Plane point sets with many squares

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Abstract

How many squares are spanned by n points in the plane? Here we study the corresponding maximum possible number $S_{\square}(n)$ of squares and determine the exact values for all $n \le 16$. For $17 \le n \le 100$ we give lower bounds for $S_{\square}(n)$ and state several conjectures. Besides that a few preliminary structural results are obtained.

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 [10]. Besides being now a classical problem in combinatorial geometry there are connections to pattern recognition problems, see e.g. [4] 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), a famous open problem introduced by Erdős [9]. The best upper bound known still is $O\big(n^{4/3}\big)$ [17], with a recent constant factor improvement, see [3].[1] From that we can conclude $C_{\mathcal{Q}}(n) \in O\big(n^{4/3}\big)$ and all congruent copies of $\mathcal{Q}$ can be found in $O\big(\#\mathcal{Q} \cdot n^{4/3} \log n\big)$ time, see [4] for more details. For $S_{\mathcal{Q}}(n)$ we have an upper bound of $n(n-1)$ and quadratic lower bound if $\mathcal{Q}$ contains only algebraic points [8]. 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 $O\big(\#\mathcal{Q} \cdot n^2 \log n\big)$ time, see e.g. [4]. However, the existence of $\lim\limits_{n\to\infty} S_{\mathcal{Q}}(n)$ is unknown for all non-trivial sets $\mathcal{Q}$. Here we want to study the maximum number $S_{\square}(n)$ 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 $S_{\square}(n)$ for the cases where n is rather small. Taking the points of an $m \times m$ integer grid gives $\liminf\limits_{n\to\infty} \frac{S_{\square}(n)}{n^2} \ge \frac{1}{12}$ (see sequence A002415 for the precise counts of squares). Taking the integer points inside circles of increasing radii gives $\liminf\limits_{n\to\infty} \frac{S_{\square}(n)}{n^2} \ge \frac{1-\frac{2}{\pi}}{4} > \frac{1}{11.008}$, see Theorem 5.3. Denote the maximum number of right isosceles triangles in an n-point set by $S_{\triangle}(n)$ and observe that each square consists of four such

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[1] This upper bound applies to all strictly convex norms, not just Euclidean distance, and can in fact be attained for certain special norms, see [19, 18].

triangles. With this, the upper bound $S_{\triangle}(n) \le \left\lfloor \frac{2}{3}(n-1)^2 - \frac{5}{3} \right\rfloor$ from [2] gives $\limsup\limits_{n\to\infty} \frac{S_\square(n)}{n^2} \le \frac{1}{6}$. In Proposition 4.33 we will show $\limsup\limits_{n\to\infty} \frac{S_\square(n)}{n^2} \le \frac{1}{8}$.

Of course similar problems can be considered in higher dimensions or with different metrics [6]. 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. [20, Theorem 1]. For results on repeated angles see e.g. [15]

The remaining part is structured as follows. In Section 2 we summarize a lot of observations, notations, and examples. The approach of constructing point sets by recursively adding further points is studied in depth in Section 3. Those parts may eventually lay the basis for further investigations. Readers interested in concrete results only are provided the following shortcuts. 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 3.17 and its direct proof stated in Remark 3.18. An explicit upper bound on the necessary grid size is stated in Proposition 3.22. 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 3.6 and Definition 3.7. With this, the determination of $S_\square(n)$ becomes a finite computational problem, cf. Proposition 3.25. Since even the number of similarity classes of point sets that can be obtained by recursive 2-extension gets large for small parameters, see Table 3.4, we determine the exact values of $S_\square(n)$ for $n \le 16$ via exhaustive 2-extension combined with a few mathematical tools in Section 4 Constructions for point sets with many squares are the topic of Section 5. The special case where each pair of squares is allowed to contain at most one common vertex is briefly discussed in Section 6. In Appendix A we list all known similarity classes of n-point sets with $n \le 100$ that attain the currently best lower bound known for the number of squares. For the corresponding counts, see Table 3.5.

A final warning and invitation. The present text is by no means a thorough and completed investigation of the problem of point sets with many squares. It is merely a collection ideas and their possible formalizations. It may turn out in the end that some of our notions are not needed or can be replaced by more appropriate concepts. Some approaches may be blind alleys. Nevertheless we hope that the present text may serve as a suitable starting point for further investigations. Everybody is warmly invited to share thoughts.[2]

2 Preliminaries

By definition an n-point set $\mathcal{P}$ is a subset of $\mathbb{R}^2$ of cardinality $\#\mathcal{P} = n$. By $S_\square(\mathcal{P})$ 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 2.1. Here we have also depicted the squares contained in the point set. By convention $\mathcal{P}^i_{n,m}$ will always denote an n-point set with $S_\square(\mathcal{P}^i_{n,m}) = m$, where i is an index distinguishing non-similar point sets. The set of points of a single (unit) square is denoted by $\mathcal{P}^1_{4,1}$; for other examples see Figure 2.1. For easier reference we label the points from 1 to n.

If situated on the integer grid, there exists a smallest circumscribing $a \times b$-grid and we may also use an ASCII art representation using "x" for chosen grid points and "." otherwise. In the

[2] At `https://www.overleaf.com/5434274833vmtzqpfthcsm` the present document can be edited or extended directly. Of course, also a post to the Sequence Fans Mailing List or a private email is an option being more low-threshold.

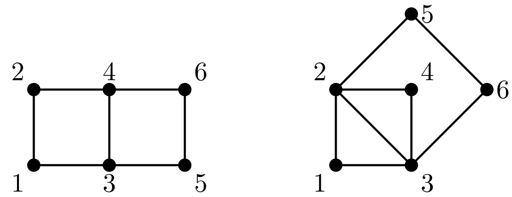

Figure 2.1: Two non-similar point sets $\mathcal{P}_{6,2}^1$ and $\mathcal{P}_{6,2}^2$ consisting of 6 points and 2 squares.

labeled version we replace the “x” by the corresponding numbers, or letters “A” to “Z” for the integers 10 to 35. In this compact notation the two point sets from Figure 2.1 are given by:

```
      .x.           .5.
xxx   xxx     246   246
xxx   xx.     135   13.
```

n	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
$S_\Box(n) \geq$	1	1	2	3	4	6	7	8	11	13	15	17	20	22	25	28	32	37
n	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37		
$S_\Box(n) \geq$	40	43	47	51	56	60	65	70	75	81	88	92	97	103	109	117		
n	38	39	40	41	42	43	44	45	46	47	48	49	50					
$S_\Box(n) \geq$	123	130	137	144	151	158	166	175	182	189	198	207	216					

Table 2.1: Lower bounds for $S_\Box(n)$ for $4 \leq n \leq 50$.

We also mix both ASCII art notations in order to represent a sequence of point sets. The starting point set $\mathcal{P}_0$ is given by the positions of the “x”. Let $n = \#\mathcal{P}_0$ and l be the largest occurring “integer” (i.e. corresponding to a number or a letter) in the representation. Then for $0 \leq i \leq l$ the point set $\mathcal{P}_i$ is given by the positions of the “x” and the positions of the “integers” at most i. By convention, the integers are chosen such that $\#\mathcal{P}_i = n + i$. With this we can certify the lower bounds in Table 2.1 by just five sequences of point sets:

```
                                          ..xxxx..
                             .6xxx7.      .xxxxxx.
                .GA78B.      5xxxxx8      2xxxxxxx
      ..7..     .931xxC      xxxxxxx      xxxxxxxx
      4xx3.     E5xxxxx      xxxxxx9      xxxxxxxx
435.  xxxx5     F4xxxxx      xxxxxxA      .xxxxxxx
xx26  xxxx6     .6xxxxx      4xxxxx3      .xxxxxx.
xx17  1xx2.     .D2xxx.      .2xxx1.      ...xx1..

4-11  12-19     20-36        37-47        48-50
```

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 2.1 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 2.1. *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 $1 \le i \le 4$, 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* $\{P_1, P_2\}$ *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 2.2.

