_{m-1})$  as the secret and public variables, where  $k_i, v_j \in \mathbb{F}_2$  for  $0 \leq i < n$  and  $0 \leq j < m$ . The output bit can be written as a polynomial  $f$  in  $\mathbb{F}_2[\mathbf{k}, \mathbf{v}]$ .

Let  $I \subseteq \{0, 1, \dots, m-1\}$  be a set of indices of public variables. A **cube** determined by  $I$  is denoted as  $C_I$ , and contains all  $2^{|I|}$  possible combinations of the values of  $v_j$ 's for  $j \in I$ , while the value of  $v_l$  remains unchanged for  $l \in \{0, 1, \dots, m-1\} \setminus I$ . We have the following equation:

$$\sum_{C_I} f = \sum_{C_I} (t_I \cdot p + q) = \sum_{C_I} t_I \cdot p + \sum_{C_I} q = p,$$

where  $t_I$  represents the product  $\prod_{i \in I} v_i$ , and there is no term of  $q$  divisible by  $t_I$ . The polynomial  $p$  is called the **superpoly** of the cube  $C_I$ . By the above definitions, the superpoly of  $C_I$  only involves the inactive public variables  $v_l$  where  $l \in \{0, 1, \dots, m-1\} \setminus I$ , and the values of these variables are often preset to constants in cube attacks. So the superpoly  $p$  is a polynomial in  $\mathbb{F}_2[\mathbf{k}]$ .

We say a polynomial  $p \in \mathbb{F}_2[\mathbf{k}]$  is balanced, if  $|\{\mathbf{k} \mid p(\mathbf{k}) = 0\}| = |\{\mathbf{k} \mid p(\mathbf{k}) = 1\}| = 2^{n-1}$ . A balanced superpoly  $p$  usually leads to a key-recovery attack. In the *offline* phase of the cube attack, attackers recover the superpoly  $p$  of a cube  $C_I$ . In the *online* phase, attackers get the value  $a$  of  $p$  by querying the encryption oracle  $2^{|I|}$  times. Since the superpoly is balanced,  $2^{n-1}$  invalid keys will be filtered out by the equation  $p = a$ . To recover the whole

key, it suffices to query the encryption oracle another  $2^{n-1}$  times. The overall number of querying times of this attack is  $2^{|I|} + 2^{n-1}$ .

Note that more balanced superpolys may filter out more invalid keys, but the complexity of obtaining the values of these superpolys increases. However, the costs of calculating these values may be lowered in a special case. That is, if several cubes and their indexes are all from the subsets of a set  $S$ , then it only needs  $2^{|S|}$  requests to calculate all the values of the superpolys. In this case, we usually call  $S$  as a **mother cube**. This technique was used in [YT21] to obtain practical cube attacks against round-reduced TRIVIUM.

## 2.2 TRIVIUM

TRIVIUM is an NLFSR-based stream cipher [DCP08]. TRIVIUM has a 288-bit internal state  $(s_0, s_1, \dots, s_{287})$  which is divided into three registers. The 80-bit secret key  $\mathbf{k} = (k_0, k_1, \dots, k_{79})$  is loaded into the first register, and the 80-bit initialization vector  $\mathbf{v} = (v_0, v_1, \dots, v_{79})$  is input to the second register. The other state bits are set to 0 except the last three bits in the third register. That is, we have

$$\begin{aligned} (s_0, s_1, \dots, s_{92}) &\leftarrow (k_0, k_1, \dots, k_{79}, 0, \dots, 0), \\ (s_{93}, s_{94}, \dots, s_{176}) &\leftarrow (v_0, v_1, \dots, v_{79}, 0, \dots, 0), \\ (s_{177}, s_{178}, \dots, s_{287}) &\leftarrow (0, 0, \dots, 0, 1, 1, 1). \end{aligned}$$

The state of TRIVIUM is updated in the following way:

$$\begin{aligned} t_1 &\leftarrow s_{65} + s_{92}, \\ t_2 &\leftarrow s_{161} + s_{176}, \\ t_3 &\leftarrow s_{242} + s_{287}, \\ z &\leftarrow t_1 + t_2 + t_3, \\ t_1 &\leftarrow t_1 + s_{90} \cdot s_{91} + s_{170}, \\ t_2 &\leftarrow t_2 + s_{174} \cdot s_{175} + s_{263}, \\ t_3 &\leftarrow t_3 + s_{285} \cdot s_{286} + s_{68}, \\ (s_0, s_1, \dots, s_{92}) &\leftarrow (t_3, s_0, \dots, s_{91}), \\ (s_{93}, s_{94}, \dots, s_{176}) &\leftarrow (t_1, s_{93}, \dots, s_{175}), \\ (s_{177}, s_{178}, \dots, s_{287}) &\leftarrow (t_2, s_{177}, \dots, s_{286}), \end{aligned}$$

where  $z$  denotes the 1-bit key stream. The state is updated 1152 times first. After the key initialization is done, the one-bit key stream is produced by every update function.

## 2.3 Graph

In this paper, a **vertex** is denoted as an uppercase letter, for instance,  $A, B, C$ . An **edge** has a direction from one vertex to another, and we differentiate the starting and ending vertexes of an edge. In Delaune et al.'s graph-based Model [DDGP22], edges also have four types.

For an edge  $e$ , we use  $\text{St}(e)$ ,  $\text{En}(e)$ , and  $\text{Type}(e)$  to denote the starting vertex, the ending vertex, and the type of  $e$ . Two edges are identical only when they have the same starting vertex, ending vertex, and type. For a vertex  $A$ , we denote by  $\text{in}(A)$  the set of incoming edges of  $A$ , and respectively, we use  $\text{out}(A)$  to represent the set of outgoing edges of  $A$ . In case we do not know the specific type of edge  $e$ , we also use  $(\text{St}(e), \text{En}(e))$  to represent  $e$  briefly. For an edge  $e$ , we define the set  $\mathbf{V}(e) := \{\text{St}(e), \text{En}(e)\}$ . Similarly, for a set of edges, say  $\mathcal{E}$ , we define  $\mathbf{V}(\mathcal{E}) := \bigcup_{e \in \mathcal{E}} \mathbf{V}(e)$ .

A graph consists of a set of vertexes and edges and is denoted as lowercase Greek letters, such as  $\alpha, \beta, \gamma, \tau$ . Given a graph  $\alpha$ , its vertexes and edges are referred as  $\mathbf{V}(\alpha)$  and  $\mathbf{E}(\alpha)$ . In this paper, we only consider the graphs without *isolated* vertexes, i.e., any vertex in the graph is either a starting or ending vertex of some edge. In this case,  $\mathbf{V}(\alpha)$  is completely determined by  $\mathbf{E}(\alpha)$ , i.e.  $\mathbf{V}(\alpha) = \mathbf{V}(\mathbf{E}(\alpha))$ .

In a graph  $\alpha$ , we say a vertex  $A$  is a **top** vertex if  $\text{in}(A) = \emptyset$ , and  $B$  is a **bottom** vertex if  $\text{out}(B) = \emptyset$ . A vertex is called an **inner** vertex if it is neither a top nor a bottom vertex in  $\alpha$ . We use  $\text{Top}(\alpha)$ ,  $\text{Bot}(\alpha)$ ,  $\text{Inner}(\alpha)$  to refer to the sets of the top, bottom, and inner vertexes of the graph  $\alpha$ . Clearly, we have  $\mathbf{V}(\alpha) = \text{Top}(\alpha) \cup \text{Bot}(\alpha) \cup \text{Inner}(\alpha)$ . For two graphs  $\alpha$  and  $\beta$ , we say  $\beta$  **contains**  $\alpha$ , or equivalently  $\alpha$  is a **subgraph** of  $\beta$ , if  $\mathbf{E}(\alpha) \subseteq \mathbf{E}(\beta)$ , and we write  $\alpha \subseteq \beta$  for short.

Given two graphs  $\alpha$  and  $\beta$ , we define  $\alpha - \beta$  and  $\alpha + \beta$  as

$$\alpha - \beta := (\mathbf{V}(\mathbf{E}(\alpha) \setminus \mathbf{E}(\beta)), \mathbf{E}(\alpha) \setminus \mathbf{E}(\beta)) \text{ and } \alpha + \beta := (\mathbf{V}(\alpha) \cup \mathbf{V}(\beta), \mathbf{E}(\alpha) \cup \mathbf{E}(\beta)).$$

where  $\mathbf{E}(\alpha) \setminus \mathbf{E}(\beta)$  is the set that  $\mathbf{E}(\alpha)$  minus  $\mathbf{E}(\beta)$ .

## 2.4 Graph-based model for TRIVIUM

In [DDGP22], Delaune et al. proposed a graph-based model to recover the superpoly of TRIVIUM when a cube is given. They constructed a directed graph in which a vertex represents a variable, and an edge from  $X$  to  $Y$  indicates that the variable  $Y$  appears in the ANF of  $X$ . The round function of TRIVIUM defines the possible transitions from a vertex to its children. Thus, a Deterministic Finite Automaton (DFA) can be deduced from the description of TRIVIUM. We rewrite these relations equivalently by Eq. (1):

$$\begin{aligned} A_r &:= C_{r-66} \oplus C_{r-111} \oplus C_{r-110} \cdot C_{r-109} \oplus A_{r-69}, \\ B_r &:= A_{r-66} \oplus A_{r-93} \oplus A_{r-92} \cdot A_{r-91} \oplus B_{r-78}, \\ C_r &:= B_{r-69} \oplus B_{r-84} \oplus B_{r-83} \cdot B_{r-82} \oplus C_{r-87}, \end{aligned} \tag{1}$$

where  $A_r, B_r, C_r$  represents the output bit of the register  $A, B,$  or  $C$  in the  $r$ -th round. There are four possible transitions to go from the output bit of each register ( $A, B,$  or  $C$ ) to its successors: three of them are simple edges, and one is the doubling edge ( $\Rightarrow$ ). The three simple transitions were named by the looping ( $\cdots \rightarrow$ ), the short ( $--\rightarrow$ ), and the long ( $\rightarrow$ ) one. For example, from the first equation in Eq. (1), the edge  $A_r \cdots \rightarrow A_{r-69}$  is a looping edge;  $A_r --\rightarrow C_{r-66}$  and  $A_r \rightarrow C_{r-111}$  are short and long edges, respectively. The doubling edge is a bit complex. The edges  $A_r \Rightarrow C_{r-110}$  and  $A_r \Rightarrow C_{r-109}$  are both doubling edges. Please note that the doubling edges  $A_r \Rightarrow C_{r-110}$  and  $A_r \Rightarrow C_{r-109}$  are two edges in the graph view, but they share the same variable in Delaune et al.'s model because they always appear or disappear simultaneously. As the doubling edges always appear in a pair, we call the edges like  $A_r \Rightarrow C_{r-110}$  and  $A_r \Rightarrow C_{r-109}$  a **pair of doubling edges**.

Delaune et al. presented a MILP implementation of the graph-based model of TRIVIUM. Here, we illustrate the model using the notations in Sec. 2.3, slightly different from the original one. Please refer to [DDGP22] for more details about the original model. All variables related to the edges are declared as Boolean variables:

$$X_e = \begin{cases} 1 & \text{if the edge } e \text{ appears in a valid graph,} \\ 0 & \text{otherwise.} \end{cases}$$

We define the validation of the graphs below, implying that not all graphs are allowable in Delaune et al.'s graph-based model.

