# Plane point sets with many squares or isosceles right triangles

SASCHA KURZ (SASCHA.KURZ@UNI-BAYREUTH.DE)\*

Department of Mathematics, University of Bayreuth, D-95440 Bayreuth, Germany

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Abstract: How many squares are spanned by n points in the plane? Here we study the corresponding maximum possible number  $S_{\Box}(n)$  of squares and determine the exact values for all  $n \leq 17$ . For  $18 \leq n \leq 100$  we give lower bounds for  $S_{\Box}(n)$ . Besides that a few preliminary structural results are obtained. For the related problem of the maximum possible number  $S_{\Box}(n)$  of isosceles right triangles we determine the exact values for  $n \leq 14$  and give lower bounds for  $15 \leq n \leq 50$ .

## 1 Introduction

Given a finite set of points  $\mathcal{Q} \subset \mathbb{R}^2$ , what is the maximum number  $S_{\mathcal{Q}}(n)$  of similar copies that can be contained in an *n*-point set in the plane? The origin of this problem can be traced back at least to Erdős and Purdy [11]. Besides being now a classical problem in combinatorial geometry there are connections to pattern recognition problems, see e.g. [5] and the references cited therein. In such applications similarity is mostly replaced by congruency, so that we denote the maximum number of congruent copies of a finite set  $\mathcal{Q} \subset \mathbb{R}^2$  that can be contained in an *n*-point set in the plane by  $C_{\mathcal{Q}}(n)$ . An easy algorithm for the corresponding congruent subset detection problem of  $\mathcal{Q}$  in  $\mathcal{P}$  is to choose two arbitrary (different) points  $q_1, q_2 \in \mathcal{Q}$  and to loop over all pairs of points  $p_1, p_2 \in \mathcal{P}$  where  $d(q_1, q_2) = d(p_1, p_2)$ , i.e., where the distances are equal. The complexity analysis of the algorithm requires one to determine  $C_{\{q_1,q_2\}}(n)$ , i.e., the maximum number of unit distances in the plane (sequence  $A186705^{1}$ ), a famous open problem introduced by Erdős [10]. The best upper bound known still is  $O(n^{4/3})$  [18], with a recent constant factor improvement, see [4].<sup>2</sup> From that we can conclude  $C_{\mathcal{Q}}(n) \in O(n^{4/3})$  and all congruent copies of  $\mathcal{Q}$  can be found in  $O(\#\mathcal{Q} \cdot n^{4/3} \log n)$  time, see [5] for more details. For  $S_{\mathcal{Q}}(n)$  we have an upper bound of n(n-1) and quadratic lower bound if Q contains only algebraic points [9]. In [14] a characterization of the point sets  $\mathcal{Q}$  with  $S_{\mathcal{Q}}(n) = \Theta(n^2)$  was obtained. All similar copies of  $\mathcal{Q}$  can be found in  $O(\#\mathcal{Q} \cdot n^2 \log n)$  time, see e.g. [5]. However, the existence of  $\lim S_{\mathcal{Q}}(n)$ is unknown for all non-trivial sets Q. Here we want to study the maximum number  $S_{\Box}(n)$ of squares contained in an n-point set in the plane (sequence A051602). We will be mainly interested in the determination of exact values or tight bounds for  $S_{\Box}(n)$  for the cases where n is rather small. Taking the points of an  $m \times m$  integer grid gives  $\liminf_{n \to \infty} \frac{S_{\Box}(n)}{n^2} \ge \frac{1}{12}$  (see sequence A002415 for the precise counts of squares). Taking the integer points inside circles of increasing

<sup>\*</sup>This paper is inspired by an extensive discussion on the Sequence Fans Mailing List with contributions from many people.

<sup>&</sup>lt;sup>1</sup>For the subsequently mentioned integer sequences see the "On-Line Encyclopedia of Integer Sequences" (OEIS) at https://oeis.org.

<sup>&</sup>lt;sup>2</sup>This upper bound applies to all strictly convex norms, not just Euclidean distance, and can in fact be attained for certain special norms, see [20, 19].

radii gives  $\liminf_{n\to\infty} \frac{S_{\Box}(n)}{n^2} \geq \frac{1-\frac{2}{\pi}}{4} > \frac{1}{11.008}$ , see the comments in sequence A051602.<sup>3</sup> Denote the maximum number of isosceles right triangles in an *n*-point set by  $S_{\mathbb{k}}(n)$  and observe that each square consists of four such triangles. With this, the upper bound  $S_{\mathbb{k}}(n) \leq \lfloor \frac{2}{3}(n-1)^2 - \frac{5}{3} \rfloor$  from [3] gives  $\limsup_{n\to\infty} \frac{S_{\Box}(n)}{n^2} \leq \frac{1}{6}$ . In Proposition 35 we will show  $\limsup_{n\to\infty} \frac{S_{\Box}(n)}{n^2} \leq \frac{1}{8}$ . For the maximum number of equilateral triangles in the plane we refer to [1, 15]. The latter reference takes the additional assumption that the *n* points must be in convex position, see also [22] for isosceles right triangles under the same assumption.

Of course similar problems can be considered in higher dimensions or with different metrics [7]. Another variant is the number of rhombi or parallelograms contained in a plane point set. Since not all rhombi or parallelograms are similar the upper bound  $O(n^2)$  does not apply and is indeed violated. For e.g. axis-parallel squares the lower bound  $\Omega(n^2)$  is violated, cf. [21, Theorem 1]. For results on repeated angles see e.g. [16]. Another interesting variant is the maximum number of unit circles spanned by n points in the plane, see e.g. [12].

The remaining part is structured as follows. Section 2 is devoted to point sets with many isosceles right triangles. The approach of constructing point sets by recursively adding the vertices of an additional square is studied in depth in Section 3. For every point set in  $\mathbb{R}^2$  there exists another point set in  $\mathbb{Z}^2$  that spans at least as many squares, see Theorem 28. An explicit upper bound on the necessary grid size is stated in Proposition 32. While there are infinitely many 7-point sets spanning two squares that are pairwise non-similar, for all numbers n of points and m of squares there exist only finitely many equivalence classes if one uses a suitable combinatorial description, see Definition 18 and Definition 19. With this, the determination of  $S_{\Box}(n)$  becomes a finite computational problem. In Section 4 we discuss bounds for  $S_{\Box}(n)$  and determine the exact values for all  $n \leq 17$ . In an appendix we list several point sets that provide lower bounds for different variants of the problem.

## 2 Plane point sets with many isosceles right triangles

By definition an *n*-point set  $\mathcal{P}$  is a subset of  $\mathbb{R}^2$  of cardinality  $\#\mathcal{P} = n$ . By  $S_{\mathbb{A}}(\mathcal{P})$  we denote the number of isosceles right triangles contained in  $\mathcal{P} \subseteq \mathbb{R}^2$ . In [3, Theorem 6] the numbers  $S_{\mathbb{A}}(3) = 1, S_{\mathbb{A}}(4) = 4, S_{\mathbb{A}}(5) = 8, S_{\mathbb{A}}(6) = 11, S_{\mathbb{A}}(7) = 15, S_{\mathbb{A}}(8) = 20, \text{ and } S_{\mathbb{A}}(9) = 28$  (sequence A186926) were determined. Each pair of points can form the edge of six different isosceles right triangles, see Figure 1, so that  $S_{\mathbb{A}}(n) \leq {n \choose 2} \cdot 6/3 = n(n-1)$ , which equals the general upper bound  $S_{\mathcal{Q}}(n) \leq n(n-1)$ . As mentioned, the improved upper bound  $S_{\mathbb{A}}(n) \leq \left\lfloor \frac{2}{3}(n-1)^2 - \frac{5}{3} \right\rfloor$ for  $n \geq 3$  was shown in [3, Theorem 5].

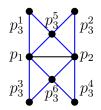


Figure 1: The third vertices of the six isosceles right triangles containing a given line segment  $\{p_1, p_2\}$  as an edge.

If  $\mathcal{P}'$  arises from an *n*-point set  $\mathcal{P}$  by picking a pair  $\{p_1, p_2\}$  of points in  $\mathcal{P}$  and setting  $\mathcal{P}' = \mathcal{P} \cup \{p_3\}$  for one of the six possibilities for  $p_3$  such that  $\{p_1, p_2, p_3\}$  forms an isosceles right triangle, then we say that  $\mathcal{P}'$  is obtained by 1-extension. If an *n*-point set  $\mathcal{P}$  is obtained by a sequence of 1-extensions starting from an arbitrary isosceles right triangle, then we say that  $\mathcal{P}$  can be obtained by 1-extension. In Table 1 we have listed the number of non-similar

<sup>&</sup>lt;sup>3</sup>https://oeis.org/A051602/a051602\_2.txt

points sets that can be obtained by 1-extension per number n of points and m of isosceles right triangles. The number of isosceles right triangles of such an n-point set is at least n - 2. E.g. a 5-point set obtained by joining two isosceles right triangles at a common vertex, such that no further isosceles right triangles are spanned, cannot be obtained by 1-extension. So, clearly not all n-point sets can be obtained by 1-extension. In Proposition 6 we will show that for points sets with at most 7 points a sufficiently large number of isosceles right triangles implies that the point set can be obtained by 1-extension. For n = 9 and  $7 \le m \le 8$  the numbers of cases are quite numerous so that we did not have determined the number of similarity types.

	n	3	4	4	4	5	5	5	5	5	5	6	6	6	6	6	6 (	6	6
	m	1	2	3	4	3	4	5	6	$\overline{7}$	8	4	5	6	7	8	9	10	11
	#	1	2	1	1	16	4	2	1	0	1	232	88	38	16	6	1 3	3	1
	$\overline{n}$	7		7		7		7		7	7	7	7	7	7	7	8		
	m	5		6		7		8		9	1(	) 11	12	13	14	15	6		
	#	5	383	2	397	10	51	49	0	164	50	) 39	17	7	6	2	1'	7240	8
n	8			8		8		8		8		8	8	8	8	8	8	8	8
m	7			8		9		10		11		12	13	14	1 1	15	16	17	18
#	89	926	6	414	75	199	25	71	23	248	38	1513	685	5 25	53	137	75	31	17
n	8	8		9		9			9		)	9	9		9		9		9
m	19	2	0	9		1	0		1	1		12	13	3	14		15		16
#	2	5		162	329	1 8	787	70	3'	79869	) [	142722	2 7	7106	362	226	146	662	7194
			9	(	9	9		9		9	9	9	9	9	9	9	9		
		-	17		18	19	9	20		21	22	23	24	25	26	27	28		
		ć	347	5	1474	8	56	31(	)	186	94	33	20	5	4	1	1		
		_																_	

Table 1: Number of non-similar points sets  $\mathcal{P}$  produced by recursive 1-extension per number of points n and isosceles right triangles m.

**Definition 1.** Let  $\mathcal{P} \subset \mathbb{R}^2$  be an arbitrary point set. A point set  $\mathcal{P}' \subseteq \mathcal{P}$  is called a 1-extension subconfiguration if  $\mathcal{P}' \subseteq \mathcal{P}$  can be obtained by 1-extension. If no proper superset of  $\mathcal{P}'$  can be obtained by 1-extension, then we call  $\mathcal{P}'$  1-extension maximal.

**Lemma 2.** Let  $\mathcal{P} \subset \mathbb{R}^2$  be an arbitrary n-point set and  $\mathcal{P}'$  be a 1-extension maximal subconfiguration. Then we have

$$S_{\mathbb{A}}(\mathcal{P}) \leq S_{\mathbb{A}}(\mathcal{P}') + 2 \cdot \binom{\#\mathcal{P}\backslash\mathcal{P}'}{2} + S_{\mathbb{A}}(\#\mathcal{P}\backslash\mathcal{P}') \leq S_{\mathbb{A}}(\#\mathcal{P}') + 2 \cdot \binom{\#\mathcal{P}\backslash\mathcal{P}'}{2} + S_{\mathbb{A}}(\#\mathcal{P}\backslash\mathcal{P}').$$

Proof. Let t be an arbitrary isosceles right triangle in  $\mathcal{P}$  that is not contained in  $\mathcal{P}'$ . Since  $\mathcal{P}'$  is 1-extension maximal either 2 or 3 vertices of t have to be contained in  $\mathcal{P} \setminus \mathcal{P}'$ . The second case can occur at most  $S_{\mathbb{A}}(\#\mathcal{P} \setminus \mathcal{P}')$  times. For the first case we observe that there are  $\binom{\#\mathcal{P} \setminus \mathcal{P}'}{2}$  pairs of points in  $\mathcal{P} \setminus \mathcal{P}'$ . Consider such a pair  $\{p_1, p_2\}$  and the third point  $p_3^i$  of an isosceles right triangle as in Figure 1. Since the triples  $\{p_3^1, p_3^2, p_1\}, \{p_3^3, p_3^4, p_1\}, \{p_3^1, p_3^3, p_2\}, \{p_3^2, p_3^4, p_1\}, \{p_5^3, p_5^6, p_1\}, \{p_3^1, p_5^3, p_1\}, \{p_3^2, p_5^5, p_2\}, \{p_3^3, p_3^6, p_1\}, \text{and } \{p_4^3, p_5^6, p_2\} \text{ form isosceles right triangles with exactly two vertices in <math>\mathcal{P}'$  at most two out of the six points  $p_3^1, \ldots, p_3^6$  can be obtained in  $\mathcal{P}'$ . Thus, the first case can occur at most  $2 \cdot \binom{\#\mathcal{P} \setminus \mathcal{P}'}{2}$  times.

Example 3. Consider the 6-point set

$$\mathcal{P} = \left\{ (0,0), (1,0), (0,1), (1,1), \left(\frac{3}{5}, \frac{6}{5}\right), \left(\frac{2}{5}, \frac{4}{5}\right) \right\}$$

and its subset  $\mathcal{P}' = \{(0,0), (1,0), (0,1), (1,1)\}$  with  $S_{\mathbb{N}}(\mathcal{P}) = 6$  and  $S_{\mathbb{N}}(\mathcal{P}') = 4$ . The 1-extension subconfiguration  $\mathcal{P}'$  is 1-extension maximal, so that the upper bound of Lemma 2 is attained with equality.