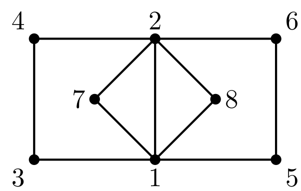

Figure 2.2: Three squares through a pair of points – point set $\mathcal{P}^1_{8,3}$.

Since each square consists of $\binom{4}{2} = 6$ pairs of points, Lemma 2.1 directly implies the upper bound $S_{\square}(n) \le \binom{n}{2}/2 = \frac{n^2}{4} + O(n)$. 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.

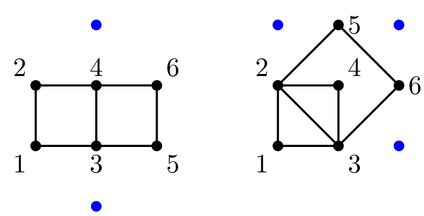

Figure 2.3: 1-extension for the point sets $\mathcal{P}^1_{6,2}$ and $\mathcal{P}^2_{6,2}$.

In Figure 2.3 we have depicted the candidate points in the 1-extension for $\mathcal{P}^1_{6,2}$ and $\mathcal{P}^2_{6,2}$ 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 2.1.(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 2.4. Note that $\mathcal{P}^1_{6,2}$ yields $\mathcal{P}^1_{7,3}$ only, while $\mathcal{P}^1_{6,2}$ produces both 7-point sets.

Even after introducing more powerful constructions of point sets with many squares later on, we will observe that none of them improves upon the lower bounds stated in Table 2.1. As demonstrated, they can all be obtained by recursive 1-extension starting from a few specific point sets. We can turn this approach into an even more systematic one. Consider the grid points in

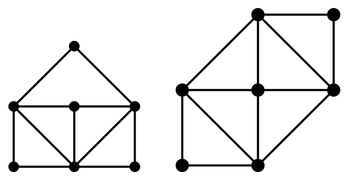

Figure 2.4: Two non-similar point sets $\mathcal{P}^1_{7,3}$ and $\mathcal{P}^2_{7,3}$.

circles with a given center and radius. For increasing radii the achievable numbers of grid points are given in A057961 for center $(0,0)$ and in A057962 for center $(0.5,0.5)$.[3] As a shorthand we write $\texttt{circle}(n)$ for a point set with n grid points obtained that way.[4] In order to treat the cases $n \le 100$ we also use the the following four point sets $\mathcal{S}_i$, where $i \in \{47, 63, 74, 91\}$ refers to the corresponding number of (grid) points.

```
                                       ....xxx....
                          ...xxx...    ..xxxxxxx..
             ...xxx...    .xxxxxxx.    .xxxxxxxxx.
...xx...     ..xxxxxx.    xxxxxxxxx    .xxxxxxxxx.
..xxxxx.     .xxxxxxx.    xxxxxxxxx    xxxxxxxxxxx
.xxxxxxx     xxxxxxxxx    xxxxxxxxx    xxxxxxxxxxx
xxxxxxxx     xxxxxxxxx    xxxxxxxxx    xxxxxxxxxxx
xxxxxxxx     xxxxxxxxx    xxxxxxxxx    .xxxxxxxxxx
.xxxxxxx     .xxxxxxxx    xxxxxxxxx    .xxxxxxxxx.
.xxxxxx.     .xxxxxxx.    .xxxxxxx.    ..xxxxxxx..
..xxxx..     ..xxxxx..    ...xxx...    ....xxxx...
```

Writing $\mathrm{conv}(\{P_1,\dots,P_l\}) \subset \mathbb{R}^2$ for the convex hull of the points $P_1,\dots,P_l$, we can also state $\mathcal{S}_{47}$ as

$$\begin{aligned} & \mathrm{conv}(\{(0,4),(0,3),(1,1),(2,0),(5,0),(7,2),(7,5),(6,6),(4,7),(3,7)\}) \cap \mathbb{Z}^2 \\ = \; & \mathrm{conv}(\{(1.5,0),(5,0),(7,2),(8,5.5),(3.5,7.5),(0,4),(-0.5,3.5)\}) \cap \mathbb{Z}^2, \end{aligned}$$

see Figure 2.5.

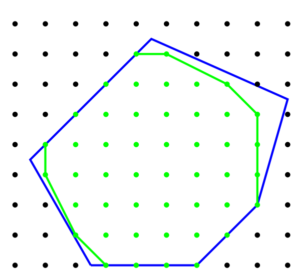

Figure 2.5: $\mathcal{S}_{47}$ as set of grid points inside a convex hexagon or decagon.

[3] Circles with general centers are considered in Section 5.

[4] Of course this construction works for specific choices of n only. For center $(0,0)$ we have $n \equiv 1 \pmod 4$ and for center $(0.5,0.5)$ we have $n \equiv 0 \pmod 4$ as necessary conditions.

Conjecture 2.2. *For $n \geq 6$ every n-point set $\mathcal{P}$ with $S_\square(\mathcal{P}) = S_\square(n)$ is similar to an n-point set $\mathcal{P}' \subset \mathbb{Z}^2$ with* $\operatorname{conv}(\mathcal{P}') \cap \mathbb{Z}^2 = \mathcal{P}'$.

Remark 2.3. *For $9 \leq n \leq 100$ the best lower bounds known for $S_\square(n)$, see Table 2.1 and Table 2.2, can be attained by the recursive application of 1-extension applied to the starting configurations* circle(9), circle(12), circle(21), circle(32), circle(37), $\mathcal{S}_{47}$, circle(52), $\mathcal{S}_{63}$, circle(69), $\mathcal{S}_{74}$, circle(76), circle(80), $\mathcal{S}_{91}$, *and* circle(97).

n	51	52	53	54	55	56	57	58	59	60	61	62	63
$S_\square(n) \geq$	226	237	245	254	263	272	282	293	303	314	324	334	346
n	64	65	66	67	68	69	70	71	72	73	74	75	76
$S_\square(n) \geq$	358	370	382	394	407	421	431	442	454	466	480	493	507
n	77	78	79	80	81	82	83	84	85	86	87	88	89
$S_\square(n) \geq$	521	535	549	564	578	593	608	623	638	653	669	686	700
n	90	91	92	93	94	95	96	97	98	99	100		
$S_\square(n) \geq$	715	731	748	765	782	799	817	836	853	870	887		

Table 2.2: Lower bounds for $S_\square(n)$ for $51 \leq n \leq 100$.