**Definition 1.** A graph  $\gamma = (\mathbf{V}, \mathbf{E})$  is valid if the following two conditions hold.

1. No isolate vertexes in  $\mathbf{V}$ , i.e., each vertex is a starting or ending vertex of some edge.
2. For any non-bottom vertex  $P$ , the size of  $\text{out}(P)$  is either 1 or 2. If  $|\text{out}(P)| = 1$ , the edge in  $\text{out}(P)$  can only be the looping, long, or short edge; otherwise,  $\text{out}(P)$  must contain a pair of doubling edges.

A solution to the graph-based MILP model should be a valid graph, and such a solution is also called a **trail** in [DDGP22]. A trail corresponds to a monomial in the superpoly.

Please remark that in Delaune et al.'s MILP model, the doubling edges are treated as a whole. Let  $A \Rightarrow B$  and  $A \Rightarrow C$  be a pair of doubling edges. Only one variable  $x$  is used to represent both  $X_{(A,B)}$  and  $X_{(A,C)}$  in the model. For instance,  $x = 1$  means both  $A \Rightarrow B$  and  $A \Rightarrow C$  appear in the trail; otherwise, neither  $A \Rightarrow B$  nor  $A \Rightarrow C$  appears.

Some constraints are added to ensure the MILP solutions are all valid graphs. The graph  $\alpha$  being valid means

$$\sum_{e \in \text{out}(A)} X_e \leq 1, \text{ for } \forall A \in V(\alpha) \setminus \text{Bot}(\alpha).$$

If there is an outgoing edge from  $A$ , then there should be an incoming edge:

$$\sum_{e \in \text{out}(A)} X_e \leq \sum_{e' \in \text{in}(A)} X_{e'}, \text{ for } \forall A \in \text{Inner}(\alpha).$$

Conversely, if there is no outgoing edge from  $A$ , then there should be no incoming edges:

$$|\text{in}(A)| \cdot \left( \sum_{e \in \text{out}(A)} X_e \right) \geq \sum_{e' \in \text{in}(A)} X_{e'}, \text{ for } \forall A \in \text{Inner}(\alpha).$$

If  $V$  is a cube variable, we use the following constraint to ensure  $V$  appears:

$$\sum_{e \in \text{in}(V)} X_e \geq 1.$$

After the MILP model was built, Delaune et al. proposed several techniques to speed up its solving. One important technique is the “3 consecutive bit” pattern technique, which rejects useless trails efficiently.

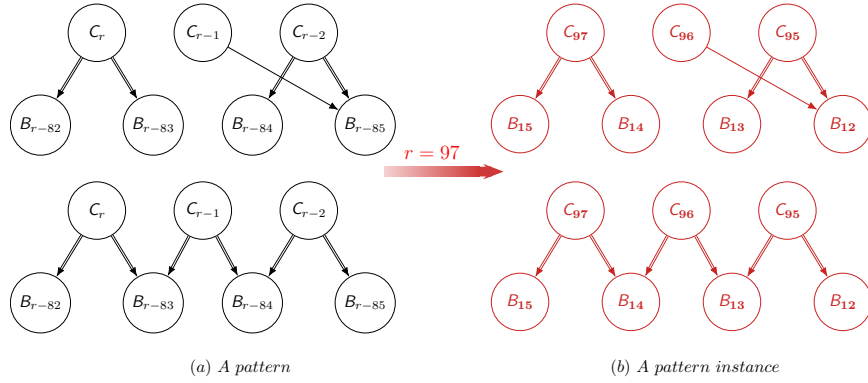
In the MILP model built for recovering a superpoly, each trail (i.e. a feasible solution to the model) corresponds to a monomial in the superpoly. To obtain the precise representation of the superpoly, one needs to calculate all trails. As the superpoly is Boolean, a monomial vanishes if it appears twice. Thus, whether a monomial “finally” appears in the representation of the superpoly is determined by how many trails correspond to this monomial. In other words, if the number of trails is even, this monomial does not appear in the superpoly. Moreover, if the number of trails related to a monomial is 3, then 2 of the 3 trails make no contributions to the superpoly. So, even numbers of trails related to the same monomial are useless in recovering the superpolys. It is generally agreed that if a MILP model has more solutions, it takes more time to solve this model. Delaune et al. proposed the “3 consecutive bit” pattern to detect the trails always appearing in pairs. In this way, they can reject an even number of trails related to the same monomial and speed up the procedure of recovering superpolys. However, Delaune et al. only used one pattern to reject pairing trails. Later, Cheng and Qiao found more patterns [CQ23], but they did not accelerate the model’s solving procedure.

**Pattern vs. pattern instance** Delaune et al. proposed the concept of pattern but did not give a rigorous definition. However, by saying a pattern, they mean a pattern instance.

**Definition 2.** Let  $\Gamma = \{\gamma_0, \gamma_1\}$  be a set of graphs. We say  $\Gamma$  is a **2-pattern instance** if  $\gamma_0$  and  $\gamma_1$  are valid,  $\gamma_0 \neq \gamma_1$ ,  $\text{Top}(\gamma_0) = \text{Top}(\gamma_1)$  and  $\text{Bot}(\gamma_0) = \text{Bot}(\gamma_1)$ .

Similarly, we can define  **$k$ -pattern instance**.

To our understanding, a “pattern” is like a “template”, where some parameters exist to be set. When the parameters are specialized, a “2-pattern” becomes a “2-pattern instance”.



**Figure 1:** 2-pattern vs. 2-pattern instance

In this sense, we think the left figure of Fig. 1 stands for a 3-consecutive bit pattern, and the right figure illustrates an instance of this pattern when  $r$  is specialized to 97.

We denote a 2-pattern by a calligraphic letter, e.g.,  $\mathcal{A}, \mathcal{B}$ . An instance  $\mathbf{a}$  of a 2-pattern  $\mathcal{A}$  is a specialization and denoted by  $\mathbf{a} = (\alpha_0, \alpha_1)$ . Given a 2-pattern instance  $\mathbf{a} = (\alpha_0, \alpha_1)$ , we define the vertexes and edges of  $\mathbf{a}$  as

$$\mathbf{V}(\mathbf{a}) = \mathbf{V}(\alpha_0) \cup \mathbf{V}(\alpha_1) \text{ and } \mathbf{E}(\mathbf{a}) = \mathbf{E}(\alpha_0) \cup \mathbf{E}(\alpha_1).$$

Besides, the top, bottom, and inner of  $\mathbf{a}$  are defined as

$$\text{Top}(\mathbf{a}) = \text{Top}(\alpha_0) = \text{Top}(\alpha_1), \text{Bot}(\mathbf{a}) = \text{Bot}(\alpha_0) = \text{Bot}(\alpha_1), \text{Inner}(\mathbf{a}) = \text{Inner}(\alpha_0) \cup \text{Inner}(\alpha_1).$$

Please note that we have  $\text{Top}(\mathbf{a}) \cup \text{Bot}(\mathbf{a}) \subseteq \mathbf{V}(\alpha_0) \cap \mathbf{V}(\alpha_1)$ , but  $\mathbf{V}(\alpha_0) \cap \mathbf{V}(\alpha_1)$  may be strictly larger than  $\text{Top}(\mathbf{a}) \cup \text{Bot}(\mathbf{a})$ . So, we should consider the different vertexes in  $\alpha_0$  and  $\alpha_1$ . For the 2-pattern  $\mathbf{a} = (\alpha_0, \alpha_1)$  we define the set of different vertexes as

$$\text{Diff}(\mathbf{a}) := \mathbf{V}(\mathbf{a}) \setminus (\mathbf{V}(\alpha_0) \cap \mathbf{V}(\alpha_1)).$$

For simplification, as we rarely discuss patterns but always talk about the instances, we call pattern instances as patterns for short if no confusion appears.

### 3 A New Graph-based Model for Recovering Superpolys

A critical step of the new attacks is to obtain numerous superpolys. However, recovering superpolys is costly, particularly when the superpoly is dense. In [DDGP22], Delaune et al. proposed a graph-based model for recovering superpolys, and this model has been proven very efficient compared with previous models, e.g. [HLM<sup>+</sup>20].

We think Delaune et al.'s graph model's improvement in efficiency mainly comes from two aspects. Firstly, in the graph-based model, the variables stand for whether the edges appear. This change in data structure decreases the number of variables and simplifies the representation of constraints. Secondly, Delaune et al. presented many techniques for speeding up the solving procedure of the constructed MILP model. We think one of their important techniques is to use the "3 consecutive bit" pattern to reject many useless solutions of the model.

However, Delaune et al. only used one 2-pattern to reject "pairing trails", which are the trails appearing in pairs. Later, Cheng and Qiao found more 2-patterns [CQ23], but they did not accelerate the model's solving procedure. We think the main obstacle is that no mathematical theory exists to show how different 2-patterns work correctly when used simultaneously.



Therefore, to recover the superpolys more efficiently, we aim to find and use more 2-patterns to reject the useless pairing trails. For this goal, we need some theories to ensure the correctness when several 2-patterns are used simultaneously.

### 3.1 Theory

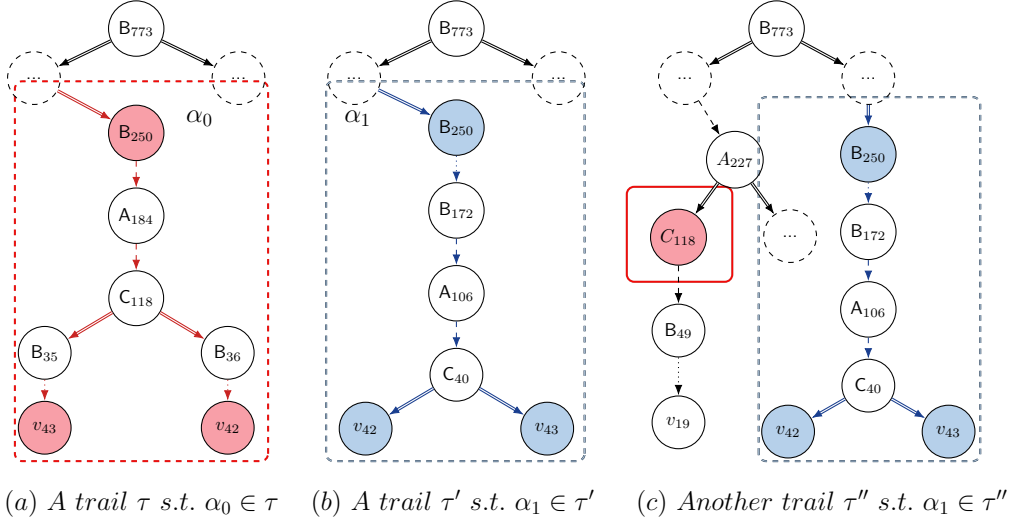
In this subsection, we study and answer the following three questions respectively.

1. Which kinds of trails can be rejected by a 2-pattern?
2. How do two 2-patterns work correctly when used simultaneously?
3. How do several 2-patterns work correctly when used simultaneously?

#### 3.1.1 Which kinds of trails can be rejected by a 2-pattern?

A trail of a graph-based MILP model corresponds to a monomial in the superpoly. It is easy to find out that only two trails related to the same monomial can be removed without bringing any error in recovering the superpoly. Let  $m$  be a monomial, and  $\mathcal{T}_m$  be the set of all trails of the graph-based model related to the monomial  $m$ .

The patterns given by Delaune et al. and Cheng-Qiao are all subgraphs of the complete trails. Intuitively, if two trails are only different in the subgraphs involved by a 2-pattern, these two trails could be rejected by the 2-pattern, e.g., the two left graphs in Fig. 2. However, to ensure a 2-pattern works correctly, the trails to be rejected have more requirements.