An easy averaging argument implies the existence of subconfigurations with relatively many isosceles right triangles:

**Lemma 4.** ([3, Lemma 8]) Let  $\mathcal{P}$  be an *n*-point set. If  $S_{\square}(A) \leq b$  for all  $\mathcal{P}' \leq \mathcal{P}$  with  $\#\mathcal{P}' = k$ , then we have

$$S_{\mathbb{L}}(\mathcal{P}) \leq \left\lfloor \binom{n}{3} \cdot b / \binom{k}{3} \right\rfloor$$

*Proof.* The point set  $\mathcal{P}$  contains  $\binom{n}{k}$  subsets of cardinality k. Since each isosceles right triangle is contained in  $\binom{n-3}{k-3}$  such subsets of cardinality k, we have

$$S_{\square}(\mathcal{P}) \le \binom{n}{k} \cdot b / \binom{n-3}{k-3} = \frac{n(n-1)(n-2)}{k(k-1)(k-2)} \cdot b.$$

Adding an arbitrary point to a 4-point set consisting of four isosceles right triangles, we obtain a 5-point set that consists of four isosceles right triangles in most cases. Such point sets obviously cannot be obtained by 1-extension. In order to avoid these trivial modifications we forbid "isolated" points. More precisely, we call an *n*-point set  $\mathcal{P}$  reduced if each point is contained in at least one isosceles right triangle.

**Lemma 5.** Let  $\mathcal{P}$  be a reduced *n*-point set and  $\widetilde{\mathcal{P}}$  be a 1-extension maximal subconfiguration. Then, we have  $\#\widetilde{\mathcal{P}} \neq \#\mathcal{P}$ .

*Proof.* Assume  $\#\widetilde{\mathcal{P}} = \#\mathcal{P}$  and let p be the unique vertex contained in  $\mathcal{P} \setminus \widetilde{\mathcal{P}}$ . Since  $\mathcal{P}$  is reduced there exist an isosceles right triangle t containing p as a vertex. Since t intersects  $\widetilde{\mathcal{P}}$  in two vertices,  $\widetilde{\mathcal{P}}$  is not 1-extension maximal – contradiction.

#### Proposition 6.

- (1) Each reduced 3-point set  $\mathcal{P}$  with  $S_{\mathbb{A}}(\mathcal{P}) \geq 1$  can be obtained by 1-extension and  $S_{\mathbb{A}}(3) = 1$ .
- (2) Each reduced 4-point set  $\mathcal{P}$  with  $S_{\square}(\mathcal{P}) \geq 2$  can be obtained by 1-extension and  $S_{\square}(4) = 4$ .
- (3) Each reduced 5-point set  $\mathcal{P}$  with  $S_{\mathbb{A}}(\mathcal{P}) \geq 3$  can be obtained by 1-extension and  $S_{\mathbb{A}}(5) = 8$ .
- (4) Each reduced 6-point set  $\mathcal{P}$  with  $S_{\mathbb{N}}(\mathcal{P}) \geq 7$  can be obtained by 1-extension and  $S_{\mathbb{N}}(6) = 11$ .
- (5) Each reduced 7-point set  $\mathcal{P}$  with  $S_{\mathbb{N}}(\mathcal{P}) \geq 11$  can be obtained by 1-ext. and  $S_{\mathbb{N}}(7) = 15$ .

*Proof.* Given the data of Table 1 it suffices to show that  $\mathcal{P}$  can be obtained by 1-extension if  $S_{\mathbb{A}}(\mathcal{P})$  is at least as large as proposed.

The statement is trivial for  $\#\mathcal{P} = 3$ . If  $\#\mathcal{P} = 4$ , then consider an arbitrary isosceles right triangle t. The statement follows from the fact that each additional isosceles right triangle t' shares an edge with t. For  $\#\mathcal{P} = 5$  we apply Lemma 4 to conclude the existence of a 4-point set  $\mathcal{P}'$  with  $S_{\mathbb{A}}(\mathcal{P}') \geq 2$ . Since  $S_{\mathbb{A}}(3) = 1 < 2$ ,  $\mathcal{P}'$  is reduced, so that  $\mathcal{P}'$  can by obtained by 1-extension due to (2). Now consider an isosceles right triangle t with vertex  $\mathcal{P}\setminus\mathcal{P}'$ . Since t intersects  $\mathcal{P}'$  in two points, also  $\mathcal{P}$  can be obtained by 1-extension, see Lemma 5. For  $\#\mathcal{P} = 6$ we apply Lemma 4 to conclude the existence of a 5-point set  $\mathcal{P}'$  with  $S_{\mathbb{A}}(\mathcal{P}') \geq 4$ . If  $\mathcal{P}'$  is reduced, then  $\mathcal{P}'$  can be obtained by 1-extension due to (3) and an isosceles right triangle t with vertex  $\mathcal{P}\setminus\mathcal{P}'$  intersects  $\mathcal{P}'$  in two vertices, so that also  $\mathcal{P}$  can be obtained by 1-extension. If  $\mathcal{P}'$  is not reduced, then  $S_{\mathbb{A}}(3) = 1$  implies the existence of a reduced 4-point set  $\mathcal{P}''$  with  $S_{\mathbb{A}}(\mathcal{P}'') = 4$  and (2) yields that  $\mathcal{P}''$  can be obtained by 1-extension. Now let  $\widetilde{\mathcal{P}}$  be a 1-extension maximal subconfiguration of  $\mathcal{P}$ , so that  $\#\widetilde{\mathcal{P}} \geq \#\mathcal{P}'' = 4$ . If  $\#\widetilde{\mathcal{P}} = 6$ , then  $\mathcal{P}$  can be obtained by 1-extension. If  $\#\widetilde{\mathcal{P}} = 5$ , then we can again consider an isosceles right triangle containing the missing sixth point as a vertex to conclude that  $\mathcal{P}$  can be obtained by 1-extension. Thus, it remains to consider the case  $\#\widetilde{\mathcal{P}} = 4$ , where Lemma 2 yields

$$S_{\mathbb{L}}(\mathcal{P}) \le S_{\mathbb{L}}(4) + 2\binom{2}{2} + S_{\mathbb{L}}(2) = 6 < 7,$$

which is a contradiction.

Now let  $\#\mathcal{P} = 7$  and  $\mathcal{P}'$  be a 1-extension maximal subconfiguration of  $\mathcal{P}$  with  $\#\mathcal{P}' < 7 = \#\mathcal{P}$ . If  $\#\mathcal{P}' \in \{5,6\}$ , then Lemma 2 gives

$$S_{\mathbb{L}}(\mathcal{P}) \le \max\left\{S_{\mathbb{L}}(5) + 2\binom{2}{2} + S_{\mathbb{L}}(2), S_{\mathbb{L}}(6) + 2\binom{1}{2} + S_{\mathbb{L}}(1)\right\} = 10 < 11,$$

which is a contradiction. If no pair of points is contained in at least two isosceles right triangles, then  $S_{\square}(\mathcal{P}) \leq \binom{\#\mathcal{P}}{2}/3$ , so that we can conclude  $\#\mathcal{P}' = 4$  in our situation. Lemma 2 then yields

$$S_{\square}(\mathcal{P}) \le S_{\square}(4) + 2\binom{3}{2} + S_{\square}(3) = 11$$

However, if the upper bound of Lemma 2 is attained, then the three points in  $\mathcal{P} \setminus \mathcal{P}'$  form an isosceles right triangle and each edge is contained in two further isosceles right triangles, which yields a subconfiguration of cardinality 5 that can be obtained by 1-extension – contradiction.

Similar as in Example 3, we can start from the (up to similarity) unique 5-point set  $\mathcal{P}'$  with  $S_{\mathbb{A}}(\mathcal{P}') = 8$  and add two further points to obtain an 7-point set  $\mathcal{P}$  with  $S_{\mathbb{A}}(\mathcal{P}) = 10$  that cannot be obtained by 1-extension.

**Lemma 7.** The maximum target value of the following integer linear program (ILP) is an upper bound for  $S_{\mathbb{A}}(n)$ , where  $N = \{1, \ldots, n\}$ :

$$\begin{aligned} \max \sum_{S \subseteq N: \#S=3} x_S \quad subject \ to \\ \sum_{S \subseteq N: \#S=3} x_S \leq S_{\mathbb{A}}(\#T) \quad \forall T \subseteq N : 4 \leq \#T \leq n-1 \\ -3y_{4,T} + \sum_{S \subseteq T: \#S=3} x_S \leq 1 \quad \forall T \subseteq N : \#T=4 \\ \begin{pmatrix} t-1 \\ 2 \end{pmatrix} (y_{t-1,R} - y_{t,T}) + \sum_{S \subseteq T: S \not\subseteq R, \#S=3} x_S \leq \binom{t-1}{2} \quad \forall R \subset T \subseteq N : \#T=t, \#R=t-1, 5 \leq t \leq n \\ x_S \in \{0,1\} \quad \forall S \subseteq N : \#S=3 \\ y_{\#T,T} \in \{0,1\} \quad \forall T \subseteq N : 4 \leq \#T \leq n \end{aligned}$$

*Proof.* Given an *n*-point set  $\mathcal{P}$  we set  $x_S = 1$  iff the three elements in *S* form the vertices of an isosceles right triangle in  $\mathcal{P}$ . For each *T* ⊆ *N* with  $4 \leq \#T \leq n$  we set  $y_{\#T,T} = 1$  iff the restriction of  $\mathcal{P}$  to *T* can by obtained by 1-extension. With this, the first set of inequalities is automatically satisfied. For the second set of inequalities we remark that either at most one of the four 3-sets  $S \subset T$  forms the vertices of an isosceles right triangle or the restriction of  $\mathcal{P}$  to *T* (of cardinality 4) can be obtained by 1-extension since there are at least two isosceles right triangles intersecting in an edge. For the third set of inequalities we observe that  $\sum_{S \subseteq T:S \subseteq R, \#S=3} x_S \leq \binom{t-1}{2}$ . So, if  $y_{t-1,R} = 0$ , then the inequality is automatically satisfied. The same is true if  $y_{t-1,R} = 1$  and  $\sum_{S \subseteq T:S \subseteq R, \#S=3} = 0$ . If  $y_{t-1,R} = 1$  and  $\sum_{S \subseteq T:S \subseteq R, \#S=3} \geq 1$ , then the restriction of  $\mathcal{P}$  to *R* can be obtained by 1-extension and there exists an isosceles right triangle that intersects *R* in two vertices, so that also the restriction of  $\mathcal{P}$  to *T* can be obtained by 1-extension of  $\mathcal{P}$  to *T* can be obtained by 1-extension and there exists an isosceles right triangle that intersects *R* in two vertices, so that also the restriction of  $\mathcal{P}$  to *T* can be obtained by 1-extension and there exists an isosceles right triangle that intersects *R* in the latter case the inequality is also satisfied. To sum up, choosing the  $x_S$  and  $y_{\#T,T}$  as stated initially yields a feasible solution of the ILP with target value  $\sum_{S \subseteq N: \#S=3} x_S = S_{\mathbb{A}}(\mathcal{P})$ . Thus, the optimal target value of the ILP is at least as large as  $S_{\mathbb{A}}(n)$ .

#### **Proposition 8.**

- (1) Each reduced 8-point set  $\mathcal{P}$  with  $S_{\mathbb{N}}(\mathcal{P}) \geq 14$  can be obtained by 1-ext. and  $S_{\mathbb{N}}(8) = 20$ .
- (2) Each reduced 9-point set  $\mathcal{P}$  with  $S_{\mathbb{A}}(\mathcal{P}) \geq 18$  can be obtained by 1-ext. and  $S_{\mathbb{A}}(9) = 28$ .

*Proof.* Given the data of Table 1 it suffices to show that  $\mathcal{P}$  can be obtained by 1-extension if  $S_{\mathbb{A}}(\mathcal{P})$  is at least as large as proposed.

Assume that  $\mathcal{P}$  is a reduced 8-point set that cannot be obtained by 1-extension and satisfies  $S_{\mathbb{L}}(\mathcal{P}) \geq 14$ . Let  $\widetilde{\mathcal{P}}$  be a 1-extension maximal subconfiguration of  $\mathcal{P}$ , so that Lemma 5 implies  $\#\widetilde{\mathcal{P}} \leq 6$ . If  $\#\widetilde{\mathcal{P}} = 6$ , then Lemma 2 implies  $S_{\mathbb{L}}(\mathcal{P}) \leq S_{\mathbb{L}}(6) + 2 \cdot \binom{2}{2} + S_{\mathbb{L}}(2) = 13$ , which is a contradiction. If  $\#\widetilde{\mathcal{P}} = 5$ , then Lemma 2 implies  $S_{\mathbb{L}}(\mathcal{P}) \leq S_{\mathbb{L}}(\widetilde{\mathcal{P}}) + 2 \cdot \binom{3}{2} + S_{\mathbb{L}}(3) = S_{\mathbb{L}}(\widetilde{\mathcal{P}}) + 7$ , so that  $S_{\mathbb{L}}(\widetilde{\mathcal{P}}) \geq 7$ . From Proposition 6.(3) and Table 1 we conclude  $S_{\mathbb{L}}(\widetilde{\mathcal{P}}) = 8$ . Next we apply the ILP from Lemma 7 with n = 8 and the additional inequalities  $y_{\#T,T} = 0$  for all  $T \subseteq N$  with  $\#T \in \{6,7,8\}$  and

$$-8y_{5,T} + \sum_{S \subseteq T: \#S=3} x_S \ge 0$$

for all  $T \subseteq N$  with #T = 5. We can computationally check that the optimal target value of this modified ILP is 12, so that statement (1) follows.