The assumption $n \geq 9$ in Remark 2.3 can of course be removed if we extend the list of starting configurations with the 2×2- (a.k.a. $\mathcal{P}^1_{4,1}$ or `circle`(4)) and the 2×3 grid rectangle. There are also other instances of the construction `circle`(n), like e.g. for $n = 16$, that attain the best lower bound known (`blbk`) for $S_\square(n)$. On the other hand, not all instances of `circle`(n) attain the `blbk`. E.g. the point set `circle`(24) contains 46 squares while a 24-point set with 47 squares is known. In Table 2.3 we perform the comparison between the circle construction and `blbk`. In Section 5 we will see that we can replace the specific point sets $\mathcal{S}_{47}$, $\mathcal{S}_{63}$, $\mathcal{S}_{74}$, and $\mathcal{S}_{91}$ in Remark 2.3 by more nicely structured point sets.

n	4	9	12	13	16	21	24	25	29	32	37	44	45	49
$S_\square$(`circle`(n))	1	6	11	11	20	37	46	50	67	88	117	163	175	204
difference to `blbk`	0	0	0	2	0	0	1	1	3	0	0	3	0	3
n	52	57	60	61	68	69	76	80	81	88	89	96	97	
$S_\square$(`circle`(n))	237	278	311	323	401	421	507	564	568	686	698	808	836	
difference to `blbk`	0	4	3	1	6	0	0	0	10	0	2	9	0	

Table 2.3: Performance of the circle construction for $n \leq 100$.

3 Recursively extending point sets

Lemma 2.1 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 vertices blue, see Figure 3.6 for an example of 2-extension applied to the unit square $\mathcal{P}^1_{4,1}$. The four horizontal or vertical blue lines yield $\mathcal{P}^1_{6,2}$ and the four skewed blue lines yield $\mathcal{P}^2_{6,2}$.

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

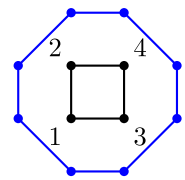

Figure 3.6: 2-extension applied to $\mathcal{P}^1_{4,1}$.

be already contained in the point set. Note that this case does not occur in our example in Figure 3.6 since there exists no 1-extension of the unit square $\mathcal{P}^1_{4,1}$ (that increases the number of points). From Lemma 2.1.(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 $\mathcal{P}^1_{4,1}$, gives us quite some non-similar n-point sets with m squares, see Table 3.4.[5]

n	4	6	7	8	8	9	9	9	10	10	10	10	11	11	11	11	12
m	1	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	1405	159	15	5	15621

n	12	12	12	12	12	12	13	13	13	13	13	13	13	13
m	6	7	8	9	10	11	6	7	8	9	10	11	12	13
#	4729	476	80	11	3	1	90573	15955	1836	482	43	14	1	1

n	14	14	14	14	14	14	14	14	14	14	15
m	6	7	8	9	10	11	12	13	14	15	7
#	1088332	403295	61386	9319	2301	356	83	10	4	2	8143021

n	15	15	15	15	15	15	15	15	15	15
m	8	9	10	11	12	13	14	15	16	17
#	1745837	273037	60632	10982	2693	460	122	26	7	2

n	16	16	16	16	16	16	16	16
m	7	8	9	10	11	12	13	14
#	101999759	44513294	8155822	1445326	360147	69230	19076	3488

n	16	16	16	16	16	16	17	17	17	17
m	15	16	17	18	19	20	8	9	10	11
#	1017	239	55	17	3	2	919429357	215082508	37029433	7414942

n	17	17	17	17	17	17	17	17	17	17	17
m	12	13	14	15	16	17	18	19	20	21	22
#	1419401	281512	52643	10546	2137	511	89	11	2	0	1

Table 3.4: 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 $m = S_\square(\mathcal{P})$.

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 $S_\square(\mathcal{P}) \geq \lceil n/2 \rceil - 1$ for $n \geq 6$. In particular, no 7-point set $\mathcal{P}$ with $S_\square(\mathcal{P}) = 2$ squares will be obtained. Note that the configuration in Figure 3.7 is non-rigid in the sense that we can twist the two squares, connected via vertex 4, without changing the

[5] There are e.g. 1 180 723 093 non-similar 17-point sets. For a publicly available implementation see `https://github.com/hvds/seq/tree/master/A051602`.

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 $S_\square(\mathcal{P})$ of squares, c.f. Section 4, there exists a similar point set that can be obtained by the recursive application of 2-extension starting from $\mathcal{P}^1_{4,1}$. More concretely, we state:

Conjecture 3.1. *For $n \geq 6$ every n-point set $\mathcal{P}$ with $S_\square(\mathcal{P}) = S_\square(n)$ is similar to an n-point set $\mathcal{P}'$ obtained by recursive 2-extension starting from $\mathcal{P}^1_{4,1}$.*

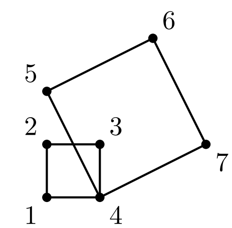

Figure 3.7: A non-rigid 7-point set $\mathcal{P}^1_{7,2}$ with two squares.

Let us briefly discuss the issue of of equivalence classes of point sets with respect to similarity. We have to consider

- translations, i.e. mappings $\mathbb{R}^2 \to \mathbb{R}^2$, $(x, y) \mapsto (x + \alpha, y + \beta)$, where $\alpha, \beta \in \mathbb{R}$ are arbitrary;
- scalings, i.e. mappings $\mathbb{R}^2 \to \mathbb{R}^2$, $(x, y) \mapsto (\lambda x, \lambda y)$, where $\lambda \in \mathbb{R}_{>0}$; and
- reflections, i.e. mappings $\mathbb{R}^2 \to \mathbb{R}^2$, $(x, y) \mapsto (x, y) - 2 \cdot \frac{xu+yv}{u^2+v^2} \cdot (u, v)$, where $u, v \in \mathbb{R}$ with $u^2 + v^2 \neq 1$.

Note that all other similarity transformations, like e.g. rotations, can be expressed by a sequence of the above transformations. The choice $(u, v) = (1, 0)$ is the reflection at the y-axis and $(u, v) = (0, 1)$ corresponds to the reflection at the x-axis. As an example we state that the following five ASCII arts all represent pairwise similar point sets.

```
                              x.x     x...x...x
          .x..      ..x..     .x.     .........
x.x.x     xxx.      .xxx      x.x     ..x...x..
.x.x.     .xxx      xxx.      .x.     .........
x.x.x     ..x.      .x..      x.x     x...x...x
```

We prefer the leftmost as a canonical representation of the point set on the integer grid. More precisely, for each n-point set $\mathcal{P} \subset \mathbb{Z}^2$ the canonical representation with “x”’s and “.”’s arranged in an $a \times b$-matrix is the lexicographically smallest one among those that minimize $a \cdot b$ and b for equal values of $a \cdot b$.

With respect to Conjecture 3.1, Table 3.5 shows the number of known pairwise dissimilar point sets attaining `blbk`. All of these are were obtained by the recursive application of 2-extension only using the best found few thousand point sets for the next iteration. For $n \leq 100$ points they are depicted in Appendix A. While this approach is rather heuristic, we nevertheless conjecture these counts to be exhaustive and challenge the reader to try to find further examples.

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.

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

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

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

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

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

n	96	97	98	99	100
#	1	1	1	2	2

Table 3.5: Number of known pairwise dissimilar point sets attaining `blbk`.

Definition 3.2. *An* incidence structure *is a triple* (P, L, I) *where* P, L *are sets and* $I \subseteq P \times L$ *is the* incidence relation.