**Figure 2:** Three trails and a 2-pattern  $\mathbf{a} = (\alpha_0, \alpha_1)$ .

**Definition 3.** Let  $\tau \in \mathcal{T}_m$  be a trail and  $\mathbf{a} = (\alpha_0, \alpha_1)$  be a 2-pattern. We say  $\tau$  is **replaceable** with respect to  $\mathbf{a}$ , if there exists  $\alpha_i$  such that  $\alpha_i \subseteq \tau$  and

$$\mathbf{V}(\tau - \alpha_i) \cap \text{Diff}(\mathbf{a}) = \emptyset. \quad (2)$$

In  $\mathcal{T}_m$ , the set consists of all replaceable trails with respect to  $\mathbf{a}$  is called the **replaceable set** of  $\mathbf{a}$  in  $\mathcal{T}_m$ , denoted by  $\text{Rep}(\mathbf{a})$ .

**Proposition 1.** Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  be a 2-pattern and  $\tau \in \mathcal{T}_m$  be a trail such that  $\alpha_0 \subseteq \tau$ . If  $\tau \in \text{Rep}(\mathbf{a})$ , then  $\tau - \alpha_0 + \alpha_1$  is also in  $\text{Rep}(\mathbf{a})$ .

*Proof.* As  $\tau$  is replaceable with respect to  $\mathbf{a}$ , we have  $\mathbf{V}(\tau - \alpha_0) \cap \text{Diff}(\mathbf{a}) = \mathbf{V}(\tau - \alpha_0) \cap (\mathbf{V}(\mathbf{a}) \setminus (\mathbf{V}(\alpha_0) \cap (\mathbf{V}(\alpha_1)))) = \emptyset$  by definition. Thus,  $\tau' := \tau - \alpha_0 + \alpha_1$  is a valid graph without any isolated vertex, which means it is also a trail.

As  $\text{Bot}(\tau) = \text{Bot}(\tau')$ , the trails  $\tau$  and  $\tau'$  correspond to the same monomial. Besides,  $\mathbf{V}(\tau - \alpha_0) \cap \text{Diff}(\mathbf{a}) = \mathbf{V}(\tau' - \alpha_1) \cap \text{Diff}(\mathbf{a}) = \emptyset$  implies  $\tau'$  is also replaceable with respect to  $\mathbf{a}$ . Thus, we have  $\tau' \in \text{Rep}(\mathbf{a})$ .  $\square$

In the above proof, we construct a special trail related to the given trail in the replaceable set. Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  be a 2-pattern and  $\tau \in \mathcal{T}_m$  be a trail such that  $\alpha_0 \subseteq \tau$ . If  $\tau \in \text{Rep}(\mathbf{a})$ , then we define  $\tau' := \tau - \alpha_0 + \alpha_1$  as the **dual trail** of  $\tau$ , and denote it as  $\text{Dual}(\tau)$ . Prop. 1 implies if  $\tau \in \text{Rep}(\mathbf{a})$ , so is  $\text{Dual}(\tau)$ . Moreover, we have  $\tau = \text{Dual}(\text{Dual}(\tau))$ , which deduces the following corollary.

**Corollary 1.** *Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  be a 2-pattern. Then the number  $|\text{Rep}(\mathbf{a})|$  is even.*

The requirement in Eq. (2) is essential to construct a new valid trail. For example in Fig. 2, the trail  $\tau''$  contains  $\alpha_1$  but  $\tau''$  is not replaceable with respect to  $\mathbf{a}$  due to the fact  $\mathbf{V}(\tau'' - \alpha_1) \cap \text{Diff}(\mathbf{a}) = \{C_{118}\}$ . This leads to that  $\tau'' - \alpha_1 + \alpha_0$  is not valid, because the vertex  $C_{118}$  has two different types of outgoing edges in  $\tau'' - \alpha_1 + \alpha_0$ , i.e. the short edge  $C_{118} \dashrightarrow B_{49}$  and the doubling edges  $C_{118} \Rightarrow B_{35}, C_{118} \Rightarrow B_{36}$ .

Next, we show how to generate constraints in MILP models to reject the pairing trails in  $\text{Rep}(\mathbf{a})$  for a given 2-pattern  $\mathbf{a} = (\alpha_0, \alpha_1)$ .

**Proposition 2.** *Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  be a 2-pattern. Denote  $\text{in}_i(V) := \text{in}(V) \cap \mathbf{E}(\alpha_i)$  and  $\text{out}_i(V) := \text{out}(V) \cap \mathbf{E}(\alpha_i)$  for  $V \in \mathbf{V}(\alpha_i)$  and  $1 \leq i \leq 2$ . The following constraints will reject all trails in  $\text{Rep}(\mathbf{a})$ :*

$$\sum_{V \in \text{Top}(\alpha_0), e \in \text{out}_0(V)} X_e + \sum_{V \in \text{Inner}(\alpha_0), e \in \text{out}_0(V)} (|\text{in}_0(V)| \cdot X_e) < \sum_{V \in \text{Inner}(\mathbf{a}), e \in \text{in}(V)} X_e + |\text{Top}(\alpha_0)|,$$

and

$$\sum_{V \in \text{Top}(\alpha_1), e \in \text{out}_1(V)} X_e + \sum_{V \in \text{Inner}(\alpha_1), e \in \text{out}_1(V)} (|\text{in}_1(V)| \cdot X_e) < \sum_{V \in \text{Inner}(\mathbf{a}), e \in \text{in}(V)} X_e + |\text{Top}(\alpha_1)|.$$

*Proof.* For any inner vertex  $V$  of the graph  $\alpha_0$ , we have

$$\sum_{e \in \text{out}_0(V)} |\text{in}_0(V)| \cdot X_e \leq \sum_{e \in \text{in}(V)} X_e, \quad (3)$$

since the basic constraint of the graph-based model requires that the number of outgoing edges of a vertex cannot exceed the number of incoming edges of this vertex.

Since  $|\text{out}(V)| \leq 1$  for any vertex  $V$  in a valid graph, then we have

$$\sum_{e \in \text{out}(V)} X_e \leq |\text{Top}(\alpha_0)|, \text{ for } V \in \text{Top}(\alpha_0). \quad (4)$$

Summing up Eq. (3) and (4) for vertexes in  $\text{Inner}(\alpha_0)$  and  $\text{Top}(\alpha_0)$ , we obtain

$$\sum_{V \in \text{Top}(\alpha_0), e \in \text{out}_0(V)} X_e + \sum_{V \in \text{Inner}(\alpha_0), e \in \text{out}_0(V)} (|\text{in}_0(V)| \cdot X_e) \leq \sum_{V \in \text{Inner}(\mathbf{a}), e \in \text{in}(V)} X_e + |\text{Top}(\alpha_0)|.$$

Considering the trails in the replaceable set  $\text{Rep}(\mathbf{a})$ , the equality holds only when a trail  $\tau \in \text{Rep}(\mathbf{a})$  contains the 2-pattern. Deleting this equality will reject this trail exactly and does not affect other others. Similarly, the second constraint rejects exactly the trail  $\tau' \in \text{Rep}(\mathbf{a})$  that covers  $\alpha_1$ .

Similarly, the second constraint rejects exactly the trail  $\tau'$  that covers  $\alpha_1$  such that  $\mathbf{V}(\tau' - \alpha_1)$  does not involve any vertex in  $\text{Inner}(\mathbf{a})$ .  $\square$

**Example 1.** For example, we consider the 2-pattern  $\mathbf{a} = (\alpha_0, \alpha_1)$  used in Fig. 2, and illustrate how to add constraints to reject trails in  $\text{Rep}(\mathbf{a})$ . From the figure, we have  $\alpha_0 = (\mathbf{V}_0, \mathbf{E}_0)$ ,  $\alpha_1 = (\mathbf{V}_1, \mathbf{E}_1)$ ,  $\mathbf{V}_0 = \{B_{250}, A_{184}, C_{118}, B_{35}, B_{36}, v_{42}, v_{43}\}$ ,  $\mathbf{E}_0 = \{(B_{250}, A_{184}), (A_{184}, C_{118}), (C_{118}, B_{35}), (C_{118}, B_{36}), (B_{35}, v_{43}), (B_{36}, v_{42})\}$ ,  $\mathbf{V}_1 = \{B_{250}, B_{172}, A_{106}, C_{40}, v_{42}, v_{43}\}$ ,  $\mathbf{E}_1 = \{(B_{250}, B_{172}), (B_{172}, A_{106}), (A_{106}, C_{40}), (C_{40}, v_{42}), (C_{40}, v_{43})\}$ . Here, we simplify the notation  $(B_{250}, A_{184})$  to  $e_{(250,184)}$  and denote its variable as  $X_{(250,184)}$ . We also abuse the notation  $X_{(36,42)}$  to represent the variable of the edge  $(B_{36}, v_{42})$ .

Therefore, the constraint corresponding to  $\alpha_0$  is:

$$X_{(250,184)} + X_{(184,118)} + X_{(118,35)} + X_{(35,43)} + X_{(36,42)} < \sum_{e \in \text{Inner}(\mathbf{a})} X_e + 1. \quad (5)$$

Please remark that  $e_{(118,35)}$  and  $e_{(118,36)}$  form a pair of doubling edges. In Delaune et al.'s graph-based model, they share the same variable  $X_{(118,35)}$  and only appear once on the left of the above constraint. Similarly, the constraint corresponding to  $\alpha_1$  is:

$$X_{(250,172)} + X_{(172,106)} + X_{(106,40)} + X_{(40,43)} < \sum_{e \in \text{Inner}(\mathbf{a})} X_e + 1. \quad (6)$$

There is another pair of doubling edges  $e_{(40,43)}$  and  $e_{(40,42)}$ , so only one variable  $X_{(40,43)}$  appears in the left.

Note that after adding these constraints in the model, the two left trails in Fig. 2 do not satisfy the above two constraints and will not be the solutions to the model. For example, if  $\alpha_0$  is a trail, the left side of Eq. (5) is 5, while the right is also 5, implying the inequality does not hold. However, the right trail in Fig. 2 satisfies the above constraints and is still a solution to the model. Because the edge  $e_{(227,118)}$  appears in the trail, which means  $X_{(227,118)} = 1$  and  $e_{(227,118)} \in \text{Inner}(\mathbf{a})$ . Thus, Eq. (5) and (6) hold, and the trail cannot be rejected. In this way, only 2 of the 3 trails are rejected; hence, no error occurs.

Now, we can answer the question proposed in the title of this subsection: not all trails that cover some subgraph of a 2-pattern can be rejected by the 2-pattern correctly, and only the trails in the replaceable set of this 2-pattern can.

### 3.1.2 How do two 2-patterns work correctly when used simultaneously?

In the practical recovery of superpolys, the number of trails rejected by a single 2-pattern instance is limited. Even in the original graph-based model, Delaune et al. also exploited many 3-consecutive bit pattern instances, and the authors also mentioned that although they found some other patterns, they cannot guarantee correctness if using different types of patterns simultaneously. In this subsection, we will solve this problem in theory. Besides, our theory also explains why many 3-consecutive bit pattern instances can work correctly when used simultaneously.

We consider the scenario where two 2-patterns  $\mathbf{a} = (\alpha_0, \alpha_1)$  and  $\mathbf{b} = (\beta_0, \beta_1)$  are applied simultaneously. If the constraints related to  $\mathbf{a}$  and  $\mathbf{b}$  are appended to the MILP model, the trails rejected by these two 2-patterns are  $\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})$ .