Assume that  $\mathcal{P}$  is a reduced 9-point set that cannot be obtained by 1-extension and satisfies  $S_{\mathbb{A}}(\mathcal{P}) \geq 19$ . Let  $\widetilde{\mathcal{P}}$  be a 1-extension maximal subconfiguration of  $\mathcal{P}$ , so that Lemma 5 implies  $\#\widetilde{\mathcal{P}} \leq 7$ . If  $\#\widetilde{\mathcal{P}} = 7$ , then Lemma 2 implies  $S_{\mathbb{A}}(\mathcal{P}) \leq S_{\mathbb{A}}(7) + 2 \cdot \binom{2}{2} + S_{\mathbb{A}}(2) = 17$ , which is a contradiction. If  $\#\widetilde{\mathcal{P}} = 6$ , then Lemma 2 implies  $S_{\mathbb{A}}(\mathcal{P}) \leq S_{\mathbb{A}}(\widetilde{\mathcal{P}}) + 2 \cdot \binom{3}{2} + S_{\mathbb{A}}(3) = S_{\mathbb{A}}(\widetilde{\mathcal{P}}) + 7$ , so that  $S_{\mathbb{A}}(\widetilde{\mathcal{P}}) = 11$ . Next we apply the ILP from Lemma 7 with n = 9 and the additional inequalities  $y_{\#T,T} = 0$  for all  $T \subseteq N$  with  $\#T \in \{7, 8, 9\}$  and

$$-11y_{6,T} + \sum_{S \subseteq T: \#S=3} x_S \ge 0$$

for all  $T \subseteq N$  with #T = 6. We can computationally check that the optimal target value of this modified ILP is 17, so that statement (2) follows.

**Proposition 9.** Each 10-point set  $\mathcal{P}$  with  $S_{\mathbb{A}}(\mathcal{P}) \geq 25$  can be obtained by 1-extension from a subconfiguration  $\mathcal{P}'$  with  $\#\mathcal{P}' \leq 9$ ,  $S_{\mathbb{A}}(\mathcal{P}') \geq 18$  that can be obtained by 1-extension. Moreover, we have  $S_{\mathbb{A}}(10) = 35$ .

Proof. From Lemma 4 we conclude the existence of a subconfiguration  $\mathcal{P}'' \subset \mathcal{P}$  with  $\#\mathcal{P}'' = 9$ and  $S_{\mathbb{A}}(\mathcal{P}'') \geq 18$ . Now let  $\mathcal{P}'$  arise from  $\mathcal{P}''$  by removing isolated vertices, so that  $\mathcal{P}'$  is reduced and  $S_{\mathbb{A}}(\mathcal{P})' \geq 18$ . Proposition 8 then yields that  $\mathcal{P}'$  can be obtained by 1-extension and  $\#\mathcal{P}' \in \{8,9\}$ .

We recursively apply 1-extension starting from all point sets  $\mathcal{P}'$  with  $\#\mathcal{P}' \in \{8,9\}$  and  $S_{\mathbb{A}}(\mathcal{P}') \geq 18$  that can be obtained by 1-extension till cardinality n = 10 is reached for  $\mathcal{P}$ . This computation yields  $S_{\mathbb{A}}(10) \geq 35$  and none of the constructed point sets strictly improves upon this lower bound.

Now let  $\widetilde{\mathcal{P}}$  be a 1-extension maximal subconfiguration of  $\mathcal{P}$  with  $\mathcal{P}' \subseteq \widetilde{\mathcal{P}}$ . From Lemma 2 and Lemma 5 we conclude  $\#\widetilde{\mathcal{P}} = \#\mathcal{P}$ , so that  $S_{\mathbb{N}}(10) = 35$ .

Using the same technique we prove the following four statements:

**Proposition 10.** Each 11-point set  $\mathcal{P}$  with  $S_{\mathbb{A}}(\mathcal{P}) \geq 34$  can be obtained by 1-extension from a subconfiguration  $\mathcal{P}'$  with  $\#\mathcal{P}' \leq 10$ ,  $S_{\mathbb{A}}(\mathcal{P}') \geq 25$  that can be obtained by 1-extension. Moreover, we have  $S_{\mathbb{A}}(11) = 43$ .

**Proposition 11.** Each 12-point set  $\mathcal{P}$  with  $S_{\mathbb{A}}(\mathcal{P}) \geq 45$  can be obtained by 1-extension from a subconfiguration  $\mathcal{P}'$  with  $\#\mathcal{P}' \leq 11$ ,  $S_{\mathbb{A}}(\mathcal{P}') \geq 34$  that can be obtained by 1-extension. Moreover, we have  $S_{\mathbb{A}}(12) = 52$ .

**Proposition 12.** Each 13-point set  $\mathcal{P}$  with  $S_{\mathbb{A}}(\mathcal{P}) \geq 58$  can be obtained by 1-extension from a subconfiguration  $\mathcal{P}'$  with  $\#\mathcal{P}' \leq 12$ ,  $S_{\mathbb{A}}(\mathcal{P}') \geq 45$  that can be obtained by 1-extension. Moreover, we have  $S_{\mathbb{A}}(13) = 64$ .

**Proposition 13.** Each 14-point set  $\mathcal{P}$  with  $S_{\mathbb{A}}(\mathcal{P}) \geq 73$  can be obtained by 1-extension from a subconfiguration  $\mathcal{P}'$  with  $\#\mathcal{P}' \leq 13$ ,  $S_{\mathbb{A}}(\mathcal{P}') \geq 58$  that can be obtained by 1-extension. Moreover, we have  $S_{\mathbb{A}}(14) = 74$ .

**Theorem 14.** We have  $S_{\mathbb{A}}(10) = 35$ ,  $S_{\mathbb{A}}(11) = 43$ ,  $S_{\mathbb{A}}(12) = 52$ ,  $S_{\mathbb{A}}(13) = 64$ ,  $S_{\mathbb{A}}(14) = 74$ , and all similarity types of the corresponding extremal configurations are listed in Appendix A.

While the bound of Lemma 4 is too weak to continue in the same manner for n > 14, we can recursively apply 1-extension keeping the best 30000 point sets in each iteration only in order to obtain heuristic lower bounds for  $S_{\mathbb{A}}(n)$ . These lower bounds are given in Table 2 and the known similarity types of attaining configurations are listed in Appendix A. For  $15 \le n \le 25$ the lower bounds of [3] are matched.

$\overline{n}$		15	16	17	18	19	20	21	22	23	24	25	26	27
$S_{\square}$	$(n) \ge$	85	97	112	124	139	156	176	192	210	229	252	271	291
γ	ı	28	3	29	30	31	32	33	34	35	36	37	38	39
L.	$S_{\square}(n) \ge$	31	14	338	363	389	417	448	473	501	531	564	594	626
	$\overline{n}$		40	41	42	43	44	45	46	47	48	49	50	
	$S_{ m b}(n)$	$\geq$	659	696	728	763	799	836	874	914	955	100	0 10	38

Table 2: Lower bounds for the number of isosceles right triangles in *n*-point sets.

### **3** Recursively extending point sets by squares

By  $S_{\Box}(\mathcal{P})$  we denote the number of squares contained in  $\mathcal{P} \subseteq \mathbb{R}^2$ . We say that  $\mathcal{P}$  can be embedded on the (integer) grid if there exists a similar point set  $\mathcal{P}'$  with  $\mathcal{P}' \subset \mathbb{Z}^2$ . In our context most of the point sets can be assumed to be finite subsets of the integer grid. Instead of listing coordinates, we may also give a graphical representation, see Figure 2. Here we have also depicted the squares contained in the point set. By convention  $\mathcal{P}_{n,m}^i$  will always denote an *n*-point set with  $S_{\Box}(\mathcal{P}_{n,m}^i) = m$ , where *i* is an index distinguishing non-similar point sets. The set of points of a single (unit) square is denoted by  $\mathcal{P}_{4,1}^1$ ; for other examples see Figure 2. For easier reference we label the points from 1 to *n*.

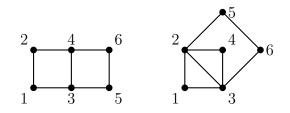


Figure 2: Two non-similar point sets  $\mathcal{P}_{6,2}^1$  and  $\mathcal{P}_{6,2}^2$  consisting of 6 points and 2 squares.

Since each square consists of four (corner) points, i.e. vertices, we have  $S_{\Box}(i) = 0$  for  $i \leq 3$ and  $S_{\Box}(4) = 1$ . Let us now consider how the vertices of two different squares can overlap. To this end we distinguish between the four edges and the two diagonals of a square. In  $\mathcal{P}_{6,2}^2$  in Figure 2 the vertices 2 and 3 form a diagonal of the square with vertices in  $\{2, 3, 5, 6\}$  as well as an edge of the square with vertices in  $\{1, 2, 3, 4\}$ .

**Lemma 15.** Let  $P_1, P_2 \in \mathbb{R}^2$  be two arbitrary distinct points. Then there exist three different choices for pairs of points  $\{P_3, P_4\}$  such that  $\{P_1, P_2, P_3, P_4\}$  spans a square. More precisely, denoting the coordinates of  $P_i$  by  $(x_i, y_i)$  for  $1 \leq i \leq 4$ , we have (up to a permutation of  $P_3$  and  $P_4$ ) that

- (a)  $(x_3, y_3) = \left(\frac{x_1 + x_2 + y_2 y_1}{2}, \frac{y_1 + y_2 + x_1 x_2}{2}\right), (x_4, y_4) = \left(\frac{x_1 + x_2 + y_1 y_2}{2}, \frac{y_1 + y_2 + x_2 x_1}{2}\right); if \{P_1, P_2\}$  is the diagonal of the square;
- (b)  $(x_3, y_3) = (x_2 \pm (y_2 y_1), y_2 \pm (x_1 x_2)), (x_4, y_4) = (x_1 \pm (y_2 y_1), y_1 \pm (x_1 x_2))$  if {P<sub>1</sub>, P<sub>2</sub>} is an edge of the square.

A graphical representation of the, up to similarity, unique point set with three squares through a common pair of points, without any further points, is given depicted in Figure 3.

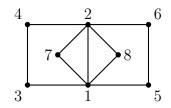


Figure 3: Three squares through a pair of points – point set  $\mathcal{P}^1_{8,3}$ .

Since each square consists of  $\binom{4}{2} = 6$  pairs of points, Lemma 15 directly implies the upper bound  $S_{\Box}(n) \leq \binom{n}{2}/2 = \frac{n^2}{4} + O(n)$ . Another easy implication is that through each triple of points there exists at most one square. So, given an *n*-point set  $\mathcal{P}$  we may consider every triple of points and compute a candidate for an (n + 1)th point by considering a square through the new point. We call this procedure 1-point extension or just 1-extension for short.

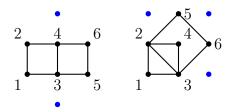


Figure 4: 1-extension for the point sets  $\mathcal{P}_{6,2}^1$  and  $\mathcal{P}_{6,2}^2$ .

In Figure 4 we have depicted the candidate points in the 1-extension for  $\mathcal{P}_{6,2}^1$  and  $\mathcal{P}_{6,2}^2$  by blue circles. Since one of the three 2-subsets of the triple of points has to be an edge of the square, we conclude from Lemma 15.(b) that the "new" point lies on the integer grid if  $\mathcal{P} \subset \mathbb{Z}^2$ . Of course it may happen that three points determine a fourth point that is already contained in the point set. Up to symmetry, i.e., similarity, the resulting point sets are depicted in Figure 5. Note that  $\mathcal{P}_{6,2}^1$  yields  $\mathcal{P}_{7,3}^1$  only, while  $\mathcal{P}_{6,2}^1$  produces both 7-point sets.

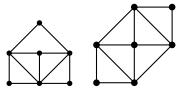


Figure 5: Two non-similar point sets  $\mathcal{P}^1_{7,3}$  and  $\mathcal{P}^2_{7,3}$ .

Lemma 15 also suggests a 2-extension procedure, i.e., for an arbitrary pair of points of an n-point set  $\mathcal{P}$  consider the three possible squares containing them. Here the candidates come in pairs of "new" points. We depict those candidates by a blue line and also color the corresponding



Figure 6: 2-extension applied to  $\mathcal{P}_{4,1}^1$ .

vertices blue, see Figure 6 for an example of 2-extension applied to the unit square  $\mathcal{P}_{4,1}^1$ . The four horizontal or vertical blue lines yield  $\mathcal{P}_{6,2}^1$  and the four skewed blue lines yield  $\mathcal{P}_{6,2}^2$ .

To simplify the notation, we will consider 1-extensions as a special case of 2-extensions, i.e., we allow that from the two "new" points one (or both, to include the degenerate case) can be already contained in the point set. Note that this case does not occur in our example in Figure 6 since there exists no 1-extension of the unit square  $\mathcal{P}_{4,1}^1$  (that increases the number of points). From Lemma 15.(a) we see that it may be possible to scale the resulting point set by a factor of two in order to stay within the integer grid. Note that in our example no scaling was necessary. Applying 2-extension recursively, starting from the unit square  $\mathcal{P}_{4,1}^1$ , gives us quite some non-similar *n*-point sets with *m* squares, see Table 3.<sup>4</sup>

	4	6	7	8	8	9	9	9	10	10	10	10	11	1	1	11	11	12	)
n	4	÷	•	•	-			-	-										2
m	T	2	3	3	4	4	5	6	4	5	6	7	5	6		7	8	5	
#	1	2	2	15	2	34	1	1	340	74	5	1	140	)5 1	59	15	5	15	5621
$\overline{n}$	12	2	12	2	12	12	12	12	13		13		13	13	1	3 1	13	13	13
m	6		7		8	9	10	11	6		$\overline{7}$		8	9	1	0 1	1	12	13
#	4'	729	47	76	80	11	3	1	905	573	1595	55	1836	482	2 4	3 1	4	1	1
$\overline{n}$		14		-	14		14		14	14	1	14	14	14	14	14	15	)	
$\eta$	<i>i</i> (	6		-	7		8		9	10	]	11	12	13	14	15	7		
#	<u>L</u>	1088	8332	2 4	4032	95	6138	6	9319	230	01 3	356	83	10	4	2	81	430	21
	1	ı	15		1	5		15	1	5	15		15	15	15	1	5	15	
	1	n	8		Q	)		10	1	1	12		13	14	15	1	6	17	
	7	<del>ļ</del>	174	583	7 2	27303		6063	<b>3</b> 2 1	0982	26	93	460	122	26	5 7		2	
$\overline{n}$	1	6			16			16		16		1(	6	16		16		16	;
m	7	7			8			9		10		1	1	12		13		14	
#	1	019	997	59	445	51329	94 8	8155	5822		5326	36	60147	69	230		076	34	88
$\overline{n}$	1	6	16	j	16	16	16	16	17			17		]	17		1	7	
m	1	5	16	3	17	18	19	20	8			9		]	0		1	1	
#		017	23		55	17	3	2		94293	357		608250		3702	9433		414	942
	$\overline{n}$	17	7		17		17	,	17		17	1	7	17 1	7	17	17	17	
	m	12	2		13		14	:	15		16	1	7	18 1	9	20	21	22	
-	#	14	4194	101	28	1512	52	643	105	646	2137	7 5	511 8	89 1	.1 :	2	0	1	

Table 3: Number of non-similar points sets  $\mathcal{P}$  produced by recursive 2-extension starting from a unit square per number of points n and squares  $m = S_{\Box}(\mathcal{P})$ .