Typically the elements of P are called *points* and the elements of L are called *lines*. If we assume $P = \{P_1, \ldots, P_n\}$ and $L = \{L_1, \ldots, L_m\}$ for an incidence structure (P, L, I), then the incidence relation I can be written as an *incidence matrix* $M = (m_{j,i}) \in \{0,1\}^{m \times n}$, where $m_{j,i} = 1$ iff L_j is incident with P_i, i.e., $(P_i, L_j) \in I$. In our application we may consider the incidence structure (P, S, I) given by $P = \{1, \ldots, n\}$, S as a subset of 4-element subsets of P for the squares, and $(p, s) \in I$ iff $p \in s$. Using the labels in Figure 2.1 the corresponding combinatorial description, i.e., (P, S), of the point sets $\mathcal{P}_{6,2}^1$ and $\mathcal{P}_{6,2}^2$ is given by $\big(\{1, \ldots, 6\}, \big\{\{1,2,3,4\}, \{3,4,5,6\}\big\}\big)$ and $\big(\{1, \ldots, 6\}, \big\{\{1,2,3,4\}, \{2,3,5,6\}\big\}\big)$, respectively. Two incidence structures (P, L, I) and (P', L', I') are called *isomorphic* if there exist bijections $\alpha\colon P \to P'$ and $\beta\colon L \to L'$ with $(p, l) \in I$ iff $(\alpha(p), \beta(l)) \in I'$. If we swap the labels 2 and 4, both in P and S, then we see that the combinatorial descriptions of $\mathcal{P}_{6,2}^1$ and $\mathcal{P}_{6,2}^2$ are isomorphic. So, the most natural choice of an incidence structure in our application is too coarse.

Definition 3.3. *A* 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* $\big\{\{v_1, v_2\}, \{v_3, v_4\}\big\}$*, where* $1 \le v_1, v_2, v_3, v_4 \le n$ *are pairwise different, and* $\big(p, \{\,\{v_1, v_2\}, \{v_3, v_4\}\,\}\big) \in I$ *iff* $p \in \{v_1, v_2, v_3, v_4\}$*. We call the elements of* S squares *and also abbreviate* (P, S, I) *by* (P, S) *or just* S *if* P *is given by the union of all vertices contained in the elements of* S*.*

Using our intuitive description of squares with edges and diagonals the interpretation is given as follows. The 2-subsets $\{v_1, v_2\}$ and $\{v_3, v_4\}$ of $\{1, \ldots, n\}$ form the diagonals of a square with vertex set $\{v_1, v_2, v_3, v_4\}$ – the four edges have the vertex sets $\{v_1, v_3\}$, $\{v_1, v_4\}$, $\{v_2, v_3\}$, and $\{v_2, v_4\}$. To simplify the notation, we abbreviate $\{\,\{v_1, v_2\}, \{v_3, v_4\}\,\}$ by $\{v_1v_2, v_3v_4\}$. In our example of the point sets $\mathcal{P}_{6,2}^1$ and $\mathcal{P}_{6,2}^2$, with the labeling given in Figure 2.1, the combinatorial descriptions are given by $\big(\{1, \ldots, 6\}, \big\{\{14, 23\}, \{36, 45\}\big\}\big)$ and $\big(\{1, \ldots, 6\}, \big\{\{14, 23\}, \{35, 26\}\big\}\big)$, respectively. It can be easily checked that the two square sets are non-isomorphic. Note that each bijection α on $\{1, \ldots, n\}$ induces a bijection β on the set of squares via $\beta\left(\{\,\{v_1, v_2\}, \{v_3, v_4\}\,\}\right) := \{\,\{\alpha(v_1), \alpha(v_2)\}, \{\alpha(v_3), \alpha(v_4)\}\,\}$.

Usually, an incidence structure (P, L, I) is called *realizable* (in the Euclidean plane) if it can be modeled by $\#P$ points and $\#L$ lines in $\mathbb{R}^2$ with the usual geometric meaning of incidence between points and lines. An example of an incidence structure (P, L, I) that is not realizable in the Euclidean plane is the Möbius–Kantor configuration with $P = \{1, \ldots, 8\}$, $L = \big\{\{1,2,3\},\{3,4,5\},\{1,5,6\},\{1,4,7\},\{3,6,8\},\{2,4,8\},\{2,6,7\},\{5,7,8\}\big\}$, and $(p,l) \in I$ iff $p \in l$, i.e. eight points and eight lines with three points on each line and three lines through each point. In our context we have to slightly adjust the definition:

Definition 3.4. *A square set (P,S), where $P = \{1,\ldots,n\}$, is called* realizable *if there 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 with diagonals $\{P_a,P_b\}$ and $\{P_c,P_d\}$ for each $\big\{\{a,b\},\{c,d\}\big\} \in S$.*

The square set $\big(\{1,\ldots,8\},\big\{\{15,36\},\{25,46\},\{58,67\}\big\}\big)$ is not realizable since the pair of vertices $\{5,6\}$ would be contained in the three vertex sets $\{1,3,5,6\}$, $\{2,4,5,6\}$, and $\{5,6,7,8\}$ of squares as an edge, which contradicts Lemma 2.1.(b).

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

Lemma 3.5.

(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[6] 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 $z_4 - z_1 = i\,(z_2 - z_1)$.

Using the labels of $\mathcal{P}^1_{6,2}$ in Figure 2.1, the two squares are given by $(1,2,4,3)$ and $(3,4,6,5)$ in clockwise order and by $(1,3,4,2)$ and $(3,5,6,4)$ in counter-clockwise order. Note that right shifts[7] of the 4-tuples preserve the orientation while reading from right to left[8] turns the clockwise ordering $\circlearrowright$ into the counter-clockwise ordering $\circlearrowleft$ and vice versa.

Definition 3.6. *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 $(\{1,\ldots,n\},S)$. For each square $s \in S$ we denote by $\overset{\leftrightarrow}{s}$ the square arising by interchanging the orientation $\circlearrowright$ and $\circlearrowleft$.[9] With this let $\overset{\leftrightarrow}{S} := \left\{\overset{\leftrightarrow}{s} \,:\, s \in S\right\}$ and $\overset{\leftrightarrow}{\mathcal{I}} := \left(P, \overset{\leftrightarrow}{S}\right)$. We also call $\overset{\leftrightarrow}{S}$ and $\overset{\leftrightarrow}{\mathcal{I}}$ the *reoriented square set.*

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 $(\alpha(p),\beta(s)) \in I'$. As for square sets, each

[6] The vector $z_3 - z_1$ rotated by a right angle in counterclockwise order gives the vector $z_1 - z_2$.

[7] For a vector $(a_1,\ldots,a_n)$ the *right-shift* is given by $(a_n,a_1,\ldots,a_{n-1})$ (and the *left-shift* is given by $(a_2,\ldots,a_n,a_1)$). As a canonical representation of the equivalence class of right-shifts (or left-shifts) of a given vector $(a_1,\ldots,a_n) \in \mathbb{R}^n$ we choose the shifted vector $(a_i,\ldots,a_n,a_1,\ldots,a_{i-1})$ where $a_i = \min\{a_1,\ldots,a_n\}$, cf. Definition 3.6.

[8] For a vector $a = (a_1,\ldots,a_n) \in \mathbb{R}^n$ the vector $(a_n,a_{n-1},\ldots,a_2,a_1)$ is denoted by $\overset{\leftrightarrow}{a}$.