**Lemma 1.** *Let  $\mathbf{a}$  and  $\mathbf{b}$  be two 2-patterns and  $m$  be a monomial. If the number  $|\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})| \subseteq \mathcal{T}_m$  is even, then the superpolys recovered by the models with and without these two 2-patterns are identical.*

*Proof.* Adding these two 2-patterns can only reject the trails in  $\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b}) \subseteq \mathcal{T}_m$ . If  $m$  appears even times, then it makes no difference to the final superpoly.  $\square$

Based on the above lemma, we have a condition for ensuring two 2-patterns work correctly. The next question is how to determine whether  $|\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})|$  is even.

According to the principle of inclusion-exclusion, we have

$$|\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})| = |\text{Rep}(\mathbf{a})| + |\text{Rep}(\mathbf{b})| - |\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})|.$$

As we have shown  $|\text{Rep}(\mathbf{a})|$  and  $|\text{Rep}(\mathbf{b})|$  are both even, the number  $|\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})|$  is even if and only if  $|\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})|$  is even.

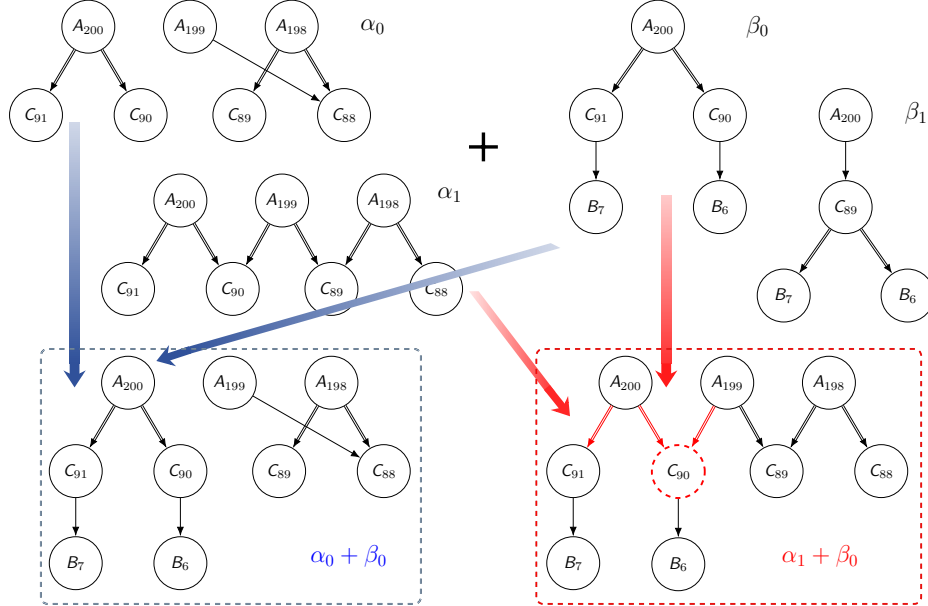
The set  $\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})$  consists of the trails covering the subgraphs from both  $\mathbf{a}$  and  $\mathbf{b}$ . Thus, we should consider the subgraphs in  $\mathbf{a}$  and  $\mathbf{b}$  together to see if contradictions occur. For two 2-patterns  $\mathbf{a} = (\alpha_0, \alpha_1)$  and  $\mathbf{b} = (\beta_0, \beta_1)$ , all possible compositions are  $\alpha_0 + \beta_0, \alpha_0 + \beta_1, \alpha_1 + \beta_0, \alpha_1 + \beta_1$ . However, it is possible that there does not exist a trail containing some  $\alpha_i + \beta_j$  at all, or although a trail covers some  $\alpha_i + \beta_j$ , its dual trail (in  $\text{Rep}(\mathbf{a})$  or  $\text{Rep}(\mathbf{b})$ ) cannot. These cases may result in  $|\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})|$  being odd. Thus, we study a special composition of the subgraphs in  $\mathbf{a}$  and  $\mathbf{b}$ .

**Definition 4.** Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  and  $\mathbf{b} = (\beta_0, \beta_1)$  be two 2-patterns. We say  $\alpha_i$  is **consistent** with  $\beta_j$  for  $0 \leq i, j \leq 1$ , if

1.  $\alpha_i + \beta_j$  is a valid graph, and
2. the following two equations hold

$$\mathbf{V}(\alpha_i - \beta_j) \cap \text{Diff}(\mathbf{b}) = \emptyset \text{ and } \mathbf{V}(\beta_j - \alpha_i) \cap \text{Diff}(\mathbf{a}) = \emptyset.$$

In the Fig. 3, we can see  $\alpha_0$  is consistent with  $\beta_0$ , but  $\alpha_1$  is not consistent with  $\beta_0$ . Although  $\alpha_1 + \beta_0$  is a valid graph, but  $\beta_0$ 's vertex  $C_{90}$  has an extra incoming edge in  $\alpha_1 + \beta_0$ , which means  $\mathbf{V}(\alpha_1 - \beta_0) \cap \text{Diff}(\mathbf{b}) = \{C_{90}\}$ .



**Figure 3:**  $\beta_0$  is consistent with  $\alpha_0$ , but inconsistent with  $\alpha_1$ .

By definition, if  $\alpha_i$  is consistent with  $\beta_j$ , then  $\beta_j$  is also consistent with  $\alpha_i$ . We use the following proposition to check whether  $\alpha_i + \beta_j$  is valid.

**Proposition 3.** Let  $\alpha$  and  $\beta$  be two valid graphs. Then  $\alpha \cup \beta$  is valid, if and only if for any vertex  $V \in \mathbf{V}(\alpha) \cap \mathbf{V}(\beta)$ ,  $V$  has identical outgoing edges in both  $\alpha$  and  $\beta$ .

Note that if  $\mathbf{V}(\alpha) \cap \mathbf{V}(\beta) = \emptyset$ , the graph  $\alpha \cup \beta$  is always valid. Moreover, we have the following proposition.

**Proposition 4.** *Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  and  $\mathbf{b} = (\beta_0, \beta_1)$  be two 2-patterns. If  $\mathbf{V}(\mathbf{a}) \cap \mathbf{V}(\mathbf{b}) = \emptyset$ , then  $\alpha_i$  is consistent with  $\beta_j$  for all  $0 \leq i, j \leq 1$ .*

*Proof.*  $\mathbf{V}(\mathbf{a}) \cap \mathbf{V}(\mathbf{b}) = \emptyset$  implies  $\mathbf{V}(\alpha_i - \beta_j) = \emptyset$ . □

Thus, the introduction of Def. 4 is intended to solve the problems appearing in the case  $\mathbf{V}(\mathbf{a}) \cap \mathbf{V}(\mathbf{b}) \neq \emptyset$ . We introduce the second condition of Def. 4 because we hope to treat the composite graph  $\alpha_i + \beta_j$  as a subgraph of a new pattern.

**Definition 5.** Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  and  $\mathbf{b} = (\beta_0, \beta_1)$  be two 2-patterns. The set  $\{\alpha_i + \beta_j \mid \alpha_i \text{ is consistent with } \beta_j \text{ for } 0 \leq i, j \leq 1\}$  is called the **composite set** of  $\mathbf{a}$  and  $\mathbf{b}$ , denoted as  $\text{Comp}(\mathbf{a}, \mathbf{b})$ .

The set  $\text{Comp}(\mathbf{a}, \mathbf{b})$  is a  $|\text{Comp}(\mathbf{a}, \mathbf{b})|$ -pattern, so we can also define the replaceable set of  $\text{Comp}(\mathbf{a}, \mathbf{b})$  in the same way as Def. 3. But in practical use, we do not directly discuss the trails in  $\text{Rep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ . We always discuss the trails in the following set

$$\text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b})) := \text{Rep}(\text{Comp}(\mathbf{a}, \mathbf{b})) \cap \text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b}),$$

where ‘‘S’’ is short for ‘‘strong’’ and we call  $\text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$  the strong replaceable set of  $\text{Comp}(\mathbf{a}, \mathbf{b})$ . By definition, for any  $\tau \in \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ , assume  $\alpha_i + \beta_j \subset \tau$ , then we have

$$\mathbf{V}(\tau - (\alpha_i + \beta_j)) \cap (\text{Diff}(\mathbf{a}) \cup \text{Diff}(\mathbf{b}) \cup \text{Diff}(\text{Comp}(\mathbf{a}, \mathbf{b}))) = \emptyset.$$

**Proposition 5.** *Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  and  $\mathbf{b} = (\beta_0, \beta_1)$  be two 2-patterns, and  $\lambda, \lambda' \in \text{Comp}(\mathbf{a}, \mathbf{b})$  be two sub-graphs. If there exists a trail  $\tau \in \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$  s.t.  $\lambda \subseteq \tau$ , then there exists  $\tau' \in \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$  s.t.  $\lambda' \subseteq \tau'$ .*

*Proof.* For  $\tau \in \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ , we have  $\tau \in \text{Rep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ . Then by the definition of replaceable set, there exists  $\tau' \in \text{Rep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$  such that  $\lambda' \subseteq \tau'$  and  $\tau - \lambda = \tau' - \lambda'$ . It suffices to show  $\tau' \in \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ . As  $\tau' \in \text{Rep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ , it suffices to show  $\tau' \in \text{Rep}(\mathbf{a})$  and  $\tau' \in \text{Rep}(\mathbf{b})$ . We next prove  $\tau' \in \text{Rep}(\mathbf{a})$ .

Firstly, assume  $\lambda' = \alpha_i + \beta_j$  for some  $i, j \in \{0, 1\}$ , since  $\lambda' \subseteq \tau'$ , we have  $\alpha_i \subseteq \tau'$ .

Secondly, since  $\tau \in \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b})) \subseteq \text{Rep}(\mathbf{a})$  and there exists some  $\alpha$  such that  $\alpha \subseteq \lambda$ , then we have  $\mathbf{V}(\tau - \lambda) \cap \text{Diff}(\mathbf{a}) \subseteq \mathbf{V}(\tau - \alpha) \cap \text{Diff}(\mathbf{a}) = \emptyset$ . By assumption, we have  $\tau - \lambda = \tau' - \lambda'$ , then we get  $\mathbf{V}(\tau' - \lambda') \cap \text{Diff}(\mathbf{a}) = \emptyset$ .

Finally, we have  $\mathbf{V}(\tau' - \alpha_i) = \mathbf{V}(\tau' - (\alpha_i + \beta_j) + (\beta_j - \alpha_i)) \subseteq \mathbf{V}(\tau' - (\alpha_i + \beta_j)) \cup \mathbf{V}(\beta_j - \alpha_i)$ . Since  $\mathbf{V}(\tau' - (\alpha_i + \beta_j)) \cap \text{Diff}(\mathbf{a}) = \mathbf{V}(\tau' - \lambda') \cap \text{Diff}(\mathbf{a}) = \emptyset$  and  $\mathbf{V}(\beta_j - \alpha_i) \cap \text{Diff}(\mathbf{a}) = \emptyset$  due to  $\beta_j$  being consistent with  $\alpha_i$ , we have  $\mathbf{V}(\tau' - \alpha_i) \cap \text{Diff}(\mathbf{a}) \subseteq (\mathbf{V}(\tau' - (\alpha_i + \beta_j)) \cup \mathbf{V}(\beta_j - \alpha_i)) \cap \text{Diff}(\mathbf{a}) = \emptyset$ .