Note that if an *n*-point set  $\mathcal{P}$  is obtained from the recursive application of 2-extension, starting from the unit square, then we have  $S_{\Box}(\mathcal{P}) \geq \lceil n/2 \rceil - 1$  for  $n \geq 6$ . In particular, no 7-point set  $\mathcal{P}$  with  $S_{\Box}(\mathcal{P}) = 2$  squares will be obtained. Note that the configuration in

<sup>&</sup>lt;sup>4</sup>There are e.g. 1180723093 non-similar 17-point sets. For a publicly available implementation by Hugo van der Sanden see https://github.com/hvds/seq/tree/master/A051602.

Figure 7 is non-rigid in the sense that we can twist the two squares, connected via vertex 4, without changing the number of squares in the point set. While the resulting point sets will be non-similar, we will discuss such transformations later on. Despite those complications, we nevertheless expect that for each *n*-point set  $\mathcal{P}$  with a sufficiently large number  $S_{\Box}(\mathcal{P})$  of squares there exists a similar point set that can be obtained by the recursive application of 2-extension starting from  $\mathcal{P}_{4,1}^1$ . More concretely, we state:

**Conjecture 16.** For  $n \ge 6$  every *n*-point set  $\mathcal{P}$  with  $S_{\Box}(\mathcal{P}) = S_{\Box}(n)$  is similar to an *n*-point set  $\mathcal{P}'$  obtained by recursive 2-extension starting from  $\mathcal{P}^1_{4,1}$ .

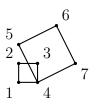


Figure 7: A non-rigid 7-point set  $\mathcal{P}_{7,2}^1$  with two squares.

Associating  $\mathbb{R}^2$  with  $\mathbb{C}$  we can state compact criteria for four points forming a square.

#### Lemma 17.

- (1) Four vertices  $z_1, z_2, z_3, z_4 \in \mathbb{C}$  of a quadrilateral in counterclockwise order form a parallelogram iff  $z_1 - z_2 + z_3 - z_4 = 0$ .
- (2) Three vertices  $z_1, z_2, z_3 \in \mathbb{C}$  form a right angle in counterclockwise order<sup>5</sup> iff  $(z_3 z_2) i = z_1 z_2$ .
- (3) Four vertices  $z_1, z_2, z_3, z_4 \in \mathbb{C}$  of a quadrilateral in counterclockwise order form a square iff  $z_1 z_2 + z_3 z_4 = 0$  and  $z_4 z_1 = i(z_2 z_1)$ .

Our next aim are combinatorial relaxations for point sets  $\mathcal{P} \subset \mathbb{R}^2$ , i.e., we want to consider discrete representations that do not list the coordinates of the points. An *incidence structure* is a triple (P, L, I) where P, L are sets and  $I \subseteq P \times L$  is the *incidence relation*.

**Definition 18.** An oriented square set is an incidence structure (P, S, I), where  $P = \{1, \ldots, n\}$  for some integer n, S consists of objects of the form  $(v_1, v_2, v_3, v_4)$ , where  $1 \le v_1, v_2, v_3, v_4 \le n$  are pairwise different with  $v_1 = \min\{v_1, v_2, v_3, v_4\}$ , and  $(p, (v_1, v_2, v_3, v_4)) \in I$  iff  $p \in \{v_1, v_2, v_3, v_4\}$ . We call the elements of S squares.

We abbreviate an oriented square set  $\mathcal{I} = (P, S, I)$  by (P, S) (since I is well defined by P and S), call #P the order of  $\mathcal{I}$  and #S the cardinality  $\#\mathcal{I}$  of  $\mathcal{I}$ . We also speak of an oriented square set S of order n referring to the oriented square set  $(\{1, \ldots, n\}, S)$ .

Two oriented square sets (P, S, I) and (P', S', I') are called *isomorphic* if there exist bijections  $\alpha \colon P \to P'$  and  $\beta \colon S \to S'$  such that  $(p, s) \in I$  iff  $(\alpha(p), \beta(s)) \in I'$ .

**Definition 19.** An oriented square set (P, S) of order n is called realizable if their exist pairwise disjoint points  $P_1, \ldots, P_n \in \mathbb{R}^2$  such that the points  $P_a, P_b, P_c, P_d$  form a square in counterclockwise ordering for each  $(a, b, c, d) \in S$ .

Of course the determination to the counterclockwise ordering is arbitrary and we may also require clockwise orderings for all squares. Given an *n*-point set  $\mathcal{P} \subset \mathbb{R}^2$  and an arbitrary labeling of the points with labels in  $\{1, \ldots, n\}$ , there exists a unique oriented square set (P, S)with  $\#S = S_{\Box}(\mathcal{P})$  that is realized by  $\mathcal{P}$ . We call (P, S) the maximal oriented square set of  $\mathcal{P}$ and also use the notation  $S(\mathcal{P})$ . For any subset  $S' \subseteq S$  the pair (P, S') is also an oriented square set realized by  $\mathcal{P}$  and we speak of an oriented square set of  $\mathcal{P}$ .

<sup>&</sup>lt;sup>5</sup>The vector  $z_3 - z_1$  rotated by a right angle in counterclockwise order gives the vector  $z_1 - z_2$ .

**Example 20.** Consider the point set  $\mathcal{P}_{6,2}^1$  with labels and coordinates as in Figure 2. The maximal oriented square set S (of order 6) of  $\mathcal{P}$  is given by  $S = \{(1,3,4,2), (3,5,6,4)\}$ . Any relabeling of the points yields an isomorphic oriented square system that is also realizable.

Next we want to consider the inverse problem, i.e., when is a given oriented square set (P, S) realizable?

**Definition 21.** Let S be an oriented square set of order n. For n complex-valued variables  $z_j$ , where  $1 \leq j \leq n$ , the linear equation system L(n, S) consists of the  $2 \cdot \#S$  equations

$$z_a - z_b + z_c - z_d = 0$$
 and  $z_d - z_a = i(z_b - z_a)$ 

for each  $s = (a, b, c, d) \in S$ .

**Lemma 22.** Let S be an oriented square set of order n. It is realizable iff the linear equation system L(n, S) admits a solution satisfying  $z_j \neq z_k$  for all  $1 \leq j < k \leq n$ .

**Example 23.** Consider the point set  $\mathcal{P}^1_{7,2}$  with coordinates and labels as in Figure 7. The maximal oriented square set of order 7 of  $\mathcal{P}^1_{7,2}$  is given by  $S = \{(1,4,3,2), (4,7,6,5)\}$ . Using Lemma 22 we can compute the full space of realizations. W.l.o.g. we assume  $z_1 = 0$  and  $z_2 = i$  for the coordinates of the points with labels 1 and 2, respectively.

Over the reals, the solution space of L(7, S) is two-dimensional and can e.g. be parameterized as

$$\begin{aligned} \mathcal{P}(u,v) &= \left\{ 0, i, 1+i, 1, 1+u+vi, 1+u+v+(v-u)i, 1+v, -ui \right\} \\ &\cong \left\{ (0,0), (0,1), (1,1), (1,0), (1+u,v), (1+u+v, v-u), (1+v, -u) \right\} \subset \mathbb{R}^2. \end{aligned}$$

The condition  $z_j \neq z_k$  for all  $1 \leq j < k \leq 7$  are equivalent to

$$(u,v) \notin \{(-1,0), (-1,1), (0,1), (0,0), (-\frac{1}{2}, -\frac{1}{2}), (-\frac{1}{2}, \frac{1}{2}), (-1,-1), (0,-1)\}.$$

For (u, v) = (0, 1) the point set  $\mathcal{P}(u, v)$  is similar to  $\mathcal{P}_{6,2}^1$ , for (u, v) = (-1, 1) we end up with  $\mathcal{P}_{6,2}^2$ . An extreme case occurs for (u, v) = (0, 0), where the vertices 4, 5, 6, and 7 are pairwise identical, *i.e.*, we end up with  $\mathcal{P}_{4,1}$ . The coordinates used in Figure 7 correspond to (u, v) = (-1, 2).

**Remark 24.** The point sets  $\mathcal{P}(u, v)$  considered in Example 23 are pairwise non-similar for different values of  $(u, v) \in \mathbb{R}^2$ . This property does not hold in general and is due to our chosen specific parameterization. If S is the maximal oriented square set for  $\mathcal{P}_{6,2}^2$ , then all solutions with pairwise different coordinates  $z_j$  correspond to similar point sets. Note that even a solution with pairwise different coordinates may correspond to a realization  $\mathcal{P}'$  of S with  $S_{\Box}(\mathcal{P}') > \#S$ .

Solutions of L(n, S) such that there exist indices  $j \neq k$  with  $z_j = z_k$  are called *degenerate*. We will now study the question when L(n, S) admits a non-degenerate solution. For convenience, we will be working over  $\mathbb{R}$  again and apply a linear transformation so that the solution space of L(n, S) is spanned by  $\lambda_1, \ldots, \lambda_l \in \mathbb{R}$ . The conditions  $z_j \neq z_k$  transfer to conditions of the form  $\sum_{j=1}^l a_j \lambda_i \neq 0$  linked as  $\vee$ -pairs, where the  $a_j$  are rational numbers.

**Lemma 25.** Let  $a_i^j \in \mathbb{Q}$  for  $1 \leq i \leq l, 1 \leq j \leq n$ , where l, n are arbitrary integers, and  $F_1, \ldots, F_f$  be arbitrary subsets of  $\{1, \ldots, n\}$ . Then there exists a vector  $x \in \mathbb{R}^l$  such that for each  $1 \leq h \leq f$  there exists an index  $j \in F_h$  such that  $\sum_{i=1}^l a_i^j x_i \neq 0$  iff for each  $1 \leq h \leq f$  there exists an index  $j \in F_h$  such that  $\binom{j}{a_1^j}, \ldots, a_l^j \neq \mathbf{0}$ .

Proof. If there exists an index  $1 \leq h \leq f$  with  $\left(a_{1}^{j}, \ldots, a_{l}^{j}\right) = \mathbf{0}$  for all  $j \in F_{h}$ , then no  $x \in \mathbb{R}^{l}$  can satisfy  $\sum_{i=1}^{l} a_{i}^{j} x_{i} \neq 0$  for an index  $j \in F_{h}$ . Otherwise, let  $j_{h} \in F_{h}$  denote an index with  $\left(a_{1}^{jh}, \ldots, a_{l}^{jh}\right) \neq \mathbf{0}$  for each  $1 \leq h \leq f$ . Now choose the  $x_{i}$  as l Q-linearly independent numbers. Then we have  $\sum_{i=1}^{l} a_{i}^{jh} x_{i} \neq 0$ , since  $\{0\} \cup \{a_{i}^{jh} : 1 \leq i \leq l\} \subset \mathbb{Q}$ , for all  $1 \leq h \leq f$ .  $\Box$ 

**Example 26.** The oriented square set of order 9 given by  $S = \{(1, 3, 4, 2), (2, 5, 9, 8), (4, 7, 6, 5)\}$  is realizable, see Figure 8. Over the reals, the solution space is six-dimensional. Note that the realization depicted in Figure 8 is on the integer grid. However, it is also possible to choose the side lengths of the three squares as 1, e, and  $\pi$ , so that no similar point set  $\mathcal{P}' \subset \mathbb{Q}^2$  exists.

Let us add (3,6,8,10) to S, i.e., we consider the oriented square set of order 10 given by  $S' = \{(1,3,4,2), (2,5,9,8), (4,7,6,5), (3,6,8,10)\}$ . Over the reals, the solution space of L(10, S') is 4-dimensional. An integer realization is given by

 $\mathcal{P}\left\{(0,5), (5,5), (0,0), (5,0), (7,1), (8,-1), (6,-2), (9,7), (11,3), (1,8)\right\} \subset \mathbb{Z}^2.$ 

If we further add (1, 10, 7, 9) to S' and denote the resulting oriented square set by S", then L(10, S'') admits a 2-dimensional solution space over the reals. From Lemma 25 we conclude that S" is non-realizable.

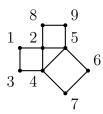


Figure 8: A non-rigid 9-point set  $\mathcal{P}_{9,3}^1$  with three squares.

Our next goal is to show that for each *n*-point set  $\mathcal{P} \subset \mathbb{R}^2$  there exists an *n*-point set  $\mathcal{P}' \subset \mathbb{Q}^2$ with  $S_{\Box}(\mathcal{P}') \geq S_{\Box}(\mathcal{P})$ . Let *S* denote a maximal oriented square set of  $\mathcal{P}$ . By assumption, L(n, S)admits a solution  $(z_1, \ldots, z_n) \in \mathbb{C}^n$  with  $z_j \neq z_k$  for all  $1 \leq j < k \leq n$ . Since the space of rational solutions is dense in the space of complex solutions and  $z_j \neq z_k$  are open conditions, there also exists a solution  $(z'_1, \ldots, z'_n) \in (\mathbb{Q}[i])^n$  with  $z'_j \neq z'_k$  for all  $1 \leq j < k \leq n$ . Just for illustration, we give an explicit construction:

**Lemma 27.** Let  $A \in \mathbb{Q}^{m \times n}$ ,  $B \in \mathbb{Q}^{l \times n}$ , and  $x \in \mathbb{R}^n$  satisfying Ax = 0 and  $Bx \neq 0$ . For each  $\varepsilon > 0$  there exists a vector  $\tilde{x} \in \mathbb{Q}^n$  such that  $A\tilde{x} = 0$ ,  $B\tilde{x} \neq 0$ , and  $||x - \tilde{x}||_{\infty} < \varepsilon$ .