[9] More precisely, if $s = (v_1,v_2,v_3,v_4)$, then, by convention, it represents the equivalence class of right-shifts $\{(v_1,v_2,v_3,v_4),(v_4,v_1,v_2,v_3),(v_3,v_4,v_1,v_2),(v_2,v_3,v_4,v_1)\}$, so that $v_1 = \min\{v_1,v_2,v_3,v_4\}$. Applying $\overset{\leftrightarrow}{\cdot}$ to all vectors in the equivalence class of right-shifts yields the set $\{(v_4,v_3,v_2,v_1),(v_3,v_2,v_1,v_4),(v_2,v_1,v_4,v_3),(v_1,v_4,v_3,v_2)\}$ corresponding to $\overset{\leftrightarrow}{s}$. By convention, we choose the canonical representation that minimizes the first entry.

bijection α naturally induces a bijection β. Any pair of bijections $\alpha\colon P \to P$, $\beta\colon S \to S$ with $(p, s) \in I$ iff $(\alpha(p), \beta(s)) \in I$ is called an *automorphism* of (P,S,I). The set of all automorphisms of $\mathcal{I} = (P, S, I)$ is called the *automorphism group* $\mathrm{Aut}(\mathcal{I})$ of $\mathcal{I}$.

Definition 3.7. *An oriented square set (P, S) of order n is called* realizable *if their exist pairwise disjoint points $P_1, \dots, P_n \in \mathbb{R}^2$ 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, i.e., consider the oriented square set $\overset{\leftrightarrow}{S}$ instead of S. Since each pair of diagonals $\{\{v_1, v_2\}, \{v_3, v_4\}\}$ with $v_1 = \min\{v_1, v_2, v_3, v_4\}$ in principle allows the two representatives (v_1, v_3, v_2, v_4) and (v_1, v_4, v_2, v_3) of the two possible equivalence classes of right-shifts, Definition 3.6 refines Definition 3.3, i.e., each square set can correspond to several different oriented square sets.

Given an n-point set $\mathcal{P} \subset \mathbb{R}^2$ and an arbitrary labeling of the points with labels in $\{1, \dots, n\}$, there exists a unique oriented square set (P, S) with $\#S = S_\square(\mathcal{P})$ 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* $\mathcal{P}$. The corresponding statements are also true for square sets.

Example 3.8. *Consider the point set $\mathcal{P}^1_{6,2}$ with labels and coordinates as in Figure 2.1. 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. The bijection α on $\{1, \dots, 6\}$ that swaps 1 with 5 and 2 with 6 is not an automorphism by our definition since the counterclockwise order of the squares is globally changed to clockwise order.*

Remark 3.9. *Let $\mathcal{P}$ be an n-point set and S be the maximal oriented square set of $\mathcal{P}$. If φ is any combination of translations, scalings, and rotations in $\mathbb{R}^2$, then the maximal oriented square set of $\varphi(\mathcal{P})$ is also given by S. If φ is an arbitrary similarity transformation in $\mathbb{R}^2$, i.e., as before but including reflections, then the maximal oriented square set of $\varphi(\mathcal{P})$ is either S or its reorientation $\overset{\leftrightarrow}{S}$.*

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

Definition 3.10. *Let S be an oriented square set of order n. For n complex-valued variables z_j, where $1 \le j \le n$, the linear equation system $L(n, S)$ consists of the $2 \cdot \#S$ equations*

$$z_a - z_b + z_c - z_d = 0 \quad \textit{and} \quad z_d - z_a = i\,(z_b - z_a)$$

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

Lemma 3.11. *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 $1 \le j < k \le n$.*

Example 3.12. *Consider the point set $\mathcal{P}^1_{7,2}$ with coordinates and labels as in Figure 3.7. 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 3.11 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

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

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

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

For $(u,v)=(0,1)$ the point set $\mathcal{P}(u,v)$ is similar to $\mathcal{P}^1_{6,2}$, for $(u,v)=(-1,1)$ we end up with $\mathcal{P}^2_{6,2}$. 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 3.7 correspond to $(u,v)=(-1,2)$.

Remark 3.13. *The point sets $\mathcal{P}(u,v)$ considered in Example 3.12 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 $\mathcal{P}^2_{6,2}$, 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 $S_\square(\mathcal{P}') > \#S$.*

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 3.14. *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 $\left(a_1^j,\ldots,a_l^j\right) \neq \mathbf{0}$.*

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 $\left(a_1^{j_h},\ldots,a_l^{j_h}\right) \neq \mathbf{0}$ for each $1 \leq h \leq f$. Now choose the x_i as l $\mathbb{Q}$-linearly independent numbers. Then we have $\sum_{i=1}^l a_i^{j_h} x_i \neq 0$, since $\{0\} \cup \left\{a_i^{j_h} \,:\, 1 \leq i \leq l\right\} \subset \mathbb{Q}$, for all $1 \leq h \leq f$. □

Example 3.15. *The oriented square set of order 9 given by $S = \big\{(1,3,4,2),(2,5,9,8),(4,7,6,5)\big\}$ is realizable, see Figure 3.8. Over the reals, the solution space is six-dimensional. Note that the realization depicted in Figure 3.8 is on the integer grid. However, it is also possible to choose the side lengths of the three squares as 1, e, and π, 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 $S' = \big\{(1,3,4,2),(2,5,9,8),(4,7,6,5),(3,6,8,10)\big\}$. Over the reals, the solution space of $L(10,S')$ is 4-dimensional. Without proof, we remark that this fact implies that each realization (if there exists any) is rigid. An integer realization is given by

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

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. Without proof, we remark that this fact already implies that S'' is non-realizable. However, the same implication can be deduced from Lemma 3.14.

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 $S_\square(\mathcal{P}') \geq S_\square(\mathcal{P})$. 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:

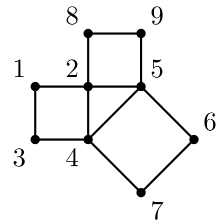

Figure 3.8: A non-rigid 9-point set $\mathcal{P}_{9,3}^1$ with three squares.

Lemma 3.16. *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 λ_i^j for all $j \in S$ and all $i \in \bar{S} := \{1 \le i \le n : i \notin S\}$ such that

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

Note that $A \in \mathbb{Q}^{m\times n}$ implies $\lambda_i^j \in \mathbb{Q}$. Set $\Lambda := \max\left\{\left|\lambda_i^j\right| : i \in \bar{S}, j \in S\right\}$, $\mu := \|Bx\|_\infty$, and $\beta := \max\{|b_{i,j}| : 1 \le i \le n, 1 \le j \le l\}$, 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 $i \in \bar{S}$. For $j \in S$ we set $\tilde{x}_j = \sum_{i \in \bar{S}} \lambda_i^j \tilde{x}_i$, so that

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

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 $B\tilde{x} \neq 0$. $\square$

Theorem 3.17. *For each n-point set $\mathcal{P} \subset \mathbb{R}^2$ there exists an n-point set $\mathcal{P}' \subset \mathbb{Q}^2$ with $S_\square(\mathcal{P}') \ge S_\square(\mathcal{P})$.*

Proof. Let S be the maximal oriented square set of order n of $\mathcal{P}$. By Lemma 3.11 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 $1 \le j < k \le n$. After a suitable transformation we can apply Lemma 3.16 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 $1 \le j < k \le n$. From Lemma 3.11 we then conclude that $\mathcal{P}' := \{z_1', \ldots, n_n'\} \subset \mathbb{Q}(i)$ realizes s. Thus, we have $S_\square(\mathcal{P}') \ge \#S = S_\square(\mathcal{P})$. $\square$

We remark that the proof of Theorem 3.17 and the parameter ε in Lemma 3.16 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 ε in the $\|\cdot\|_\infty$-metric, i.e., $\mathcal{P}'$ arises from $\mathcal{P}$ by a sufficiently small perturbation.