Thus, we have proved  $\tau' \in \text{Rep}(\mathbf{a})$ . Similarly, we can prove  $\tau' \in \text{Rep}(\mathbf{b})$ , and the proposition is proved. □

**Corollary 2.** *Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  and  $\mathbf{b} = (\beta_0, \beta_1)$  be two 2-patterns. If  $|\text{Comp}(\mathbf{a}, \mathbf{b})|$  is even, then  $|\text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))|$  is even.*

*Proof.* By Prop. 5, for any  $\tau \in \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ , we can find another  $|\text{Comp}(\mathbf{a}, \mathbf{b})| - 1$  trails in  $\text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ , which means  $|\text{Comp}(\mathbf{a}, \mathbf{b})|$  divides  $|\text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))|$ . □

**Lemma 2.** *Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  and  $\mathbf{b} = (\beta_0, \beta_1)$  be two 2-patterns. We have  $\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b}) = \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ .*

*Proof.* On one hand, we have  $\text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b})) = \text{Rep}(\text{Comp}(\mathbf{a}, \mathbf{b})) \cap \text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b}) \subseteq \text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})$ .

On the other hand, we prove the inclusion  $\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b}) \subseteq \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ . It suffices to show that for any  $\tau \in \text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})$ , we have  $\tau \in \text{Rep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ .

Firstly, suppose  $\alpha_0 \subseteq \tau$  and  $\beta_0 \subseteq \tau$ , we prove  $\alpha_0 + \beta_0 \in \text{Comp}(\mathbf{a}, \mathbf{b})$ . Clearly,  $\alpha_0 + \beta_0$  is valid as they are both sub-graphs of  $\tau$ . Since  $\tau \in \text{Rep}(\mathbf{a})$ , we have  $\mathbf{V}(\tau - \alpha_0) \cap \text{Diff}(\mathbf{a}) = \emptyset$  according to Def. 3. Note that  $\mathbf{V}(\beta_0 - \alpha_0) \subseteq \mathbf{V}(\tau - \alpha_0)$ , we can deduce  $\mathbf{V}(\beta_0 - \alpha_0) \cap \text{Diff}(\mathbf{a}) = \emptyset$ . Similarly, we have  $\mathbf{V}(\alpha_0 - \beta_0) \cap \text{Diff}(\mathbf{b}) = \emptyset$ . According to Def. 4, it follows that  $\alpha_0 + \beta_0 \in \text{Comp}(\mathbf{a}, \mathbf{b})$ .

Secondly, we prove that  $\tau \in \text{Rep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ . As  $\alpha_0 + \beta_0 \subseteq \tau$ , it suffices to prove  $\mathbf{V}(\tau - (\alpha_0 + \beta_0)) \cap \text{Diff}(\text{Comp}(\mathbf{a}, \mathbf{b})) = \emptyset$ , and we prove this by contradiction. Assume there exists a vertex  $V$  in  $\mathbf{V}(\tau - (\alpha_0 + \beta_0)) \cap \text{Diff}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ . The fact  $V \in \text{Diff}(\text{Comp}(\mathbf{a}, \mathbf{b}))$  indicates that  $V$  can only lie in  $\text{Diff}(\mathbf{a}) \cup \text{Diff}(\mathbf{b})$ . Since  $\tau \in \text{Rep}(\mathbf{a})$ , we have  $\mathbf{V}(\tau - \alpha_0) \cap \text{Diff}(\mathbf{a}) = \emptyset$ . Thus,  $\mathbf{V}(\tau - (\alpha_0 + \beta_0)) \cap \text{Diff}(\mathbf{a}) \subseteq \mathbf{V}(\tau - \alpha_0) \cap \text{Diff}(\mathbf{a}) = \emptyset$ . Similarly, we have  $\mathbf{V}(\tau - (\alpha_0 + \beta_0)) \cap \text{Diff}(\mathbf{b}) = \emptyset$ . But by assumption,  $V \in \mathbf{V}(\tau - (\alpha_0 + \beta_0))$  and  $V \in \text{Diff}(\mathbf{a}) \cup \text{Diff}(\mathbf{b})$ , which is a contradiction. So we must have  $\mathbf{V}(\tau - (\alpha_0 + \beta_0)) \cap \text{Diff}(\text{Comp}(\mathbf{a}, \mathbf{b})) = \emptyset$ . Hence,  $\tau \in \text{Rep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$  and  $\tau \in \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ .

To sum up, we have proved  $\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b}) = \text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$ .  $\square$

Lem. 2 establishes the relation between the sets  $\text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))$  and  $\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})$ . Our goal is to determine whether  $|\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})|$  is even by counting the subgraphs in the set  $\text{Comp}(\mathbf{a}, \mathbf{b})$ . For this aim, we have the following main theorem.

**Theorem 1.** *Let  $\mathbf{a} = (\alpha_0, \alpha_1)$  and  $\mathbf{b} = (\beta_0, \beta_1)$  be two 2-patterns. If  $|\text{Comp}(\mathbf{a}, \mathbf{b})|$  is even, then both  $|\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})|$  and  $|\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})|$  are even.*

*Proof.* According to Prop. 2, If  $|\text{Comp}(\mathbf{a}, \mathbf{b})|$  is even, then  $|\text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b}))|$  is also even. Moreover, by Lem. 2, we have that  $\text{SRep}(\text{Comp}(\mathbf{a}, \mathbf{b})) = \text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})$ . So we have both  $|\text{Rep}(\mathbf{a}) \cap \text{Rep}(\mathbf{b})|$  and  $|\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})|$  are even.  $\square$

We emphasize that Theorem 1 only provides a sufficient condition on  $|\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})|$  being even. So if  $|\text{Comp}(\mathbf{a}, \mathbf{b})|$  is odd, the number  $|\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})|$  may be odd or not. But a new question arises, i.e., *what if  $|\text{Comp}(\mathbf{a}, \mathbf{b})|$  is odd?* One simple method is not using the 2-pattern  $\mathbf{a}$  and  $\mathbf{b}$  simultaneously. As we will find many 2-patterns during the computations, discarding some does not affect the solving efficiency very much.

### 3.1.3 How do several 2-patterns work correctly when used simultaneously?

In practical computations, two 2-patterns may still not be adequate to reject as many pairing trails as we hope. We need more 2-patterns to work simultaneously. Let  $\mathbf{p}_0, \mathbf{p}_1, \dots, \mathbf{p}_{l-1}$  be  $l$  2-patterns. These 2-patterns work correctly only when the number of trails in  $\text{Rep}(\mathbf{p}_0) \cup \text{Rep}(\mathbf{p}_1) \cup \dots \cup \text{Rep}(\mathbf{p}_{l-1}) \subseteq \mathcal{T}_m$  is even. We next present a sufficient condition on  $|\text{Rep}(\mathbf{p}_0) \cup \text{Rep}(\mathbf{p}_1) \cup \dots \cup \text{Rep}(\mathbf{p}_{l-1})|$  being even. We need another lemma first.

**Lemma 3.** *Let  $\mathbf{p}_0, \mathbf{p}_1, \dots, \mathbf{p}_{l-1} (l \geq 3)$  be  $l$  2-patterns. If for any two 2-patterns  $\mathbf{p}_i$  and  $\mathbf{p}_j$ , we have  $|\text{Comp}(\mathbf{p}_i, \mathbf{p}_j)| = 4$ , then  $|\text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \dots \cap \text{Rep}(\mathbf{p}_{l-1})|$  is even.*

*Proof.* Let  $\tau$  be a trail in  $\text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \dots \cap \text{Rep}(\mathbf{p}_{l-1})$ . As  $\tau \in \text{Rep}(\mathbf{p}_0)$ , there exists  $\tau'$  be a dual trail of  $\tau$  in  $\text{Rep}(\mathbf{p}_0)$ . We next show  $\tau' \in \text{Rep}(\mathbf{p}_i)$  for all  $1 \leq i < l$ .

As  $|\text{Comp}(\mathbf{p}_0, \mathbf{p}_i)| = 4$ , we suppose  $\mathbf{p}_0 = (\alpha_0, \alpha_1)$ ,  $\mathbf{p}_i = (\beta_0, \beta_1)$ ,  $\alpha_0 + \beta_0 \subseteq \tau$ , and  $\alpha_1 \subseteq \tau'$ . Because  $\tau'$  is a dual trail of  $\tau$  in  $\text{Rep}(\mathbf{p}_0)$ ,  $\alpha_0 + \beta_0 \subseteq \tau$  and  $|\text{Comp}(\mathbf{p}_0, \mathbf{p}_i)| = 4$ , we have  $\alpha_1 + \beta_0 \subseteq \tau'$ .

Note that  $\mathbf{V}(\tau' - \beta_0) = \mathbf{V}(\tau' - (\beta_0 + \alpha_1) + (\alpha_1 - \beta_0)) \subseteq \mathbf{V}(\tau' - (\alpha_1 + \beta_0)) \cup \mathbf{V}(\alpha_1 - \beta_0)$ . Since  $\tau$  and  $\tau'$  are dual trails in  $\text{Rep}(\mathbf{p}_0)$ , we have  $\mathbf{V}(\tau' - (\alpha_1 + \beta_0)) \cap \text{Diff}(\mathbf{p}_i) = \mathbf{V}(\tau - \alpha_0 - \beta_0) \cap \text{Diff}(\mathbf{p}_i) = \emptyset$  due to  $\tau \in \text{Rep}(\mathbf{p}_i)$ . Again because of  $|\text{Comp}(\mathbf{p}_0, \mathbf{p}_i)| =$

4,  $\alpha_1$  is consistent with  $\beta_0$ , we have  $\mathbf{V}(\alpha_1 - \beta_0) \cap \text{Diff}(\mathbf{p}_i) = \emptyset$ . So in all, we have  $\mathbf{V}(\tau' - \beta_0) \cap \text{Diff}(\mathbf{p}_i) \subseteq (\mathbf{V}(\tau' - (\alpha_1 + \beta_0)) \cup \mathbf{V}(\alpha_1 - \beta_0)) \cap \text{Diff}(\mathbf{p}_i) = \emptyset$ . Hence,  $\tau'$  lies in  $\text{Rep}(\mathbf{p}_i)$ .

Because for any  $\tau \in \text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{l-1})$ , there exists  $\tau' \in \text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{l-1})$ , the number  $|\text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{l-1})|$  is even.  $\square$

Next, we present the second theorem in this paper.

**Theorem 2.** *Let  $\mathbf{p}_0, \mathbf{p}_1, \dots, \mathbf{p}_{l-1}$  ( $l \geq 3$ ) be 2-patterns. If the following conditions hold*

1. *For any two 2-patterns  $\mathbf{p}_i$  and  $\mathbf{p}_j$ , the number  $|\text{Comp}(\mathbf{p}_i, \mathbf{p}_j)|$  is even;*
2. *For any three 2-patterns  $\mathbf{p}_i, \mathbf{p}_j, \mathbf{p}_k$ , as most one of  $\mathbf{V}(\mathbf{p}_i) \cap \mathbf{V}(\mathbf{p}_j)$ ,  $\mathbf{V}(\mathbf{p}_i) \cap \mathbf{V}(\mathbf{p}_k)$ , and  $\mathbf{V}(\mathbf{p}_j) \cap \mathbf{V}(\mathbf{p}_k)$  is non-empty.*

*Then  $|\text{Rep}(\mathbf{p}_0) \cup \text{Rep}(\mathbf{p}_1) \cup \cdots \cup \text{Rep}(\mathbf{p}_{l-1})|$  is even.*

*Proof.* Based on Cor. 1, the number  $|\text{Rep}(\mathbf{p}_1)|, |\text{Rep}(\mathbf{p}_2)|, \dots, |\text{Rep}(\mathbf{p}_l)|$  are all even. For any two 2-patterns  $\mathbf{p}_i$  and  $\mathbf{p}_j$ , the  $|\text{Comp}(\mathbf{p}_i, \mathbf{p}_j)|$  is even means that  $|\text{Rep}(\mathbf{p}_i) \cap \text{Rep}(\mathbf{p}_j)|$  is even by Theorem 1.