*Proof.* Choose a basis  $S \subseteq \{1, \ldots, n\}$  of  $\{x \in \mathbb{R}^n : Ax = 0\}$ , i.e., choose  $\lambda_i^j$  for all  $j \in S$  and all  $i \in \overline{S} := \{1 \le i \le n : i \notin S\}$  such that

$$\{x \in \mathbb{R}^n : Ax = 0\} = \left\{ x \in \mathbb{R}^n : x_j = \sum_{i \in \bar{S}} \lambda_i^j x_i \quad \forall j \in S \right\}.$$

Note that  $A \in \mathbb{Q}^{m \times n}$  implies  $\lambda_i^j \in \mathbb{Q}$ . Set  $\Lambda := \max\left\{ \left| \lambda_i^j \right| : i \in \overline{S}, j \in S \right\}, \mu := \|Bx\|_{\infty}$ , and  $\beta := \max\left\{ |b_{i,j}| : 1 \le i \le n, 1 \le j \le l \right\}$ , where  $B = (b_{i,j})$ . W.l.o.g. we assume that  $\beta n \varepsilon < \mu$ . Set  $\varepsilon' := \min\left\{ \varepsilon, \frac{\varepsilon}{n\Lambda} \right\}$  and choose  $\tilde{x}_i \in \mathbb{Q}$  such that  $|x_i - \tilde{x}_i| < \varepsilon' \le \varepsilon$  for all  $i \in \overline{S}$ . For  $j \in S$  we set  $\tilde{x}_j = \sum_{i \in \overline{S}} \lambda_i^j \tilde{x}_i$ , so that

$$|x_j - \tilde{x}_j| = \left|\sum_{i \in \bar{S}} \lambda_i^j \cdot (x_i - \tilde{x}_i)\right| \le \sum_{i \in \bar{S}} \left|\lambda_i^j \cdot (x_i - \tilde{x}_i)\right| < n\Lambda\varepsilon' \le \varepsilon,$$

which implies  $||x - \tilde{x}||_{\infty} < \varepsilon$ . Next we compute

$$\|Bx - B\tilde{x}\|_{\infty} = \max_{1 \le j \le l} \left| \sum_{i=1}^{n} b_{i,j} \cdot (x_i - \tilde{x}_i) \right| \le \beta \cdot \sum_{i=1}^{n} |x_i - \tilde{x}_i| < \beta n\varepsilon < \mu,$$

so that  $B\tilde{x} \neq 0$ .

**Theorem 28.** For each n-point set  $\mathcal{P} \subset \mathbb{R}^2$  there exists an n-point set  $\mathcal{P}' \subset \mathbb{Q}^2$  with  $S_{\Box}(\mathcal{P}') \geq S_{\Box}(\mathcal{P})$ .

Proof. Let S be the maximal oriented square set of order n of  $\mathcal{P}$ . By Lemma 22 the existing realization  $\mathcal{P}$  corresponds to a solution  $(z_1, \ldots, z_n) \in \mathbb{C}^n$  of L(n, S) satisfying  $z_j \neq z_k$  for all  $1 \leq j < k \leq n$ . After a suitable transformation we can apply Lemma 27 to construct a solution  $(z'_1, \ldots, z'_n) \in (\mathbb{Q}(i))^n$  of L(n, S) satisfying  $z'_j \neq z'_k$  for all  $1 \leq j < k \leq n$ . From Lemma 22 we then conclude that  $\mathcal{P}' := \{z'_1, \ldots, n'_n\} \subset \mathbb{Q}(i)$  realizes s. Thus, we have  $S_{\Box}(\mathcal{P}') \geq \#S = S_{\Box}(\mathcal{P})$ .

We remark that the proof of Theorem 28 and the parameter  $\varepsilon$  in Lemma 27 would allow the stronger statement that we can assume the existence of a pairing between the points of  $\mathcal{P}$  and the points of  $\mathcal{P}'$  where the pairs of points have distance at most  $\varepsilon$  in the  $\|\cdot\|_{\infty}$ -metric, i.e.,  $\mathcal{P}'$  arises from  $\mathcal{P}$  by a sufficiently small perturbation.

**Corollary 29.** For each n-point set  $\mathcal{P} \subset \mathbb{R}^2$  there exists an n-point set  $\mathcal{P}' \subset \mathbb{Z}^2$  with  $S_{\Box}(\mathcal{P}') \geq S_{\Box}(\mathcal{P})$ .

**Corollary 30.** For each n-point set  $\mathcal{P} \subset \mathbb{R}^2$  obtained by 2-extension there exists an n-point set  $\mathcal{P}' \subset \mathbb{Z}^2$  with  $S_{\Box}(\mathcal{P}') = S_{\Box}(\mathcal{P})$ .

**Remark 31.** Theorem 28 can be directly generalized to: For each n-point set  $\mathcal{P} \subset \mathbb{R}^2$  and each  $\emptyset \neq \mathcal{Q} \subset \mathbb{Q}^2$  there exists an n-point set  $\mathcal{P}' \subset \mathbb{Q}^2$  with  $S_{\Box}(\mathcal{P}') \geq S_{\Box}(\mathcal{P})$ . I.e., one can choose  $\mathcal{Q}$  as an isosceles right triangle  $\bowtie$ .

The approach, based on linear equation systems over the rationals, also works for e.g. rectangles or axis-parallel squares and rectangles. For an equilateral triangle Q we have a similar statement replacing the Gaussian rationals (integers) by the Eisenstein rationals (integers).

**Proposition 32.** For each n-point set  $\mathcal{P} \subset \mathbb{R}^2$  there exists an n-point set  $\mathcal{P}' \subset \{0, 1, \dots, \Lambda\}^2$ with  $S_{\Box}(\mathcal{P}') \geq S_{\Box}(\mathcal{P})$  and  $\Lambda \leq 25^n$ .

*Proof.* Let S be the maximal oriented square set of order n of  $\mathcal{P}$ . By Lemma 22 the existing realization  $\mathcal{P}$  corresponds to a solution  $(z_1, \ldots, z_n) \in \mathbb{C}^n$  of L(n, S) satisfying  $z_j \neq z_k$  for all  $1 \leq j < k \leq n$ . W.l.o.g. we assume that real and imaginary parts of the  $z_j$  are non-negative and that

$$\max\{\left|\operatorname{Re}(z_j) - \operatorname{Re}(z_k)\right|, \left|\operatorname{Im}(z_j) - \operatorname{Im}(z_k)\right|\} \ge 1$$

for all  $1 \leq j < k \leq n$ . Consider the following linear program with variables  $x_j, y_j \in \mathbb{R}_{>0}$  for  $1 \leq j \leq n$ . We convert the equations of L(n, S) into their real counterparts using the  $x_j$  and  $y_j$  variables (4m equations). If  $\operatorname{Re}(z_j) - \operatorname{Re}(z_k) \ge 1$  we add the constraint  $x_j - x_k \ge 1$  and if  $\operatorname{Re}(z_i) - \operatorname{Re}(z_k) \leq -1$  we add the constraint  $x_k - x_i \geq 1$ , where  $1 \leq j < k \leq n$ . Similarly, If  $\operatorname{Im}(z_j) - \operatorname{Im}(z_k) \ge 1$  we add the constraint  $y_j - y_k \ge 1$  and if  $\operatorname{Im}(z_j) - \operatorname{Im}(z_k) \le -1$  we add the constraint  $y_k - y_j \ge 1$ , where  $1 \le j < k \le n$ . As target we choose the minimization of  $\sum_{j=1}^{n} x_j + \sum_{j=1}^{n} y_j$ , so that the LP is bounded. The existence of the solution  $(z_1, \ldots, z_n) \in \mathbb{C}^n$ implies that the LP is also feasible. Note that all coefficients of the LP formulation are contained in  $\{-1, 0, 1\}$  and that each constraint contains at most four non-zero coefficients on the left-hand side. Consider a basic solution of the LP, i.e., a solution of the uniquely solve able equation system  $A \cdot (x, y)^{\top} = b$ , where A is a suitable submatrix of the coefficient matrix of the LP and b a suitable subvector of the corresponding right hand side. For a variable  $x_j$  (or  $y_j$ ) let  $A^{x_j}$  (or  $A^{y_j}$  denote the matrix arising from A when the column corresponding to  $x_j$  (or  $y_j$ ) is replaced by b. With this Cramer's rule yields  $x_j = \det(A^{x_j})/\det(A)$  and  $y_j = \det(A^{y_j})/\det(A)$  for all  $1 \leq j \leq n$ . Using the Leibniz formula for determinants we conclude  $|\det(A^{x_j})|, |\det(A^{y_j})| \leq 5^{2n}$ for all  $1 \leq j \leq n$  (and  $|\det(A)| \leq 4^{2n}$ ). Now observe that  $\tilde{x}_j := x_j \cdot \det(A) = \det(A^{x_j})$ ,  $\tilde{y}_j := y_j \cdot \det(A) = \det(A^{y_j})$  is also a solution with  $\tilde{x}_j, \tilde{y}_j \in \mathbb{N}$  and  $|\tilde{x}_j|, |\tilde{y}_j| \leq 25^n$ , where  $1 \leq j \leq n$ .  Having the combinatorial structure of oriented square sets at hand, we can also treat nonrigid *n*-point sets using a finite number of cases only. We have to abandon the idea of classifying point sets up to similarity and consider equivalence classes of point sets distinguished by different oriented square sets. This causes some complications but allows us to determine  $S_{\Box}(n)$  exactly by a finite amount of computation, depending on n – in principle. Note that for the unit distance problem  $C_{\{q_1,q_2\}}(n)$  mentioned in the introduction, some extremal examples are not rigid, see e.g. [6, Section 5.1] or [17]. However, since the numbers in Table 3 provide a lower bound for the number of non-isomorphic realizable connected oriented square sets with order n and cardinality m, exhaustive enumerations will become computationally infeasible if n gets too large. So, in the subsequent section develop tools and criteria that allow us to obtain classification results for special values of n and m without having the full classification for all n' < n and m' < m at hand.

## 4 Bounds for $S_{\Box}(n)$

Let  $\leq$  denote the lexicographical ordering on  $\mathbb{R}^2$  and  $\mathcal{P} \subset \mathbb{R}^2$  be an arbitrary point set. Assume that the vertices of a square s in  $\mathcal{P}$  are given by  $v_1 \prec v_2 \prec v_3 \prec v_4$ . With this, we denote the six pairs of vertices by  $e_1 := \{v_1, v_2\}, e_2 := \{v_1, v_3\}, e_3 := \{v_2, v_4\}, e_4 := \{v_3, v_4\}, d_1 := \{v_1, v_4\},$ and  $d_2 := \{v_2, v_3\}$ . Observe that the  $e_i$  form the edges and the  $d_i$  form the diagonals of s. We call  $e_1$  the *leftmost edge* and  $e_2$  the *second leftmost edge* of s. In the following auxiliary result we determine the possible types of pairs of points in their three squares where they are contained, cf. Figure 9.

**Lemma 33.** Let a = (0, 0),  $b_1 = (u, v)$ , and  $b_2 = (v, -u)$ .

- (1) For  $0 \le u < v$  the squares through  $\{a, b_1\}$  are given by vertices  $a \prec b_1 \prec b_2 \prec (u+v, v-u)$ ,  $(-v, u) \prec (u-v, u+v) \prec a \prec b_1$ , and  $\frac{1}{2}(u-v, u+v) \prec a \prec b_1 \prec \frac{1}{2}(u+v, v-u)$ . The corresponding types of  $\{a, b_1\}$  are  $e_1$ ,  $e_4$ , and  $d_2$ , respectively.
- (2) For  $0 \le u < v$  the squares through  $\{a, b_2\}$  are given by vertices  $a \prec b_1 \prec b_2 \prec (u+v, v-u)$ ,  $(-u, -v) \prec a \prec (v - u, -u - v) \prec b_2$ , and  $a \prec \frac{1}{2}(v - u, -u - v) \prec \frac{1}{2}(u + v, v - u) \prec b_2$ . The corresponding types of  $\{a, b_2\}$  are  $e_2$ ,  $e_3$ , and  $d_1$ , respectively.
- (3) For  $0 < v \le u$  the squares through  $\{a, b_1\}$  are given by vertices  $a \prec b_2 \prec b_1 \prec (u+v, v-u)$ ,  $(-v, u) \prec a \prec (u-v, u+v) \prec b_1$ , and  $a \prec \frac{1}{2}(u-v, u+v) \prec b_1 \prec \frac{1}{2}(u+v, v-u)$ . The corresponding types of  $\{a, b_1\}$  are  $e_2$ ,  $e_3$ , and  $d_1$ , respectively..
- (4) For  $0 < v \le u$  the squares through  $\{a, b_2\}$  are given by vertices  $a \prec b_2 \prec b_1 \prec (u+v, v-u)$ ,  $(-u, -v) \prec (v - u, -u - v) \prec a \prec b_2$ , and  $\frac{1}{2}(v - u, -u - v) \prec a \prec b_2 \prec \frac{1}{2}(u + v, v - u)$ . The corresponding types of  $\{a, b_2\}$  are  $e_1$ ,  $e_4$ , and  $d_2$ , respectively.

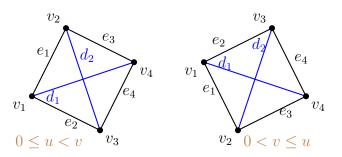


Figure 9: The lexicographical ordering of the vertices and the types of pairs of vertices of a square.

**Corollary 34.** Let  $\mathcal{P} \subset \mathbb{R}^2$  be an arbitrary point set. No pair of different points in  $\mathcal{P}$  can form both the leftmost edge of a square and the second leftmost edge of another square.