Remark 3.18. *Theorem 3.17 can also be proven directly:*
Let $(z_1, \ldots, z_n) \in \mathbb{C}^n$ be such a configuration (so the z_j's are distinct).There exists a function $s\colon [1, m] \times [1, 4] \to [1, n]$ such that for all $j \in [1, m]$, the set $\{z_{s(j,1)}, z_{s(j,2)}, z_{s(j,3)}, z_{s(j,4)}\}$ spans a square, and these four vertices are ordered counterclockwise. This is equivalent to the system of $2m$ equations $z_{s(j,1)} - z_{s(j,2)} + z_{s(j,3)} - z_{s(j,4)} = 0$, $z_{s(j,4)} - z_{s(j,1)} = i(z_{s(j,2)} - z_{s(j,1)})$. This is a linear system of $2m$ equations in n unknowns with coefficients in the field $\mathbb{Q}(i)$ of Gaussian rationals. By elementary linear algebra, the space of rational solutions of this system is dense in the space of complex solutions. Since there exists a complex solution where all variables are distinct (which is an open condition), there exists a rational solution where all variables are distinct. Such a solution, when properly scaled, represents an n-point grid-configuration spanning at least m squares.

Corollary 3.19. *For each n-point set $\mathcal{P} \subset \mathbb{R}^2$ there exists an n-point set $\mathcal{P}' \subset \mathbb{Z}^2$ with $S_\square(\mathcal{P}') \geq S_\square(\mathcal{P})$.*

Corollary 3.20. *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 $S_\square(\mathcal{P}') = S_\square(\mathcal{P})$.*

Remark 3.21. *Theorem 3.17 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 $S_\square(\mathcal{P}') \geq S_\square(\mathcal{P})$. I.e., one can choose $\mathcal{Q}$ as an isosceles right triangle ⊾.*

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 $\mathcal{Q}$ we have a similar statement replacing the Gaussian rationals (integers) by the Eisenstein rationals (integers).

Proposition 3.22. *For each n-point set $\mathcal{P} \subset \mathbb{R}^2$ there exists an n-point set $\mathcal{P}' \subset \{0, 1, \ldots, \Lambda\}^2$ with $S_\square(\mathcal{P}') \geq S_\square(\mathcal{P})$ and $\Lambda \leq 25^n$.*

Proof. Let S be the maximal oriented square set of order n of $\mathcal{P}$. By Lemma 3.11 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

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

for all $1 \leq j < k \leq n$. Consider the following linear program with variables $x_j, y_j \in \mathbb{R}_{\geq 0}$ 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 $\mathrm{Re}(z_j) - \mathrm{Re}(z_k) \geq 1$ we add the constraint $x_j - x_k \geq 1$ and if $\mathrm{Re}(z_j) - \mathrm{Re}(z_k) \leq -1$ we add the constraint $x_k - x_j \geq 1$, where $1 \leq j < k \leq n$. Similarly, If $\mathrm{Im}(z_j) - \mathrm{Im}(z_k) \geq 1$ we add the constraint $y_j - y_k \geq 1$ and if $\mathrm{Im}(z_j) - \mathrm{Im}(z_k) \leq -1$ we add the constraint $y_k - y_j \geq 1$, where $1 \leq j < k \leq n$. 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 revisit the idea of 1- and 2-extension and generalize it to oriented square sets. This way, we can also treat non-rigid 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 $S_{\square}(n)$ exactly by a finite amount of computation, depending on n – in principle.

The first such algorithm simply loops over all oriented square sets of order n and checks whether they are realizable (using Lemma 3.11 and Lemma 3.14).

In many of the cases a given oriented square set S of order n will be non-realizable, e.g. if there exist $(v_1, v_2, v_3, v_4), (v_5, v_6, v_7, v_8) \in S$ with $\#\{v_1, \ldots, v_8\} \le 5$. Moreover, in many cases there will even exist a (proper) subconfiguration, i.e., an oriented square set S' of order $n' \le n$ with $S' \subsetneq S$, that also is non-realizable (as is the case in the previous example). Of course, every subconfiguration of a given realizable oriented square set S is realizable itself and we can build up S step by step.

Definition 3.23. *Let S be an oriented square set of order n that is a subconfiguration of an oriented square set S' of order n'. We say that S' can be obtained from S by i-extension if $0 \le i \le n' - n$. The i-extensions of S consist of all oriented square sets S' such that S' is an i-extension of S.*

Note that every realizable oriented square set S can be obtained by a sequence $S_0 \to S_1 \to \cdots \to S_l = S$ of 4-extensions starting from the empty oriented square set $S_0 = \emptyset$ of order 0, where all intermediate oriented square sets S_i are realizable for $0 \le i \le l$. We say that S can be obtained from S' by i-extension if such a sequence exists that starts at S', ends at S, and where all intermediate steps are obtained by i-extension. If we just say that S can be obtained by 4-extension, then we implicitly set $S' = S_0$.

Definition 3.24. *An oriented square set S of order n is called* disconnected *if there exists a proper non-empty subset M of $\{1, \ldots, n\}$ such that for each square $(v_1, v_2, v_3, v_4) \in S$ we have $\#\big(\{v_1, v_2, v_3, v_4\} \cap M\big) \in \{0, 4\}$, i.e., the vertices of the square are either all in M or all disjoint to M. We call S* connected *if it is not disconnected.*

Let S be an oriented square set of order n that is disconnected and M be a suitable corresponding subset of $\{1, \ldots, n\}$. Partitioning the squares $s \in S$ into two subsets S_4 and S_0, according to the number of vertices contained in M, we can decompose $(\{1, \ldots, n\}, S)$ into two oriented square sets $\mathcal{I}_1 = (M, S_4)$ and $\mathcal{I}_2 = \big(\overline{M}, S_0\big)$, where $\overline{M} := \{1 \le i \le n : i \notin M\}$. With this we can state that S is realizable iff $\mathcal{I}_1$ and $\mathcal{I}_2$ are. Note that every realizable connected oriented square set $S \ne \emptyset$ can be obtained by a sequence $S_1 \to S_2 \to \cdots \to S_l = S$ of 3-extensions starting from the "unit square" $(\{1, 2, 3, 4\}, (1, 2, 3, 4))$ of order 4, where all intermediate oriented square sets S_i are realizable and connected for $1 \le i \le l$. For $i \le 3$ we say that S can be obtained by i-extension if it can be obtained by i-extension starting from the unit square.