Now, consider the case of  $r$  2-patterns  $\mathbf{p}_0, \mathbf{p}_1, \dots, \mathbf{p}_{r-1}$  ( $3 \leq r \leq l$ ), and we want to prove  $|\text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{r-1})|$  is even.

Clearly, if there exists  $\mathbf{p}_i$  and  $\mathbf{p}_j$  such that  $|\text{Comp}(\mathbf{p}_i, \mathbf{p}_j)| = 0$  and  $0 \leq i < j \leq r$ , then  $\text{Rep}(\mathbf{p}_i) \cap \text{Rep}(\mathbf{p}_j) = \emptyset$  and  $|\text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{r-1})| = 0$ . So next, we only need to consider the case that for any  $\mathbf{p}_i$  and  $\mathbf{p}_j$ , we have  $|\text{Comp}(\mathbf{p}_i, \mathbf{p}_j)| \neq 0$ .

Another simple case is that if for any two 2-patterns  $\mathbf{p}_i$  and  $\mathbf{p}_j$ ,  $|\text{Comp}(\mathbf{p}_i, \mathbf{p}_j)| = 4$ , then  $|\text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{r-1})|$  is even by Lem. 3.

The last unproved case is that there exist two 2-pattern  $\mathbf{p}_i$  and  $\mathbf{p}_j$  such that the number  $|\text{Comp}(\mathbf{p}_i, \mathbf{p}_j)| = 2$ . Similar to the proof in Lem. 3, we assume  $\tau \in \text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{r-1})$ , and we try to construct a  $\tau'$  such that  $\tau' \in \text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{r-1})$ , then this case is also proved.

Assume  $|\text{Comp}(\mathbf{p}_0, \mathbf{p}_1)| = 2$ , and there are two composite graphs  $\gamma_0$  and  $\gamma_1$  in  $\text{Comp}(\mathbf{p}_0, \mathbf{p}_1)$ . We assume  $\gamma_0 \subseteq \tau$ , and then denote  $\tau'$  be the graphs  $\tau - \gamma_0 + \gamma_1$ . Clearly we have  $\tau' \in \text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1)$  by the construction of  $\tau'$ . It suffices to show  $\tau' \in \text{Rep}(\mathbf{p}_i)$  for  $2 \leq i < r$ . The proof is quite similar to Lem 3's proof. The only difference is that  $\alpha_i$  becomes  $\gamma_i$ . Note that by the second condition of the theorem, we have  $|\text{Comp}(\mathbf{p}_0, \mathbf{p}_i)| = |\text{Comp}(\mathbf{p}_1, \mathbf{p}_i)| = 4$ , so both  $\gamma_0$  and  $\gamma_1$  are consistent with the subgraphs in  $\mathbf{p}_i$ . Next, we can use a similar proof as done in Lem. 3 to show that if  $\tau \in \text{Rep}(\mathbf{p}_i)$ , then  $\tau' \in \text{Rep}(\mathbf{p}_i)$  holds too. It follows that  $\tau' \in \text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{r-1})$ , and hence,  $|\text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{r-1})|$  is even.

To sum up, we have proved  $|\text{Rep}(\mathbf{p}_0) \cap \text{Rep}(\mathbf{p}_1) \cap \cdots \cap \text{Rep}(\mathbf{p}_{r-1})|$  is even for  $3 \leq r \leq l$ . By the principle of inclusion-exclusion,  $|\text{Rep}(\mathbf{p}_0) \cup \text{Rep}(\mathbf{p}_1) \cup \cdots \cup \text{Rep}(\mathbf{p}_{l-1})|$  is even.  $\square$

Theorem 1 and 2 solve the second and third problems proposed in the front of this section by providing sufficient conditions on ensuring  $|\text{Rep}(\mathbf{a}) \cup \text{Rep}(\mathbf{b})|$  and  $|\text{Rep}(\mathbf{p}_0) \cup \text{Rep}(\mathbf{p}_1) \cup \cdots \cup \text{Rep}(\mathbf{p}_{l-1})|$  being even. These conditions can easily be conducted without solving the model. So, to use more 2-patterns to reject useless trails, the remaining problem is how to obtain the 2-patterns, which will be solved in the next subsection.

### 3.2 Algorithm

In this subsection, we first present an algorithm for extracting 2-patterns from given trails. Next, we provide an algorithm for selecting 2-patterns from the candidates to meet the conditions of Theorem 2. Finally, we provide an algorithm for recovering superpolys, automatically finding and exploiting new 2-patterns to reject useless trails.

### 3.2.1 Extracting 2-patterns from trails

The idea of this algorithm is simple. Given two trails related to the same monomial, they form a large 2-pattern naturally since the vertexes at the top and bottom of them are identical. Our method is to delete the common edges from these two trails if the remaining graphs, after deleting the edges, also have the same top and bottom vertexes. We repeat this deleting procedure until no common edges can be deleted anymore.

---

**Algorithm 1:** Extracting a 2-pattern from two trails
 

---

**Input** : Two trails  $\tau$  and  $\tau'$  related to the same monomial.  
**Output** : A 2-pattern  $\mathbf{a} = (\alpha_0, \alpha_1)$ .

```

1 begin
2    $(\alpha_0, \alpha_1) \leftarrow (\tau, \tau')$ 
3   for  $e \in \mathbf{E}(\tau) \cap \mathbf{E}(\tau')$  do
4     if  $\text{Top}(\alpha_0 - e) = \text{Top}(\alpha_1 - e)$  and  $\text{Bot}(\alpha_0 - e) = \text{Bot}(\alpha_1 - e)$  then
5        $(\alpha_0, \alpha_1) \leftarrow (\alpha_0 - e, \alpha_1 - e)$ 
6   return  $(\alpha_0, \alpha_1)$ 

```

---

In Alg. 1, we abuse the graph minus operator “-” for simplification. By writing “ $\alpha_0 - e$ ”, we mean the graph  $\alpha_0 - (\{\text{St}(e), \text{En}(e)\}, \{e\}) = (\mathbf{V}(\mathbf{E}(\alpha_0) \setminus \{e\}), \mathbf{E}(\alpha_0) \setminus \{e\})$ .

### 3.2.2 Selecting 2-patterns from candidates

Given a set of candidate 2-patterns, there are many ways of selecting 2-patterns such that conditions of Theorem 2 are met. We use a greedy approach to select as many “small” 2-patterns as possible. We think one 2-pattern is smaller if it involves fewer vertexes. We have the following algorithm for selecting 2-patterns.

---

**Algorithm 2:** Selecting 2-patterns from candidates
 

---

**Input** : A set of candidate 2-patterns  $\{\mathbf{a}_0, \mathbf{a}_1, \dots, \mathbf{a}_{m-1}\}$ .  
**Output** : A set of 2-patterns  $\{\mathbf{p}_0, \mathbf{p}_1, \dots, \mathbf{p}_{l-1}\}$  such that  
 (1)  $|\text{Comp}(\mathbf{p}_i, \mathbf{p}_j)|$  is even for  $0 \leq i < j < l$ ;  
 (2) as most one of  $\mathbf{V}(\mathbf{p}_i) \cap \mathbf{V}(\mathbf{p}_j)$ ,  $\mathbf{V}(\mathbf{p}_i) \cap \mathbf{V}(\mathbf{p}_k)$ , and  $\mathbf{V}(\mathbf{p}_j) \cap \mathbf{V}(\mathbf{p}_k)$  is non-empty for  $0 \leq i < j < k < l$ .

```

1 begin
2    $T \leftarrow \{\mathbf{a}_0, \mathbf{a}_1, \dots, \mathbf{a}_{m-1}\}$ 
3    $D \leftarrow \emptyset$  # selected 2-patterns
4   while  $T \neq \emptyset$  do
5      $\mathbf{a} \leftarrow$  a 2-pattern with the least vertexes in  $T$ 
6      $T \leftarrow T \setminus \{\mathbf{a}\}$ 
7      $f \leftarrow \text{True}$ 
8     if  $\exists \mathbf{p} \in D$  s.t.  $|\text{Comp}(\mathbf{a}, \mathbf{p})|$  is odd then
9        $f \leftarrow \text{False}$ 
10    if  $\exists \mathbf{p}, \mathbf{p}' \in D$  s.t.  $\mathbf{V}(\mathbf{p}) \cap \mathbf{V}(\mathbf{p}') \neq \emptyset$  and  $(\mathbf{V}(\mathbf{p}) \cup \mathbf{V}(\mathbf{p}')) \cap \mathbf{V}(\mathbf{a}) \neq \emptyset$  then
11       $f \leftarrow \text{False}$ 
12    if  $f = \text{True}$  then
13       $D \leftarrow D \cup \{\mathbf{a}\}$ 
14  return  $D$ 

```

---



**Algorithm 3:** A new algorithm for recovering superpolys**Input** : A graph-based MILP model  $\mathcal{M}$  built for recovering a superpoly.**Output** : Trails corresponding to the monomials in the superpoly.

---

```

1 begin
2    $T \leftarrow \{\mathcal{M}\}$  # unsolve models
3    $S \leftarrow \emptyset$  # trails of the models
4    $C \leftarrow \emptyset$  # candidate 2-patterns
5    $P \leftarrow \emptyset$  # selected 2-patterns
6   while  $T \neq \emptyset$  do
7      $\mathcal{M}' \leftarrow$  an unsolved model in  $T$ 
8      $T \leftarrow T \setminus \{\mathcal{M}'\}$ 
9     solve  $\mathcal{M}'$  by adding the constraints of 2-patterns in  $P$ 
10    if  $\mathcal{M}'$  cannot be solved after obtaining 100000 trails then
11      extract 2-patterns from the obtained trails, and append the 2-patterns
12      to  $C$ 
13      split  $\mathcal{M}'$  into sub-models, and append them to  $T$ 
14    else
15      extract 2-patterns from the obtained trails, and append the 2-patterns
16      to  $C$ 
17      append trails to  $S$ 
18     $P \leftarrow$  select 2-patterns from  $C$ 
19  return  $S$ 

```

---

**3.2.3 A new graph-based algorithm for recovering superpolys**

As we hope to find new 2-patterns and use them to reject pairing trails in the subsequent computations, the graph-based model cannot be solved as a whole; otherwise, the found 2-patterns will be useless. Thus, we split the original graph-based algorithm into several sub-models and solve them not at the same time. Our split strategy is trivial. That is, we solve one sub-model first, and if the model cannot be solved completely after finding more than 100000 trails, then we split the model into sub-models. Since each vertex in the graph-based model only has four edges, and at most one edge is valid, we enumerate the possible cases to generate four submodels.

Whenever we obtain some trails of the submodels, we extract the 2-patterns from these trails and select a set of 2-patterns such that the conditions in Theorem 2 are met. These 2-patterns are added to the consequent unsolved models to reject possible pairing trails.

Please note that in Line 11, although the model  $\mathcal{M}'$  is not solved completely, we can also extract 2-patterns from the obtained trails related to the same monomials.

In our experiments, we also implemented this algorithm in parallel to speed up Alg. 3 further. We use multi-threads to solve the sub-models, respectively, and the sets  $C$  and  $P$  are shared among these threads.

**4 A New Practical Cube Attack via Numerous Superpolys**

The cube attack consists of two phases: the offline phase and the online phase. In the offline phase, the attackers “generate” superpolys, while in the online phase, the evaluations of superpolys are assumed to be available, so the superpolys become a system of equations. To get the secret key of the cipher, the attackers need to solve the system constructed by the superpolys. To make the system easier to solve, previous practical cube attacks

try to search for some “good” superpolys, for example, linear superpolys or superpolys with balanced bits. This makes the system easy to solve but increases the difficulty of generating superpolys.