## **Proposition 35.** For $n \ge 1$ we have $S_{\Box}(n) \le \frac{n^2-1}{8}$ .

*Proof.* Let  $\mathcal{P} \subset \mathbb{R}^2$  be an arbitrary *n*-point set. Using a suitable similarity transformation we can assume that at most  $\frac{n+1}{2}$  points have negative and  $\frac{n+1}{2}$  points have positive *x*-coordinates, while the *y*-axis is free of points. By  $a_{ij}$  we denote the number of squares such that exactly *i* of its vertices have negative coordinates, where  $0 \leq i, j \leq 4$  with i + j = 4. If necessary by reflecting in the *y*-axis we can assume  $a_{31} + a_{40} \geq a_{13} + a_{04}$ . Let *s* be an arbitrary square of  $\mathcal{P}$  with vertices  $v_1 \prec v_2 \prec v_3 \prec v_4$  such that  $v_1$  and  $v_2$  have negative *x*-coordinates. Counting pairs of points with negative *x*-coordinate that are of type  $e_1$  or type  $e_2$  gives

$$a_{22} + 2a_{31} + 2a_{40} \le \binom{\frac{n+1}{2}}{2} = \frac{n^2 - 1}{8}$$

so that

$$S_{\Box}(\mathcal{P}) = a_{22} + a_{31} + a_{40} + a_{13} + a_{04} \le a_{22} + 2a_{31} + 2a_{40} \le \frac{n^2 - 1}{8}.$$

The underlying idea of the proof of Proposition 35 fits into the framework of a general method based on ordering relations as introduced in [2, 13].

Next we want to determine the exact values of  $S_{\Box}(n)$  for small values of n. First we introduce more notation. For brevity, an *n*-point set  $\mathcal{P} \in \mathbb{R}^2$  with  $S_{\Box}(\mathcal{P}) = m$  is also called (n, m)configuration in this section. We also use intuitive notations like  $(n, \geq m)$ -configuration. Any (n, m)-configuration where a pair of points is contained in at least two different squares contains one of the (6, 2)-configurations  $\mathcal{P}_{6,2}^1$  or  $\mathcal{P}_{6,2}^2$  as subconfiguration, see Figure 2. For arbitrary point sets  $\mathcal{F}_1, \ldots, \mathcal{F}_l$  we denote by  $S_{\Box}(n; \mathcal{F}_1, \ldots, \mathcal{F}_l)$  the maximum value of  $S_{\Box}(\mathcal{P})$  where  $\mathcal{P}$  is an *n*point set such that no subset of its points is similar to  $\mathcal{F}_i$  for an index  $1 \leq i \leq l$ . Besides trivial cases like  $S_{\Box}(n; \mathcal{P}_{4,1}^1) = 0$  and  $S_{\Box}(n; \mathcal{P}_{6,2}^*, \mathcal{P}_{7,2}^1) = \lfloor n/4 \rfloor$ , the exact value of  $S_{\Box}(n; \mathcal{F}_1, \ldots, \mathcal{F}_l)$  is hard to determine if n is not too small. Nevertheless, this notation helps to better structure the subsequent arguments.

Let A(n, d, w) denote the maximum size of a binary code with word length n, minimum Hamming distance d, and constant weight w, see e.g. [8] for details and bounds. A binary code of size m, length n, minimum Hamming distance 6, and constant weight 4 is in one-to-one correspondence to a set S of m four-subsets of  $\{1, \ldots, n\}$  such that  $\#(a \cap b) \leq 1$  for all  $a, b \in S$ with  $a \neq b$ . Thus, we have

$$S_{\Box}(n; \mathcal{P}_{6,2}^{\star}) := S_{\Box}(n; \mathcal{P}_{6,2}^{1}, \mathcal{P}_{6,2}^{2}) \le A(n, 6, 4) \le \left\lfloor n \cdot \left\lfloor \frac{n-1}{3} \right\rfloor / 4 \right\rfloor = \frac{n^{2}}{12} + O(n).$$

The values A(n, 6, 4) are known exactly, see [8, Theorem 6], and we list the first few in Table 4, cf. sequence A004037.

$\overline{n}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
A(n, 6, 4)	0	0	0	1	1	1	2	2	3	5	6	9	13	14	15	20	20

Table 4: The exact values of A(n, 6, 4) for  $n \leq 17$ .

Our next goal is to use the results obtained by exhaustive recursive 2-extension starting from a unit square, see Table 3.

**Definition 36.** Let  $\mathcal{P} \subset \mathbb{R}^2$  be an arbitrary point set. A point set  $\mathcal{P}' \subseteq \mathcal{P}$  is called a 2-extension subconfiguration if  $\mathcal{P}'$  can be obtained by recursive 2-extension starting from a unit square. If there is no proper superset of  $\mathcal{P}'$  that can also be obtained by recursive 2-extension starting from  $\mathcal{P}'$ , then we call  $\mathcal{P}'$  2-extension maximal.

For an arbitrary point set  $\mathcal{P} \subset \mathbb{R}^2$  we define  $S_{\square-3\square}(\mathcal{P}) := S_{\square}(\mathcal{P}) - 3S_{\square}(\mathcal{P})$  and denote the corresponding maximum value of an *n*-point set by  $S_{\square-3\square}(n)$ .

**Lemma 37.** Let  $\mathcal{P} \subset \mathbb{R}^2$  be an arbitrary n-point set and  $\mathcal{P}'$  be a 2-extension maximal subconfiguration. Then we have

$$S_{\Box}(\mathcal{P}) \le S_{\Box}(\mathcal{P}') + S_{\square-3\Box}(\mathcal{P} \setminus \mathcal{P}') \le S_{\Box}(n') + S_{\square-3\Box}(n-n'),$$

where  $n' := \# \mathcal{P}'$ .

*Proof.* Let s be an arbitrary square in  $\mathcal{P}$  that is not contained in  $\mathcal{P}'$ . Since  $\mathcal{P}'$  is 2-extension maximal either 3 or 4 vertices of s have to be contained in  $\mathcal{P} \setminus \mathcal{P}'$ . In the first case the 3 vertices form a right isosceles triangle. In the second case the 4 vertices form a square that contains four right isosceles triangles. Note that each right isosceles triangle uniquely determines a square.  $\Box$ 

**Lemma 38.** We have  $S_{\square-3\square}(n) = 0$  for  $n \le 2$ ,  $S_{\square-3\square}(3) = 1$ ,  $S_{\square-3\square}(4) = 3$ ,  $S_{\square-3\square}(5) = 5$ ,  $S_{\square-3\square}(6) = 7$ ,  $S_{\square-3\square}(7) = 10$ ,  $S_{\square-3\square}(8) = 14$ , and  $S_{\square-3\square}(9) = 18$ .

*Proof.* The statements are obvious for  $n \leq 3$ . In Appendix B we present point sets attaining the mentioned values for  $S_{\square-3\square}(\mathcal{P})$ . Looping over all *n*-point sets with  $n \leq 9$  that can be obtained by 1-extension does not yield point sets with larger values, so that the result is implied by Proposition 6 and Proposition8. Let  $\mathcal{P}'$  be a 2-extension maximal subconfiguration of  $\mathcal{P}$  with maximum possible cardinality. Note that we have  $\#\mathcal{P}' \geq 6$ .

**Theorem 39.** We have  $S_{\Box}(n) = 0$  for  $n \leq 3$ ,  $S_{\Box}(4) = S_{\Box}(5) = 1$ ,  $S_{\Box}(6) = 2$ ,  $S_{\Box}(7) = 3$ ,  $S_{\Box}(8) = 4$ ,  $S_{\Box}(9) = 6$ ,  $S_{\Box}(10) = 7$ ,  $S_{\Box}(11) = 8$ ,  $S_{\Box}(12) = 11$ , and  $S_{\Box}(13) = 13$ . Moreover, for  $n \leq 12$  the extremal examples can be obtained by recursive 2-extension starting from the unit square and are listed in Appendix C.

Proof. The statements are obvious for  $n \leq 4$ . As shown by the examples in Appendix C, the mentioned values can indeed be attained. If there are at least two squares and  $S_{\Box}(\mathcal{P}) = S_{\Box}(\#\mathcal{P})$ , then the values in Table 4 imply  $\#\mathcal{P} = 13$ , so that we can assume the existence of a pair of points that is contained in at least two different squares. By recursively applying Lemma 37 and Lemma 38 we conclude  $\#\mathcal{P}' = \#\mathcal{P}$ .

In order to show that all 13-point sets with 13 squares can be obtained by recursive 2extension starting from the unit square it remains to show  $S_{\Box}(13, \mathcal{P}_{6,2}^{\star}) < 13$ . Starting from the upper bound  $S_{\Box}(n, \mathcal{P}_{6,2}^{\star}) \leq A(n, 6, 4)$ , we remark that  $S_{\Box}(n, \mathcal{P}_{6,2}^{\star})$  is the largest size of a binary code with word length n, minimum Hamming distance 6, and constant weight 4 that can be represented by n (pairwise different) points in the Euclidean plane  $\mathbb{R}^2$  such that the codewords are given by the squares spanned by the point set. In other words, we consider the maximum number of squares spanned by an n-point set such that no pair of points is contained in two different squares.

Trivially we have  $S_{\Box}(n, \mathcal{P}_{6,2}^{\star}) = 0$  for  $n \leq 3$  and  $S_{\Box}(n, \mathcal{P}_{6,2}^{\star}) = 1$  for  $4 \leq n \leq 6$ . It is also easy to find examples showing  $S_{\Box}(7, \mathcal{P}_{6,2}^{\star}) = S_{\Box}(8, \mathcal{P}_{6,2}^{\star}) = 2$  and  $S_{\Box}(9, \mathcal{P}_{6,2}^{\star}) = 3$ , so that the upper bound  $S_{\Box}(n, \mathcal{P}_{6,2}^{\star}) = A(n, 6, 4)$  is attained. Examples showing showing  $S_{\Box}(10, \mathcal{P}_{6,2}^{\star}) \geq 4$ ,  $S_{\Box}(11, \mathcal{P}_{6,2}^{\star}) \geq 5$ ,  $S_{\Box}(12, \mathcal{P}_{6,2}^{\star}) \geq 6$ , and  $S_{\Box}(13, \mathcal{P}_{6,2}^{\star}) \geq 7$  are given in Appendix D.

Example 40. Consider the (realizable) oriented square set

 $S = \{(1, 2, 3, 4), (4, 5, 6, 7), (3, 8, 9, 7), (2, 10, 9, 5)\}$ 

of order 10 and cardinality 4. It can be obtained by 1-extension from the (realizable) oriented square set  $\{(1,2,3,4), (4,5,6,7), (3,8,9,7)\}$  of order 9 and cardinality 3. The, up to similarity, unique representation of S is depicted in Figure 10. Thus, (3,9,4,6) also has to be a square, so that (3,8,9,7) and (3,9,4,6) share two common vertices.

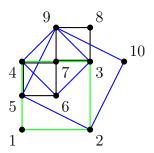


Figure 10: Four squares implying a fifth square.

The approach to check the realizability of S via the linear equation system L(n, S) with the additional inequalities  $z_j \neq z_k$  can be easily extended to also explicitly forbid squares not contained in S. Transforming the formulation over  $\mathbb{C}$  to a formulation over  $\mathbb{R}$  we stay within the setting of Lemma 25, so that we can check the existence of solutions algorithmically.

An easy averaging argument implies the existence of subconfigurations with relatively many squares:

**Lemma 41.** Let  $\mathcal{P}$  be an  $(n, \geq m)$ -configuration. For each  $1 \leq n' < n$  there exists an  $(n', \geq l)$ -subconfiguration, where  $l = \left[m \cdot \binom{n-4}{n'-4} / \binom{n}{n'}\right]$ .

*Proof.* The average number x of squares contained in an n'-subset of  $\mathcal{P}$  satisfies  $\binom{n}{n'} \cdot x / \binom{n-4}{n'-4} = m$ , so that  $x = m \cdot \binom{n-4}{n'-4} / \binom{n}{n'}$ .

For a given *n*-point set  $\mathcal{P}$  let the degree of every vertex be the number of squares in which it is contained,  $\delta_{\min}$  be the minimum, and  $\delta_{\max}$  be the maximum degree.

**Lemma 42.** Let  $\mathcal{P}$  be an (n, m)-configuration and  $\delta_{\min}$  be its minimum degree. Then we have  $\delta_{\min} \leq \lfloor 4m/n \rfloor$ ,  $\delta_{\max} \geq \lceil 4m/n \rceil$ , and there exists an  $(n - 1, m - \delta_{\min})$ -subconfiguration.

*Proof.* For the average degree  $\delta$  we have  $n\delta = 4m$ , so that  $\delta = 4m/n$ . Removing a vertex with degree  $\delta_{\min}$  from  $\mathcal{P}$  gives the desired subconfiguration.

Via exhaustive enumeration of oriented square sets we have verified  $S_{\Box}(10, \mathcal{P}_{6,2}^{\star}) = 4$ ,  $S_{\Box}(11, \mathcal{P}_{6,2}^{\star}) = 5$ , and  $S_{\Box}(12, \mathcal{P}_{6,2}^{\star}) = 6$ , so that Lemma 41 implies  $S_{\Box}(13, \mathcal{P}_{6,2}^{\star}) \leq 9$  and  $S_{\Box}(14, \mathcal{P}_{6,2}^{\star}) \leq 13$ .

Conjecture 43.

$$S_{\Box}(13, \mathcal{P}_{6,2}^{\star}) = 7$$

#### Lemma 44.

$$S_{\Box}(13, \mathcal{P}_{6,2}^{\star}) \le 8$$

*Proof.* Let  $\mathcal{P}$  be a 13-point set such that no pair of squares shares a common pair of vertices. Since the maximum degree of  $\mathcal{P}$  is at least 3, we assume that the squares contained in  $P = \{\{1, 2, 3, 4\}, \{1, 5, 6, 7\}, \{1, 8, 9, 10\}\}$  are spanned by  $\mathcal{P}$ . For  $2 \leq i \leq 13$  let  $C_i := \{1, \ldots, 13\} \setminus \{i\}$  and  $s_i$  be the number of squares of  $\mathcal{P}$  that are not contained in P and whose vertices are contained in  $C_i$ . Since  $S_{\Box}(12, \mathcal{P}_{6,2}^{\star}) = 6$ , we have  $s_i \leq 4$  for  $2 \leq i \leq 10$  and  $s_i \leq 3$  for  $11 \leq i \leq 13$ . Since the vertices of each square are contained in at least 8 of the  $C_i$ , we have

$$S_{\Box}(\mathcal{P}) \le \#P + \left\lfloor \frac{\sum_{i=2}^{13} s_i}{8} \right\rfloor \le 3 + \lfloor 45/8 \rfloor = 8.$$

With this, we can conclude  $S_{\Box}(14, \mathcal{P}_{6,2}^{\star}) \leq \lfloor 14 \cdot 8/10 \rfloor = 11$  from Lemma 41.