Let us relate our previous notion of i-extension for point sets $\mathcal{P}$ with i-extension for oriented square sets S. So, let $\mathcal{P} \subset \mathbb{R}^2$ be an arbitrary n-point set and $\mathcal{P}' \subseteq \mathbb{R}^2$ be another non-equal n'-point set that arises by direct 2-extension, i.e., without intermediate steps. By S and S' we denote the corresponding maximal oriented square sets of order n of $\mathcal{P}$ and of order n' of $\mathcal{P}'$ respectively. W.l.o.g. we assume that $\mathcal{P} \subset \mathcal{P}'$ and that the points of $\mathcal{P}$ are labeled with $\{1, \ldots, n\}$. For those points of $\mathcal{P}'$ that are contained in $\mathcal{P}$ we assign the same labels and choose new labels in $\{n+1, \ldots, n'\}$ for the others. There exists a square $s' = (v_1, v_2, v_3, v_4) \in S' \backslash S$ with $\#\big(\{v_1, v_2, v_3, v_4\} \cap \{n+1, \ldots, n'\}\big) = n' - n \le 2$ whose vertices in $\{1, \ldots, n\}$ constitute the 2-extension $\mathcal{P} \to \mathcal{P}'$. In many cases we have $S \cup \{s'\} \subsetneq S'$, i.e., the addition of a new square induces several more squares. In the context of i-extension for oriented square sets we have to add some via additional 0-extensions. If the realizations of S are rigid, i.e., up to similarity there exist unique coordinates, then we can compute unique coordinates for the extension and can directly read off the necessary 0-extensions from there. As noted before, recursively applying 2-extension stays within the set of oriented square sets whose realizations are rigid. This changes if we consider 3-extension, where we have to represent the set of possible realizations via solution spaces of linear inequality systems, see Lemma 3.11 and Lemma 3.14. 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. [5, Section 5.1] or [16].

Proposition 3.25. *Each connected (realizable) oriented square set can be obtained by* 3*-extension from* $\mathcal{P}^1_{4,1}$.

Since the numbers in Table 3.4 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 Section 4 we sketch a few preliminary ideas how to 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 Determination of exact values of $S_\square(n)$ for small n

The exact values of $S_{\triangle}(n)$ for $n \le 9$ were determined recently, see [2]. For the unit distance problem, the exact values of $C_{\{q_1,q_2\}}(n)$ and the attaining extremal configurations are known since the diploma thesis of Schade [16] for $n \le 14$ and $C_{\{q_1,q_2\}}(15) = 37$ was recently determined in [3]. Here we first classify the extremal configurations attaining $S_\square(n)$ for $n \le 9$ and then determine the exact values of $S_\square(n)$ for $n \le 16$. Not all of the notation introduced in Section 2 and in Section 3 will be necessary for this aim. However, the target is to push these limits a bit further and we will present several preliminary results in this direction.

First we introduce even more notation. For brevity, an n-point set $\mathcal{P} \in \mathbb{R}^2$ with $S_\square(\mathcal{P}) = m$ is also called (n,m)*-configuration* in this section. We also use intuitive notations like $(n, \ge m)$-configuration. As noted in Section 2, any (n,m)-configuration where a pair of points is contained in at least two different squares contains one of the $(6,2)$-configurations $\mathcal{P}^1_{6,2}$ or $\mathcal{P}^2_{6,2}$ as subconfiguration. For arbitrary point sets $\mathcal{F}_1, \ldots, \mathcal{F}_l$ we denote by $S_\square(n; \mathcal{F}_1, \ldots, \mathcal{F}_l)$ the maximum value of $S_\square(\mathcal{P})$ where $\mathcal{P}$ is an n-point set such that no subset of its points is similar to $\mathcal{F}_i$ for an index $1 \le i \le l$. Besides trivial cases like $S_\square\big(n; \mathcal{P}^1_{4,1}\big) = 0$ and $S_\square\big(n; \mathcal{P}^\star_{6,2}, \mathcal{P}^1_{7,2}\big) = \lfloor n/4 \rfloor$, the exact value of $S_\square(n; \mathcal{F}_1, \ldots, \mathcal{F}_l)$ 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. [7] 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 $\#(a \cap b) \le 1$ for all $a, b \in S$ with $a \ne b$. Thus, we have

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

The values $A(n,6,4)$ are known exactly, see [7, Theorem 6], and we list the first few in Table 4.6, cf. sequence A004037. Given the lower bounds from Section 2, we can easily check

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

Table 4.6: The exact values of $A(n,6,4)$ for $n \le 16$.

that $S_\square\big(n;\mathcal{P}^\star_{6,2}\big) = S_\square(n)$ may only be possible if $n \le 4$, $n \in \{13,16\}$, or $n > 100$.[10] The point sets $\mathcal{P}^1_{4,1}$, $\mathcal{P}^1_{7,2}$, and $\mathcal{P}^1_{9,3}$ show $S_\square\big(n;\mathcal{P}^\star_{6,2}\big) = A(n,6,4)$ for $n \le 9$. Example 3.15 shows $S_\square\big(10;\mathcal{P}^\star_{6,2}\big) \ge 4$ and indicates that this lower bound might be tight. We will reconsider the problem in Section 6.

The situation of point sets where each pair of points is contained in at most two different squares can be described by the forbidden configuration $\mathcal{F}_1 = \mathcal{P}^1_{8,3}$. A similar argument to the preceding shows that

$$S_\square\big(n;\mathcal{P}^1_{8,3}\big) \le \left\lfloor n \cdot \left\lfloor \frac{2(n-1)}{3} \right\rfloor /4 \right\rfloor = \frac{n^2}{6} + O(n).$$

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

Lemma 4.1. *Let $\mathcal{P}$ be an $(n, \ge m)$-configuration. For each $1 \le n' < n$ there exists an $(n', \ge l)$-subconfiguration, where $l = \left\lceil m \cdot \binom{n-4}{n'-4} / \binom{n}{n'} \right\rceil$.*

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

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

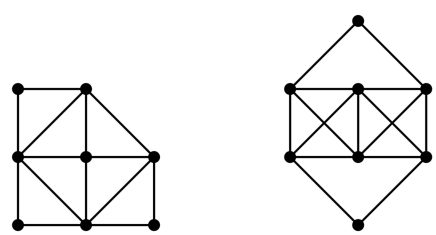

Figure 4.9: Two non-similar point sets $\mathcal{P}^1_{8,4}$ and $\mathcal{P}^2_{8,4}$ consisting of 8 points and 4 squares.

So, let us determine $S_\square(n)$ for $n \le 9$ and classify the attaining point sets. The cases $n \le 5$ are trivial, so that we assume $6 \le n \le 9$. Let $\mathcal{P}$ be an n-point set with $S_\square(\mathcal{P}) = S_\square(n)$. As observed

[10] By a careful analysis of the asymptotics of the circle construction one can show that $S_\square\Big(n;\mathcal{P}^\star_{6,2}\Big) = S_\square(n)$ is impossible for $n > 16$ in general.

before, $\mathcal{P}^1_{6,2}$ or $\mathcal{P}^2_{6,2}$ is a subconfiguration of $\mathcal{P}$. Each $(7,\geq 3)$-configuration can then be obtained by 1-extension giving $\mathcal{P}^1_{7,3}$ and $\mathcal{P}^2_{7,3}$, as discussed earlier. Starting from there, 1-extension yields the two 8-point sets in Figure 4.9, so that Lemma 4.1 implies $S_\square(8) = 4$. If $\mathcal{P}$ is another non-similar $(8,4)$-configuration, then Lemma 4.2 implies that all vertices have degree 2. By applying (direct) 2-extension to $\mathcal{P}^1_{6,2}$ and $\mathcal{P}^2_{6,2}$ we can quickly verify that this is impossible. Applying Lemma 4.1 to a $(9,\geq 6)$-configuration $\mathcal{P}$ yields the existence of an $(8,\geq 4)$-subconfiguration. Thus, $\mathcal{P}$ can be obtained by 1-extension from $\mathcal{P}^1_{8,4}$ or $\mathcal{P}^2_{8,4}$. The resulting unique possibility is depicted in Figure 4.10.