Unfortunately, it becomes challenging to find sufficient good superpolys when the round number of stream ciphers is high. To mount the cube attacks to a higher number of rounds, we prefer using numerous “not-so-good” superpolys. Here, “not so good” superpolys refer to the ones that are not linear or not balanced at all. Generally, the system constructed by these “not so good” superpolys is hard to solve. However, we noticed that superpolys corresponding to stream ciphers, e.g. TRIVIUM, are often “sparse” and “asymmetrical” in variables, and if the number of these superpolys is “adequate” enough, then the system becomes easy to solve. Here, “sparse” means the numbers of monomials in the superpolys are not huge, and the “asymmetry” of variables refers to the fact that some secret variables may appear in most of the superpolys, but some other variables only appear in a few superpolys. This asymmetry will help us to determine the guessing order of variables later. By saying “adequate” superpolys, we mean that the system becomes easier to solve only when there are a large number of superpolys. For example, when we attacked 832-round TRIVIUM if all 1373 superpolys were used, the solution of the system could often be found in seconds, but if only 500 ones were used, the system sometimes could not be solved.

Actually, if there is a system constructed by adequate, sparse, and asymmetrical superpolys, one direct way of solving this system is to use a solver, e.g., the SAT solver or the Gröbner basis method. However, we found that the system cannot be solved within a durable time for some selected keys in our experiment. Besides, the complexity of using the SAT or the Gröbner basis method directly are complicated to analyze. So we prefer a “testing method” for solving the systems. Specifically, we guess the value of a key, say  $x_0$  and check whether a contradiction occurs in the system. If  $x_0 = 1$  leads to a contradiction, then we must have  $x_0 = 0$ . The idea is very efficient in our experiments, and most of the values of the keys can be determined in this way.

Next, we show the new cube attack in more detail.

**Offline Phase:** The first step is to search for a “good” mother cube such that the superpolys of the sub-cubes of this mother cube are sparse. The second step is to recover numerous superpolys of the sub-cubes. This “good” mother cube is not very difficult to find because we only require it to be sparse. Once the mother cube is determined, a large amount of superpolys of its sub-cubes are recovered. According to our experiences, 1200 superpolys should be adequate for conducting a practical attack.

**Online Phase:** The values of the superpolys can be determined by inquiring about the oracle, and the number of inquiries depends on the size of the mother cube. Next, we obtain the true values of some secret variables by using a testing method, and the values of the undetermined secret variables can be obtained by enumeration.

**The complexity of this attack** Assume the size of the mother cube is  $s$ . We can obtain the true values of  $m$  secret variables by the testing method, and there are  $n - m$  undetermined variables. If the testing method can be finished quickly, then it takes about  $2^s + 2^{(n-m)}$  inquiries about the oracle to solve for the true key.

Note that the *testing method* for determining the values of the variables is the most crucial step in this attack. This method is given by the following algorithm.

Here are some explanations on Alg. 4.

1. The step in Line 6 is important to the testing method. Any solver of polynomial systems can be used here in theory. In early experiments, we used the CryptoMiniSat solver [SNC09]. Later, we noticed that the “groebner\_basis()” function in Singular (ver 4.4.0) [DGPS24] is more efficient than CryptoMiniSat for practical testing.
2. In the practical attacks, the solving in Line 6 takes not too much time. For example, to conduct a key-recovery attack against 832-round TRIVIUM, we used 1373 superpolys.