#### Conjecture 45.

$$S_{\Box}(16, \mathcal{P}_{6,2}^{\star}) < 20 = A(16, 6, 4)$$

In the following our aim is to find criteria that guarantee a relatively large 2-extension maximal subconfiguration of a point set  $\mathcal{P}$ .

**Definition 46.** Let  $\mathcal{P} \subset \mathbb{R}^2$  be an arbitrary non-empty point set and  $p \in \mathcal{P}$ . A decomposition (at p) is a list of subsets  $\mathcal{P}_i \subseteq \mathcal{P}$ , where  $1 \leq i \leq l$ , whose pairwise intersection equals p and the vertices of each square containing p are contained in one of the  $\mathcal{P}_i$ . The integer  $l \geq 1$  is called the cardinality of the decomposition.

We speak of a 2-extension maximal decomposition if

- for each square s of P the intersection of the set of vertices of s with each P<sub>i</sub> has a cardinality in {0,1,4} and
- all  $\mathcal{P}_i$  can be obtained by recursive 2-extension starting from the unit square.

**Example 47.** Let  $\mathcal{P}$  be the point set from Figure 10. Slightly abusing notation we will use the depicted labels of the points instead of their coordinates. For vertex p = 2, a decomposition of  $\mathcal{P}$  at p is given by  $\mathcal{P}_1 = \{2, 1, 3, 4\}, \mathcal{P}_2 = \{2, 5, 9, 10\}$  with cardinality 2. Another decomposition of  $\mathcal{P}$  at p = 2 is given by  $\mathcal{P}_1 = \{2, 1, 3, 4, 5, 9, 10\}$  with cardinality 1. Note that both decompositions (at p = 2) are also decompositions (at p = 2) of  $\mathcal{P}' = \{1, 2, 3, 4, 5, 9, 10\} \subset \mathcal{P}$ . The latter decomposition is not a 2-extension maximal decomposition of  $\mathcal{P}'$  at p = 2 since  $\mathcal{P}_1$  cannot be obtained by recursive 2-extension starting from the unit square. The first decomposition, the one with cardinality 2, is indeed a 2-extension maximal decomposition of  $\mathcal{P}'$  at p = 2.

Now let  $\mathcal{P}'' = \mathcal{P} \setminus \{1\}$  and p = 9. Two decompositions of  $\mathcal{P}''$  (or  $\mathcal{P}$ ) at p = 9 are given by  $\mathcal{P}_1 = \{9, 3, 4, 6, 7, 8\}, \mathcal{P}_2 = \{9, 2, 5, 10\}$  and  $\mathcal{P}_1 = \{9, 2, 3, 4, 5, 6, 7, 8, 10\}$ , respectively. Note that e.g.  $\mathcal{P}_1 = \{9, 3, 7, 8\}, \mathcal{P}_2 = \{9, 3, 4, 6\}, \mathcal{P}_3 = \{9, 2, 5, 10\}$  is not a decomposition of  $\mathcal{P}''$  (or  $\mathcal{P}$ ) at p = 9. The first decomposition is not a 2-extension maximal decomposition of  $\mathcal{P}''$  at p = 9 while the second is. The unique 2-extension maximal decomposition of  $\mathcal{P}$  at p = 9 is given by  $\mathcal{P}$  itself.

**Definition 48.** Let  $\mathcal{P} \subset \mathbb{R}^2$  be an arbitrary non-empty point set and  $p \in \mathcal{P}$ . The neighborhood of p in  $\mathcal{P}$  is the smallest subset  $\mathcal{P}' \subseteq \mathcal{P}$  that contains p and all vertices of squares of  $\mathcal{P}$  that contain p.

**Example 49.** Let  $\mathcal{P}$  be the point set from Figure 10. Slightly abusing notation we will use the depicted labels of the points instead of their coordinates. The neighborhood of p = 9 in  $\mathcal{P}$  is given by  $\{2, 3, 4, 5, 6, 7, 8, 9, 10\} = \mathcal{P} \setminus \{1\}$  and the neighborhood of p = 2 in  $\mathcal{P}$  is given by  $\{1, 2, 3, 4, 5, 9, 10\}$ .

Let  $\mathcal{P}$  be the neighborhood of a given vertex  $p \in \mathcal{P}$ , i.e., every vertex in  $\mathcal{P} \setminus \{p\}$  is contained in a square that contains p as a vertex. With this, the *neighborhood graph*  $\mathcal{G}$  (of p) consists of the vertices of  $\mathcal{P}$  except the "root vertex" p. Two vertices x, y in  $\mathcal{G}$  form an edge  $\{x, y\}$  (in the graph theory sense) iff p, x, and y are the vertices of a square in  $\mathcal{P}$ . Note that the square corresponding to an edge in  $\mathcal{G}$  is indeed unique (for each edge). Let  $C_1, \ldots, C_r$  be the connected components of  $\mathcal{G}$ . By  $\mathcal{P}_1, \ldots, \mathcal{P}_r$  we denote the subsets of  $\mathcal{P}$  such that the points in  $\mathcal{P}_i$  are given by p and the vertices of  $C_i$ . So, every square of  $\mathcal{P}$  that contains p as a vertex is contained in exactly one of the point sets  $\mathcal{P}_i$ .

**Lemma 50.** Using the above notation, every  $\mathcal{P}_i$  can be obtained by recursive 2-extension starting from every square containing vertex p. Moreover,  $\mathcal{P}_1, \ldots, \mathcal{P}_r$  is a decomposition of  $\mathcal{P}$  at p.

*Proof.* Let  $y \in \mathcal{P}_i \setminus \{p\}$  be an arbitrary vertex and s and arbitrary square in  $\mathcal{P}_i$  that contains p as a vertex. With this, let  $x \neq p$  be an arbitrary vertex of the square s and consider a path  $(x_0, \ldots, x_l)$  in  $C_i$  with  $x_0 = x$  and  $x_l = y$ . For  $0 \leq i < l$  the edge  $\{x_i, x_{i+1}\}$  corresponds to a square  $s_i$  in  $\mathcal{P}_i$  with vertices p,  $x_i$ , and  $x_{i+1}$ . W.l.o.g. we assume that the vertex x and the path in  $C_i$  are chosen in such a way such that  $s = s_0$ . Now we observe that we can reach the square  $s_i$  from the square  $s_{i-1}$  by a 2-extension step for all 0 < i < l. (It may happen that  $s_{i-1} = s_i$ .)

It remains to check that the conditions of Definition 46 are satisfied for  $\mathcal{P}_1, \ldots, \mathcal{P}_r$ .

For an arbitrary point set  $\mathcal{P} \subset \mathbb{R}^2$  and an arbitrary point  $p \in \mathcal{P}$  consider the neighborhood  $\mathcal{P}'$  of p in  $\mathcal{P}$ . Let  $\mathcal{P}_1, \ldots, \mathcal{P}_r$  be a decomposition of  $\mathcal{P}'$  at p according to Lemma 50. The possible candidate for the  $\mathcal{P}_i$  are enumerated in Table 5 including the information of the maximum possible degree of p in  $\mathcal{P}_i$ .

	n	4	6	7	8	8	9	9	9	10	1(	) [	10	10	11	11	. 1	1	11	1:	2 1	2
1	m	1	2	3	3	4	4	5	6	4	5	(	3	7	5	6	7	7	8	5	6	
=	#	1	2	2	5	1	12	1	1	11	1(	) 5	5	1	79	14	1 3	3	2	20	5  7	9
	$\delta_{\max}$	1	2	3	3	3	4	4	4	4	5	ŗ	5	5	5	5	6	5	6	5	6	
$\overline{n}$		12	12	12	1	3	13	1	3	13	13	13	3	14	14	14	E	14	]	14	14	14
m	'	7	8	9	6	5	7	8		9	10	11	1	6	7	8		9	]	10	11	12
#		18	10	2		398	159			11	4	2		64	533	25		131		42	4	4
$\delta_{\rm max}$	ax	6	6	7	- 6		7	7		7	8	8		6	7	7		8	8	3	9	9
	n	15	5	15		15		5	15			15	15			5	16		16		16	
	m	7		8		9		0	11			13	14			-	8	~	9		10	
	#		594	11	91	50		02	77				4	1		59	281	2	214	16	1204	1
	$\delta_{\max}$	7		8		8	8		9	1(		10	8	7	7		8		9		9	
	n	1	6	16		16	16	16	10			16	1	7	17		17		17		17	
	m		1	12		13	14	15	10			18	8		9		10		11		12	
	#		91	160		87	25	3	3	3		1		539	635		4130		209		1107	
_	$\delta_{\max}$			10		10	11	9	9	8		8	8		9		9		10		10	
	n		17	17		17	17		17	17	17		7	17	17	18		18		18		
	m		13	14		15	16		17	18	19		0	21	22	8		9		10		
	#		528	22		121			11	11	3	3		0	1	392		122	93		568	
	$\delta_{\rm ma}$		11	11		12	12		10	10	7	8		0	8	8		9		10		-
n	1		18		18		18		18	18		18		18	18	18	18		18	18	18	18
m	1		12		13		14		15	16		17		18	19	20	21		22	23	24	25
#		840		76		272	122		480			102		63	29	19	7	E.		2	0	1
$\delta_{\max}$	<u>,</u> 1	0	10		11	-	12		12	13	3	13		11	11	11	9	1	10	9	0	9

Table 5: Number of non-similar neighborhood points sets  $\mathcal{P}$  (of vertex 1) that are produced by recursive 2-extension starting from a unit square (and including vertex 1 in each step) per number of points n and squares  $m = S_{\Box}(\mathcal{P})$ .

#### **Theorem 51.** We have $S_{\Box}(14) = 15$ , $S_{\Box}(15) = 17$ , $S_{\Box}(16) = 20$ , and $S_{\Box}(17) = 22$ .

Proof. Examples attaining the stated number of squares are given in Appendix C. Now let  $\mathcal{P}$  be an *n*-point set with  $n \in \{14, 15, 16, 17\}$  and more squares than proposed in our statement. Let  $\widetilde{\mathcal{P}}$  be a 2-extension maximal subconfiguration of maximum cardinality. From Lemma 37 and Lemma 38 we conclude  $\#\widetilde{\mathcal{P}} \leq 6$  if  $n \in \{14, 15\}$  and  $\#\widetilde{\mathcal{P}} \leq 7$  if  $n \in \{16, 17\}$ . From Lemma 42 we conclude  $\delta_{\max} \geq 5$  if  $n \in \{14, 15\}$  and  $\delta_{\max} \geq 6$  if  $n \in \{16, 17\}$ . Now let p be a vertex with maximum degree in  $\mathcal{P}$  and  $\mathcal{P}'$  be the neighborhood of p in  $\mathcal{P}$ . Let  $\mathcal{P}_1, \ldots, \mathcal{P}_r$  be a decomposition of  $\mathcal{P}'$  at p according to Lemma 50. W.l.o.g. we assume  $\#\mathcal{P}_1 \geq \cdots \geq \#\mathcal{P}_r$ . Additionally, we have the conditions  $\#\mathcal{P}_i \leq \#\widetilde{\mathcal{P}}$  for  $1 \leq i \leq r, 1 + \sum_{i=1}^r (\#\mathcal{P}_i - 1) \leq n$ , and  $\sum_{i=1}^r \delta_{\max}(\mathcal{P}_i) \geq \delta_{\max}(\mathcal{P})$ . This leaves only very few choices for  $(\#\mathcal{P}_1, \ldots, \#\mathcal{P}_r)$ , which we enumerate in the following.

- n = 14: (6, 6, 4);
- n = 15: (6, 6, 4);
- n = 16: (7,7), (7,7,4), (6,6,6);
- n = 17: (7,7), (7,7,4), (6,6,6).

If there would exist indices  $1 \leq i, j \leq r$  with  $i \neq j$  and a square s in  $\mathcal{P}'$  such that at least two vertices on s are contained in  $\mathcal{P}_i$  and at least one vertex of s would be contained in  $\mathcal{P}_j$ , then  $\mathcal{P}_i \cup \mathcal{P}_j$  can be obtained by recursive 2-extension starting from the unit square. However, since  $\#(\mathcal{P}_i \cup \mathcal{P}_j) = \#\mathcal{P}_i + \mathcal{P}_j - 1$  this would yield a contradiction to the maximum possible size of  $\widetilde{\mathcal{P}}$ . Thus, we have  $S_{\Box}(\mathcal{P}') \leq \sum_{i=1}^n S_{\Box}(\#\mathcal{P}_i)$ .

For n = 14 we compute  $S_{\Box}(\mathcal{P}) = S_{\Box}(\mathcal{P}') \leq 5 < 16$ . For n = 15 we have  $\delta_{\max} = 5$  and  $S_{\Box}(\mathcal{P}') \leq 5$ . The unique vertex outside of  $\mathcal{P}'$  can have degree at most 5 so that  $S_{\Box}(\mathcal{P}) \leq 5+5 = 10 < 18$ . For n = 16 and  $(\#\mathcal{P}_1, \ldots, \#\mathcal{P}_r) = (7, 7, 4)$  or (6, 6, 6) we have  $S_{\Box}(\mathcal{P}) = S_{\Box}(\mathcal{P}') \leq 7 < 21$ . For n = 16 the only remaining case is  $(\#\mathcal{P}_1, \ldots, \#\mathcal{P}_r) = (7, 7)$  with  $\delta_{\max} = 6$ . Here, each square s not contained in  $\mathcal{P}'$  can have at most one vertex with  $\mathcal{P}_1$  or  $\mathcal{P}_2$  in common since we would obtain a contradiction to  $\#\tilde{P} \leq 7$ . Thus each such square uses at least two out of the three vertices in  $\mathcal{P} \setminus \mathcal{P}'$ , so that

$$S_{\square}(\mathcal{P}) \le S_{\square}(\mathcal{P}') + \frac{3 \cdot \delta_{\max}}{2} \le 6 + 9 = 15 < 21.$$

For n = 17 we have  $\delta_{\max} \leq 7$ . If  $(\#\mathcal{P}_1, \ldots, \#\mathcal{P}_r) = (7, 7, 4)$  or (6, 6, 6), then we have  $S_{\Box}(\mathcal{P}') \leq 7$ , so that

$$S_{\Box}(\mathcal{P}) \le S_{\Box}(\mathcal{P}') + (\#\mathcal{P} - \#\mathcal{P}') \cdot \delta_{\max} \le 7 + 7 = 14 < 23.$$

For n = 17 the only remaining case is  $(\#\mathcal{P}_1, \ldots, \#\mathcal{P}_r) = (7,7)$  with  $\delta_{\max} = 6$ . Here, each square s not contained in  $\mathcal{P}'$  can have at most one vertex with  $\mathcal{P}_1$  or  $\mathcal{P}_2$  in common since we would obtain a contradiction to  $\#\tilde{P} \leq 7$ . Thus each such square uses at least two out of the four vertices in  $\mathcal{P} \setminus \mathcal{P}'$ , so that

$$S_{\Box}(\mathcal{P}) \le S_{\Box}(\mathcal{P}') + \frac{4 \cdot \delta_{\max}}{2} \le 6 + 12 = 18 < 23.$$

Of course we can apply an incomplete 2-extension approach considering point sets with "many" squares for the next iteration only, see Table 6 and Table 9 (in Appendix C).

$\overline{n}$	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18 1	19 20	21
$S_{\Box}(n) \ge$	1	1	2	3	4	6	7	8	11	13	15	17	20	22	25 2	28 32	37
$\overline{n}$	22	23	3 2	24	25	26	27	28	3 29	30	31	32	- 33	34	35	36	37
$S_{\Box}(n) \ge$	40	43	3 4	17	51	56	60	65	5 70	75	81	88	92	97	103	109	117
$\overline{n}$	- 38	3	39		40	41	4	2	43	44	45	4	6	47	48	49	50
$S_{\Box}(n) \ge$	12	23	130	)	137	$14^{-1}$	1 1	51	158	166	175	51	82	189	198	207	216

Table 6: Lower bounds for  $S_{\Box}(n)$  for  $4 \le n \le 50$ .

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## Appendix

Here we list the known equivalence classes of *n*-point sets attaining the best lower bounds known blbk for  $S_{\mathcal{Q}}(n)$  for different variants of  $\mathcal{Q}$ . All of our examples are situated on subsets of the integer grid  $\mathbb{Z}^2$ . By an "x" we denote a chosen point and by "." a grid point that is not part of the point set. The occurring numbers just state the numbers of points and we separate different number of points by "|".

## A Dissimilar point sets for isosceles right triangles

Here we are interested in the (known) similarity classes of point sets that attain  $S_{\mathbb{A}}(n)$  for  $n \leq 14$  or match the lower bounds stated in Table 2. The number of similarity classes is listed in Table 7.

$\overline{n}$		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
#	£ 1	1	1	1	1	2	5	1	1	1	2	2	1	1	1	1	2	2	1	1
n	22	2	23	24	- 4	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39
#	2		1	1	]	L	1	3	2	2	1	2	1	1	1	1	1	1	1	1
				_	n	4	0 4	1	42	43	44	45	46	47	48	49	50			
					#	1	1		1	2	2	3	3	1	2	1	1			

Table 7: Number of known dissimilar point sets attaining blbk for isosceles right triangles.

x.x.	
.x.   xx.   xxx x.x.   x.x.x xxx. xxx .xxx .xx.   xxx	xxx.
xx   xx   xxx   xxx   xxx .xxx   .x.xxxx x.x. xxxx   xxx	XXXX
x.   xx   .x.   .x.   .x. x.x.   x.x.x x.x. xxx	xxx.
	10
	10
	x
.x.x  x.x  x	.x
xx.x.   .x.x   x.x.x.   .x.x.x.   .x.	х.х.
xxx.   .xxxxx.   .xxx. x.x.x   x.x.x.   .xxx.x   x.xxx.x   x.xx	xx.x
xxxx   xxxxx x xxxx   xxxxx .   .xxx.x   x.x.x.   .x.x.x.   .x.x.	х.х.
xxx.   .xxx. xxxx   .xxx. x.x.x   x.x.x.   .x.x  x.x  x	.x
.x  xxx.  xx.x.  x  x  x  x.	х
11   12   13   14   15   16   17	
.x.x   .x.x.x.      x.x	x.x
.x.xx.x	.x.x.x.
x.x.xx.x.x.   .xxxx.x.x.   .xxx.   .xxx.   x.xxx.xxxx	x.xxx.x
.xxx.x x.xxx.x   xxxxx x.xxx.x   xxxxx   .x.x.x. x.xxx.x.	.xxx.x.
x.xxxx.x.x.   xxxxx.x.x.   xxxxx   xxxxx   x.x.x.x xxxxxx	x.x.x.x
.x.x.xx.x   xxxxxx.x   xxxxx   xxxxx   .x.x.x. xxxxx.	.x.x.x.
x.xx   .x.xx   .x.x.   .xxx.  x.x	x.x
18   19   20   21   22	23

I	I	I		x.x			x.x	x.x.x
x.x	x.x	x.x	.x.x.x.	.x.x.x.	.x.x	.x	.x.x.	x x.x.x.x.
.x.x.x.	.x.x.x.	.x.x.x	x.x.x.	x.xxx.x.	х.х.	x.x.	x.x.x	.xx.x.x.x
x.xxx.x	x.xxx.x	x.xxx.x.	.x.xxx.x	. xxxxx . x	.x.x	.x.x	.x.xx	x.x x.xxx.x.
.xxxxx.	.xxxxx.	.xxxxx.x	x.xxxxx.	x.xxx.x.	x.xx	x.x.	x.xxx	.xx.x.x.x
x.x.x.x	x.xxx.x	x.xxx.x.	.x.xxx.x	.x.x.x.	.x.x	.x.x	.x.x.	x.x x.x.x.x.
.x.x.x.	.x.x.x.	.x.x.x	x.x.x.	x.x	х.х.	x.x.	x.x	.xx.x.x.
x.x	x.x	x.x	x.x	x	.x.x	.x	x.	xx
24	25	26	27			I	28	
	I			x.	x	x	.x	x.x
.x.x.x	.x.x.x	x.x.x.	x.x.x	x.x	x	x.	x.x	x.x.x
x.x.x.x	x.x.x.x.	.x.x.x.x.	.x.x.x.	xx.x.	x.x.	.x.x	.x.x.	.x.x.x.x.
.x.x.x.x .	.x.x.x.	x.x.x.x.	x.x.x.x	.x x.x.x	x.x.x	x.x.	x.x.x	x.x.x.x.x
x.xxx.x	x.xxx.x.	.x.xxx.x.	.x.xxx.	xx.xx	x.x.	.x.x	xx.x.	.x.xxx.x.
.x.x.x.x x	.x.x.x.x	x.x.x.x.x	x.x.x.x	.x x.x.x	x	x.x.	x.x.x	x.x.x.x.x
x.x.x.x	x.x.x.x.	.x.x.x.x.	.x.x.x.	xx.x.	x.x.	.x.x	.x.x.	.x.x.x.x.
.x.x.x	.x.x.x	x.x.x.	x.x.x	x.x	x	x.	x.x	x.x.x
x.x	x.x	x.x	x.x.		x	x		x.x
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x.x.x.	I		I	.x.x.x	.x.	.x.x.	x.x.	.x.x.x.x.
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47
      | 48
                    | 49
                           | 50
```

## B Dissimilar point sets attaining the value in Lemma 38

The enumeration of all *n*-point sets with  $n \leq 9$  that can be obtained by 1-extension yields the following point sets attaining  $S_{\square -3\square}(n)$  as mentioned in Lemma 38:

```
| XXX .X. | X.X. XXX. XXX X.X.X XXX.X | X.X.X
   xx | xxx | .x. xxx | .xxx .x. .x. .xx.. .x... | .xxx.
x. | .x. | x.. .x. | ..x. x... x.x ..x.. ..x.. | ..x..
                                               | 7
3 | 4
       | 5
                   6
                   | x.x.. .x...
x.x. x.x.. | x.x.. | .xxx. ..x.x
.xxx .xx.. | .xxx. | ..x.x .xxx.
..x. ..x.x | ..x.x | .x... x.x..
.x....x.... | .x... | ...x.. ....x.
7
           8
                   | 9
```

We remark that the only possible case where  $S_{\mathbb{A}-3\square}(n)$  might be attained a point set that cannot be obtained by 1-extension is given by n = 7 and  $\S_{\mathbb{A}}(\mathcal{P}) = 10$ . However, Lemma 2 then implies that  $\mathcal{P}$  contains a 5-point set  $\mathcal{P}'$  with  $S_{\mathbb{A}}(\mathcal{P}') = 8$  as a subconfiguration. Since  $\mathcal{P}'$  contains a square, we have  $S_{\mathbb{A}-3\square}(\mathcal{P}) \leq 7$ . Thus, the above list is exhaustive.

## C Dissimilar point sets attaining blbk for $S_{\Box}(n)$

Here we list the known equivalence classes of *n*-point sets attaining blbk for  $S_{\Box}(n)$  mentioned in Table 8 for  $n \leq 100$ . Here the numbers just state the numbers of points and we separate different number of points by "|".

$\overline{n}$	4	6	7 8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
#	1	2	2 2	1	1	5	1	1	2	2	2	4	3	5	1	1	1	3
$\overline{n}$	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41
#	1	1	1	2	2	1	4	1	1	2	4	2	3	1	1	2	1	2
$\overline{n}$	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59
#	2	6	2	1	1	7	2	1	4	1	1	1	2	1	5	3	1	1
$\overline{n}$	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77
#	1	1	9	3	2	2	1	4	1	1	2	4	2	8	1	3	2	1
$\overline{n}$	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95
#	3	4	2	4	3	2	2	1	4	1	1	1	2	2	1	2	2	5
						$\overline{n}$	n 9	6 9	7 9	8 9	9 1	00						
							≠ 1	1	1	2	2							

Table 8: Number of known pairwise dissimilar point sets attaining blbk for  $S_{\Box}(n)$ .

xx.   xxx xx.   .xx. xxx   xxx   xxx.   xxxx xxxx xxxx xxxx .xxx.
xx   xxx xxx   xxx xxx   xxxx   xxx   xxxx   xxxx xxx. xxxx xxx. xxxx
xx   xxx .x.   .xxx   .xx. xx.   xxx   xxx.   .xxx
4 6 7 8 9 10 11
.xx.   xxx.   xxx. xxxx   .xxx. xxxx   .xxx. xxxx   xxxx. xxxxx xxxx. xxxx.
xxxx   xxxx   xxxx x xxxx   xxxxx xxxx   xxxxx xxxx xxxx xxxx xxxxx xxxxx xxxxx xxxx
xxxx   xxxx   xxxx xxxx   xxxx xxxx   xxxxx   xxxxxxx. xxxx xxxx
.xx.   .xx.   .xxx .xx.   .xxx. xxx.   .xxx. xxxx  xxxxxx. xxxx.
12   13   14   15   16   17
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$\overline{n}$	51	52	53	54	55	56	57	58	59	60	61	62	63
$S_{\Box}(n) \ge$	226	237	245	254	263	272	282	293	303	314	324	334	346
$\overline{n}$	64	65	66	67	68	69	70	71	72	73	74	75	76
$S_{\Box}(n) \ge$	358	370	382	394	407	421	431	442	454	466	480	493	507
$\overline{n}$	77	78	79	80	81	82	83	84	85	86	87	88	89
$S_{\Box}(n) \ge$	521	535	549	564	578	593	608	623	638	653	669	686	700
$\overline{n}$		90	91	92	93	94	95	96	97	98	99	100	
C (	$\sim (\sim$	715	791	719	765	782	700	017	836	853	870	887	

Table 9: Lower bounds for  $S_{\Box}(n)$  for  $51 \le n \le 100$ .

## D Point sets with many squares such that no pair of points is contained in two different squares

Point sets showing  $S_{\Box}(10, \mathcal{P}_{6,2}^{\star}) \geq 4$ ,  $S_{\Box}(11, \mathcal{P}_{6,2}^{\star}) \geq 5$ ,  $S_{\Box}(12, \mathcal{P}_{6,2}^{\star}) \geq 6$ , and  $S_{\Box}(13, \mathcal{P}_{6,2}^{\star}) \geq 7$  are given by:

x.xx.. .x.x.. ....x. xxxx.. .xxx. .xx.. .xx.. x..x. x.x.. . . . . . . x.xx. .x.x. .xx.. x.x.. .x... .x...x ....x. .xx.x xx.x.. x.xx. xx.x. .x... xx.x. x.x.x .x.xx ....xx x..x.. .x...x xxx.. ..xx. xxx.. xx...x x..x. x.xx. .xx.. ..x.. ..xx. .x.x. ..x.. ...x.. ...x.. .x... .x... 10

			I	.xxxx
	xxxx	.x.xx	.xxxx	x.
x.xx.	X.	x.	x.x  x.	.xx  xx
xx.	.xx	xx	.xx.x  xx	.xxx.   .xx
			xxx   .xx	
			x.   xx	
.x	x	x	.xx  x	.xx  x
11			12	13

## E Point sets with many squares determining the same directions

In the introduction we mentioned the problem of the maximum number  $S_{\parallel \square}(n)$  of axis-parallel squares spanned by n points. We may also say that the counted squares determine the same directions. Looping over the point sets that can be obtained by recursive 2-extension gives the lower bounds  $S_{\parallel \square}(4) \ge 1$ ,  $S_{\parallel \square}(6) \ge 2$ ,  $S_{\parallel \square}(7) \ge 2$ ,  $S_{\parallel \square}(8) \ge 3$ ,  $S_{\parallel \square}(9) \ge 5$ ,  $S_{\parallel \square}(10) \ge 5$ ,  $S_{\parallel \square}(11) \ge 6$ ,  $S_{\parallel \square}(12) \ge 8$ ,  $S_{\parallel \square}(13) \ge 8$ ,  $S_{\parallel \square}(14) \ge 9$ ,  $S_{\parallel \square}(15) \ge 11$ ,  $S_{\parallel \square}(16) \ge 14$ , and  $S_{\parallel \square}(17) \ge 14$ :

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