**Algorithm 4:** A testing method for solving the system

---

**Input** : A large set  $F$  of superpoly equations, e.g.  $F = \{p_0 = 1, p_1 = 0, \dots\}$ .  
**Output** : A solution to  $F$ , e.g.  $\{k_0 = 1, k_1 = 0, \dots, k_{n-1} = 1\}$ .

```

1 begin
2    $R \leftarrow \emptyset$  # a set of equations recording the determined key values.
3    $U \leftarrow \{k_0, k_1, \dots, k_{n-1}\}$  # the set containing all secret variables
4   for  $k \in U$  do
5     for  $v \in \{0, 1\}$  do
6       solve the system  $F \cup R \cup \{k = v\}$  by a solver
7       if there is no solution to the system  $F \cup R \cup \{k = v\}$  then
8          $R \leftarrow R \cup \{k = 1 - v\}$ 
9          $U \leftarrow U \setminus \{k\}$ 
10  for  $\forall v \in \mathbb{F}_2^{|U|}$  do
11    # assume  $U = \{u_0, u_1, \dots, u_{l-1}\}$ 
12    if  $R \cup \{(u_0, \dots, u_{l-1}) = v\}$  is a solution to  $F$  then
13      return  $R \cup \{(u_0, \dots, u_{l-1}) = v\}$ 

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Testing the values of the 80 secret variables takes about 8 ~ 9 hours by using an ordinary PC. The values of about 77 variables on average can be determined, which means recovering the key completely can be done practically by enumerating the values of the other 3 variables.

3. The asymmetry of the superpolys speeds up the solving in Line 6. Take the attack on 832-round TRIVIUM as an example. There are 1373 superpolys in total, and all 80 key variables appear. But  $k_{58}$  appears in 1344 superpolys,  $k_{59}$  in 1307 ones, ...,  $k_9$  in 23 ones. We used this asymmetry to determine the testing order, i.e., we test the variables in the order  $k_{58}, k_{59}, \dots, k_9$  Line 4. We found this order sped up the testing in our experiments compared to some other orders.
4. The sparsity of the superpolys also speeds up the solving in Line 6 because the sparsity leads to fewer constraints in the SAT solver and also makes the Buchberger algorithm (in Singular) more efficient.
5. In practical attacks, we used a progressive way to speed up Alg. 4. Specifically, we generate several subsets of  $F$ , say  $F_1 \subset F_2 \subset \dots \subset F_m = F$ . The first set  $F_1$  consists of the simplest superpolys, e.g., superpolys whose numbers of monomials are smaller than 100. The second set  $F_2$  consists of those whose monomial numbers are smaller than 200. .... In the test, we check the values of the secret variables with  $F_1$  first. We may obtain the values of some secret variables quickly, and we can preset these values to the secret variables in  $F_2$  and test the values of the undetermined variables. If  $F_2$  is inadequate to determine all the bits of the key, we use the set  $F_3$ , and so on. If all the superpolys in  $F$  have been used, and there are still some secret variables that cannot be determined, then we enumerate these secret variables' values to find the true target key in Line 10 ~ 13.

## 5 Applications to TRIVIUM

We applied the new approach to attacking TRIVIUM practically. Firstly, we tested the effectiveness of the new proposed Alg. 3 in Sec. 5.1. Next, the new attacks on 820- and

832-round TRIVIUM are shown in Sec. 5.2.

## 5.1 Effectiveness of the new 2-patterns

In this section, we test the number of trails rejected by Alg. 3 compared to the original graph-based models. The goal of rejecting more pairing trails is to speed up the computation of recovering superpolys, so we also show the timings for each example.

As examples, we use the cubes from [DDGP22] and [CQ23]. Besides, we also use some sub-cubes that we used to attack 832-round TRIVIUM. The data are shown in Tab. 2 and 3. In the tables, we compare three algorithms, including the original graph-based algorithm in [DDGP22], our paralleled version of the graph-based algorithm, and Alg. 3. We present the number of all trails solved from the models, the number of monomials in the superpolys, and the trails related to the appearing monomials in the superpolys. The timings are obtained from a platform with AMD Threadripper 3970X with 32 cores and 256 GB memory, running Ubuntu 20.04.

**Table 2:** Comparisons of the original graph-based algorithm ([DDGP22]), paralleled graph-based algorithm (Parallel), and the paralleled graph-based algorithm with new 2-patterns (Parallel + Pat.) on recovering the superpolys of 840-, 841-, 842-, and 843-round TRIVIUM. To test the effectiveness of the optimal 2-patterns, some previously found optimal 2-patterns were added to these models used by Parallel + Pat. in advance.

Round	Alg.	Patterns	#all trails	#mon.	#mon. trails	Time (sec.)
840	[DDGP22]	3CBP	8025	41	667	309.74
	Parallel	3CBP	8025	41	667	295.13
	Parallel + Pat.	143	<b>2564</b>	41	<b>373</b>	<b>290.85</b>
841	[DDGP22]	3CBP	18905	55	2617	1796.15
	Parallel	3CBP	18905	55	2617	1253.32
	Parallel + Pat.	184	<b>2971</b>	55	<b>595</b>	<b>1214.57</b>
842	[DDGP22]	3CBP	720779	975	191435	13941.10
	Parallel	3CBP	720779	975	191435	6345.27
	Parallel + Pat.	345	<b>322199</b>	975	214719	<b>5435.98</b>
843	[DDGP22]	3CBP	–	–	–	>20000
	Parallel	3CBP	5658914	359514	1681158	5980.24
	Parallel + Pat.	983	<b>3972087</b>	359514	<b>1323591</b>	<b>5190.65</b>

$$I_{840} = \{0, \dots, 79\} \setminus \{70, 72, 74, 76, 78\},$$

$$I_{841} = \{0, \dots, 79\} \setminus \{8, 78\},$$

$$I_{842} = \{0, \dots, 79\} \setminus \{18, 34\},$$

$$I_{843} = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 34, 36, 38, 40, 42, 45, 47, 49, 51, 53, 55, 57, 60, 62, 64, 66, 68, 70, 72, 77, 75, 79\}.$$

From Tab. 2 and Tab. 3, we can see that the parallel version of the graph-based algorithm is much faster than its original version, and the new algorithm is even more efficient. The total numbers of trails are significantly reduced in the new algorithm, which we think is the main reason for the speed-up. The speed-up brought by decreasing the number of trails is not obvious for simple examples, e.g., the second example in Tab. 3, but it becomes significant for complicated ones, e.g., the last three examples in Tab. 3.

## 5.2 A practical attack against 820- and 832-round TRIVIUM

The practical attacks consist of three steps.

The **first step** is to search for a mother cube with only a few terms and a low degree. We used some cube indexes in [YT21] and replaced some cube indexes with random. We

**Table 3:** Comparisons of the original graph-based algorithm ([DDGP22]), paralleled graph-based algorithm (Parallel), and the paralleled graph-based algorithm with new 2-patterns (Parallel + Pat.) on recovering the superpolys of 832-round TRIVIUM.

Cube	Alg.	Patterns	#all trails	#mon.	#mon. trails	Time (sec.)
$I_1$	[DDGP22]	3CBP	435185	4917	14431	2259.81
	Parallel	3CBP	435185	4917	14431	655.03
	Parallel + Pat.	91	<b>26573</b>	4917	<b>7411</b>	<b>196.56</b>
$I_2$	[DDGP22]	3CBP	81666	5184	13092	172.32
	Parallel	3CBP	81666	5184	13092	<b>115.89</b>
	Parallel + Pat.	51	<b>32616</b>	5184	<b>6132</b>	144.58
$I_3$	[DDGP22]	3CBP	215101	6097	13949	569.85
	Parallel	3CBP	215101	6097	13949	281.69
	Parallel + Pat.	76	<b>82161</b>	6097	<b>13269</b>	<b>184.95</b>
$I_4$	[DDGP22]	3CBP	1289438	8220	35306	20630.81
	Parallel	3CBP	1289438	8220	35306	2715.23
	Parallel + Pat.	131	<b>67728</b>	8220	<b>20624</b>	<b>295.97</b>
$I_5$	[DDGP22]	3CBP	–	–	–	>20000
	Parallel	3CBP	1732002	10636	121068	3504.03
	Parallel + Pat.	107	<b>170622</b>	10636	<b>51018</b>	<b>367.17</b>
$I_6$	[DDGP22]	3CBP	915843	10827	149717	10794.13
	Parallel	3CBP	915843	10827	149717	1977.31
	Parallel + Pat.	265	<b>204497</b>	10827	<b>46635</b>	<b>411.58</b>

$$I_1 = S_{832} \setminus \{12, 29, 54\}, I_2 = S_{832} \setminus \{14, 25, 31, 54\}, I_3 = S_{832} \setminus \{1, 29, 55, 68\}, \\ I_4 = S_{832} \setminus \{1, 29\}, I_5 = S_{832} \setminus \{15, 31, 67\}, I_6 = S_{832} \setminus \{29, 31, 73\}.$$

recovered many superpolys using the new algorithm and selected the cube with the lowest degree. For attacking 820- and 832-round TRIVIUM, we use two mother cubes:

$$S_{820} = \{1, 3, 5, 6, 8, 9, 10, 12, 14, 16, 18, 20, 21, 22, 23, 24, 25, 26, 27, 29, 31, 33, 35, 37, \\ 38, 40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62, 64, 67, 69, 71, 73, 75, 77, 79\},$$

$$S_{832} = \{0, 1, 2, 4, 6, 8, 10, 11, 12, 13, 14, 15, 17, 19, 21, 23, 25, 26, 28, 29, 30, 31, 32, 34, 36, 38, \\ 40, 43, 45, 47, 49, 51, 53, 54, 55, 58, 60, 61, 62, 64, 66, 67, 68, 69, 71, 73, 75, 77, 79\},$$

where  $|S_{820}| = 45$  and  $|S_{832}| = 49$ .

The **second step** is to recover numerous superpolys of the sub-cubes using Alg. 3. Note that Alg. 3 can recover any superpoly if the time and space are unlimited, because this algorithm keeps splitting the sub-models until the sub-models can eventually be solved. For the sake of efficiency, we set a limit on the running time in the practical attacks. That is, we cut down the program if the superpoly was not recovered completely within 7200 seconds. Finally, we obtained 1912 superpolys of the sub-cubes of  $S_{820}$ , and 1373 ones for the 832-round TRIVIUM. The implementation of Alg. 3 is based on the Gurobi solver [Gur24].

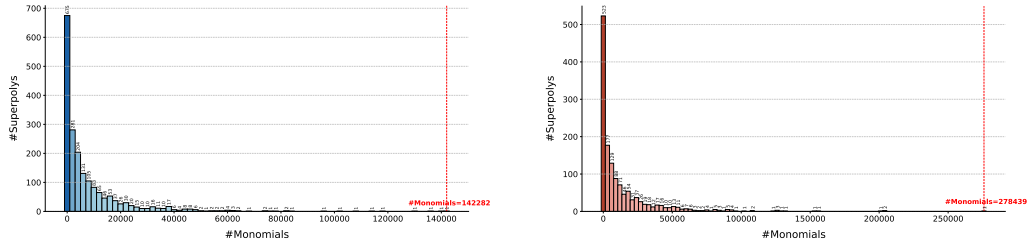
The statistics of the features of the superpolys are shown as follows.

**Table 4:** The number of superpolys of different sizes of cubes.

Round	Cube size	38	39	40	41	42	43	44	45	46	47	48	49
820	#S.polys	1	68	406	572	634	201	29	1				
832	#S.polys						137	420	369	321	104	21	1

In Tab. 4, most of the superpolys used for attacking 820-round TRIVIUM come from the sub-cubes of size 40, 41, and 42. We think this phenomenon results from two reasons.

Firstly, the number of sub-cubes with sizes 43 and 44 is limited, so the number of superpolys related to these sub-cubes is small. Secondly, the algebraic degrees of the superpolys corresponding to the cube sizes smaller than 39 are usually high, so we did not recover many of them. A similar phenomenon also happens to the superpolys for attacking 832-round TRIVIUM.

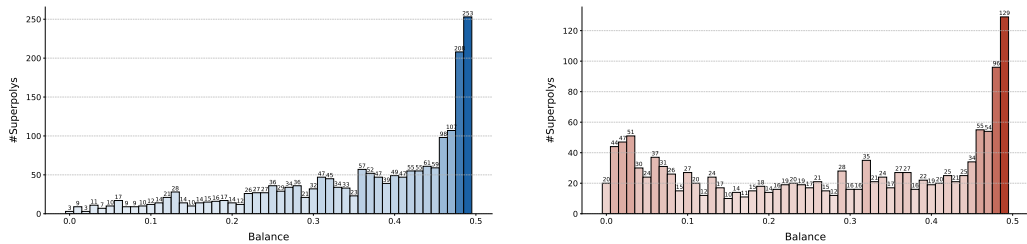


(a) The number of monomials of superpolys for attacking 820-round TRIVIUM.

(b) The number of monomials of superpolys for attacking 832-round TRIVIUM.

**Figure 4:** The distributions of monomials in superpolys.

Fig. 4 presents the distributions of the numbers of monomials. Most of the superpolys used for practical attacks contain small numbers of monomials. The largest superpolys for attacking 820- and 832-round TRIVIUM have 142282 and 278429 monomials, respectively. Besides, the degrees of 1205 superpolys used for attacking 832-round TRIVIUM are not smaller than 10.



(a) The distributions of the balance of superpolys for attacking 820-round TRIVIUM.

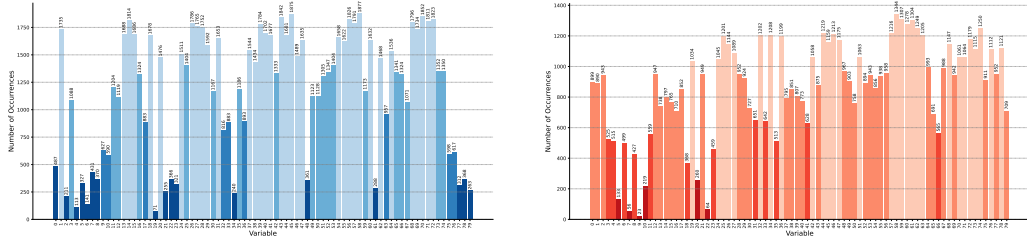
(b) The distributions of the balance of superpolys for attacking 832-round TRIVIUM.

**Figure 5:** The distributions of the balance of superpolys.

The distributions of the balance of superpolys are shown in Fig. 5. We cannot obtain the rigorous balance value of each superpoly because there are 80 variables, so we calculate a rough balance value by assigning 10000 random values to each superpoly. Many of the superpolys used for practical attacks have good balance values.

All these recovered superpolys were used in our practical attack. Not every superpoly involves all 80 key variables, but each key variable appears in some superpolys. Fig. 6 shows that the numbers of appearing times of the key variables are not uniformly distributed, reflecting the variables' asymmetry. This asymmetry is used to determine the testing order of variables in Alg. 4. This order sped up the testing in our experiments compared to some other orders.

The **final step** is to solve the system constructed by the obtained superpolys by Alg. 4. The superpolys are fixed in the online phase, but the evaluations of these superpolys are determined by the specific values of the secret variables. It is impossible to test whether the systems can be solved by Alg. 4 practically for all keys, so we chose  $2^{14}$  keys for testing the practical attacks against 820- and 832-round TRIVIUM.

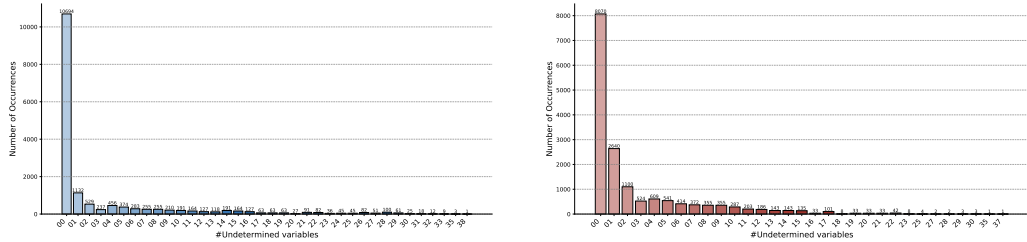


(a) The appearing times of variables in the superpolys for attacking 820-round TRIVIUM.

(b) The appearing times of variables in the superpolys for attacking 832-round TRIVIUM.

**Figure 6:** The appearing times of variables in the superpolys.

In the experiments, we generated random keys and calculated the evaluations of superpolys. Some bits of the keys were determined using Alg. 4. Specifically, for testing the value of each variable  $k$ , we solved the system  $F_i \cup R \cup \{k = 0\}$  and  $F_i \cup R \cup \{k = 1\}$  in Line 8 of Alg. 4 by the CryptoMiniSat solver [SNC09] or the Gröbner basis function in Singular [DGPS24]. This test can be done quickly due to the sparsity of the systems if the systems have no solutions; otherwise, we stop the program once CryptoMiniSat finds one solution, or the Gröbner basis cannot return the results within 100 seconds. If the system  $F_i \cup R \cup \{k = 0\}$  has no solution, then we can determine that  $k = 1$ . The average times of this step for 820- and 832-round TRIVIUM are about 3 and 9 hours, respectively. The distributions of the numbers of undetermined bits are shown in Fig. 7. The platform ( $2 \times$  AMD EPYC 7763 64 cores, 2 TB memory) is used to finish these experiments.



(a) The number of undetermined secret variables for 820-round TRIVIUM.

(b) The number of undetermined secret variables for 832-round TRIVIUM.

**Figure 7:** The number of undetermined secret variables.

From Fig. 7, all  $2^{14}$  tested keys can be recovered completely with no more than  $2^{38}$  or  $2^{37}$  enumerations for 820- and 832-round TRIVIUM, which could be done practically. Specifically, 65.27% and 49.26% of the target keys can be directly recovered without extra enumerations; 76.86% and 75.28% of the experiments need to enumerate the values of at most 3 variables; more than 99% target keys can be recovered by guessing the values of at most 30 bits. Although we only test a small proportion of the key space  $2^{80}$ , we are confident that our new attack has practical significance in recovering random keys.

In all, the overall time complexities of attacking 820- and 832-round TRIVIUM are about  $2^{45} + 2^{38}$  and  $2^{49} + 2^{37}$ .

**Remark** We found both the SAT and GB methods cannot solve all the systems directly w.r.t. the keys selected in our experiments. Specifically, they cannot solve the systems with more than 30 undetermined variables in Fig. 7. However, Alg. 4 could obtain all target key values practically. Besides, the complexities of using SAT/GB directly are complicated to analyze. In our attack, if the values of  $m$  variables are determined, enumerating the values

of the other  $80 - m$  variables will obtain the true key. In experiments, the testing approach only costs a few hours, so the complexity of Alg. 4 is dominated by the enumeration complexity  $2^{(80-m)}$ , which is slightly clearer.

## 6 Conclusions

In this paper, we propose a new cube attack by using numerous superpolys. To recover these numerous superpolys, we improved Delaune et al.'s graph-based model by using more 2-patterns to reject useless pairing trails, and experimental data show our technique did improve the efficiency of recovering superpolys. Using these numerous, sparse, and asymmetric superpolys, we obtain practical attacks against 820- and 832-round TRIVIUM. Although we cannot prove our attack is valid to all keys in theory, we believe it is very useful and practical. Our attacks and algorithms for recovering superpolys can be applied to attack other stream ciphers directly.

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