Proposition 4.3. *We have $S_\square(6) = 2$, $S_\square(7) = 3$, $S_\square(8) = 4$, $S_\square(9) = 6$ and the corresponding extremal configurations are given by $\mathcal{P}^1_{6,2}$, $\mathcal{P}^2_{6,2}$, $\mathcal{P}^1_{7,3}$, $\mathcal{P}^2_{7,3}$, $\mathcal{P}^1_{8,4}$, $\mathcal{P}^2_{8,4}$, $\mathcal{P}^1_{9,6}$.*

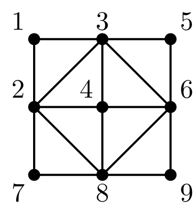

Figure 4.10: The unique point set $\mathcal{P}^1_{9,6}$ consisting of 9 points and 6 squares.

Our next goal is to use the results obtained by exhaustive recursive 2-extension starting from a unit square, see Table 3.4.

Definition 4.4. *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 $\mathcal{P}'$ maximizes $\#\mathcal{P}'$, with respect to this property, then we call $\mathcal{P}'$ 2-extension maximal.*

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

Lemma 4.5. *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*

$$S_\square(\mathcal{P}) \leq S_\square(\mathcal{P}') + S_{\triangle-3\square}(\mathcal{P}\backslash\mathcal{P}') \leq S_\square(n') + S_{\triangle-3\square}(n-n'),$$

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 $\mathcal{P}\backslash\mathcal{P}'$. 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. $\square$

Lemma 4.6. *We have*

(1) $S_{\triangle-3\square}(n) = 0$ *for* $n \leq 2$;

(2) $S_{\triangle-3\square}(3) = 1$;

(3) $S_{\triangle-3\square}(4) = 3$; *and*

(4) $5 \leq S_{\triangle-3\square}(5) \leq 7$.

(5) $S_{\triangle-3\square}(6) \leq 10$.

(6) $S_{\triangle-3\square}(7) \leq 14$.

(7) $S_{\triangle-3\square}(8) \leq 19$.

(8) $S_{\triangle-3\square}(9) \leq 27$.

Proof. The statements are obvious for $n \leq 3$. For $n \geq 4$ we assume w.l.o.g. that one of the right isosceles triangles has vertices $(0,0)$, $(1,0)$, and $(0,1)$. In Figure 4.11 we have depicted this triangle in black. All points that span at least one additional right isosceles triangle with two of the black vertices are marked by a blue circle also stating the resulting increase of the corresponding $(\triangle - 3\square)$-value. Thus, we have $S_{\triangle-3\square}(4) = 3$ with an, up to similarity, unique extremal example. For $\mathcal{P} = \{(0,0),(0,1),(1,0),(0.5,0.5),(0.5,0)\}$ we have $S_{\triangle-3\square}(\mathcal{P}) = 5$ and $\#\mathcal{P} = 5$. Now let $\mathcal{P}$ be an arbitrary 5-point set. If $\mathcal{P}$ contains a square, then we can easily check that an additional point can contribute at most 4 to the $(\triangle - 3\square)$-value. Thus we assume that $\mathcal{P}$ does not contain a square. Since each right isosceles triangle is contained in two 4-subsets of the points and the five 4-subsets of the points each contain at most 3 right isosceles triangles we have

$$5 \leq S_{\triangle-3\square}(\mathcal{P}) \leq \left\lfloor \frac{5 \cdot 3}{2} \right\rfloor = 7.$$

For (4)-(8) we can proceed as follows. Obviously we have $S_{\triangle-3\square}(n) \leq S_{\triangle}(n)$. The exact values of $S_{\triangle}(n)$ and the corresponding attaining similarity classes of points sets were determined in [2] for all $n \leq 9$. For $n \geq 4$ all of these examples contain at least one square, so that $S_{\triangle-3\square}(n) \leq S_{\triangle}(n) - 1$ for $4 \leq n \leq 9$. □

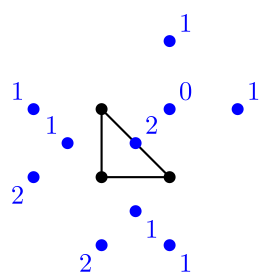

Figure 4.11: Possibilities for triangle-1-extension.

In order to allow slightly stronger statements, let us call an (n,m)-configuration $\mathcal{P}$ *reduced* if each point is contained in at least one square.

Proposition 4.7.

(1) Each reduced $(6, \geq 0)$*-configuration can be obtained by recursive* 2*-extension.*

(2) Each reduced $(7, \geq 3)$*-configuration can be obtained by recursive* 2*-extension.*

(3) Each reduced $(8, \geq 3)$*-configuration can be obtained by recursive* 2*-extension.*

(4) Each reduced $(9, \geq 4)$*-configuration can be obtained by recursive* 2*-extension.*

(5) Each reduced $(10, \geq 6)$*-configuration can be obtained by recursive* 2*-extension.*

Proof. Let $\mathcal{P}$ be an arbitrary reduced (n, m)-configuration matching one of the listed cases. Since $\mathcal{P}$ is reduced we have $S_\square(\mathcal{P}) \geq 1$, i.e., $\mathcal{P}^1_{4,1}$ is contained as a reduced subconfiguration that can be obtained by recursive 2-extension. From $S_\square(n; \mathcal{P}^\star_{6,2}) \leq A(n, 6, 4)$ and the values in Table 4.6 we can conclude that $\mathcal{P}$ contains $\mathcal{P}^1_{6,2}$ or $\mathcal{P}^2_{6,2}$ as a subconfiguration which both are reduced and can be obtained from recursive 2-extension. Now let $\mathcal{P}'$ be a 2-extension maximal subconfiguration of $\mathcal{P}$, so that $6 \leq \#\mathcal{P}' \leq \#\mathcal{P}$. If we can show $\#\mathcal{P}' = \#\mathcal{P}$ in all cases, then our statements are true.

If $\#\mathcal{P} - \#\mathcal{P}' \leq 2$, then Lemma 4.6.(1) yields $S_\square(\mathcal{P}) = S_\square(\mathcal{P}')$, which implies $\#\mathcal{P}' = \#\mathcal{P}$ since $\mathcal{P}$ is reduced. Thus, we can assume $\#\mathcal{P} - \#\mathcal{P}' \geq 3$ and $\#\mathcal{P} \geq 9$ in the following.

Assume $\#\mathcal{P} - \#\mathcal{P}' = 3$. If $\#\mathcal{P} = 9$, then we have $\#\mathcal{P}' = 6$, and $S_\square(\mathcal{P}') \leq 2$, so that Lemma 4.6.(2) yields $S_\square(\mathcal{P}) \leq 3$. If $\#\mathcal{P} = 10$, then we have $\#\mathcal{P}' = 7$, and $S_\square(\mathcal{P}') \leq 3$, so that Lemma 4.6.(2) yields $S_\square(\mathcal{P}) \leq 4$.

If $\#\mathcal{P} - \#\mathcal{P}' \geq 4$, then we have $\#\mathcal{P} = 10$, $\#\mathcal{P}' = 6$, and $S_\square(\mathcal{P}') \leq 2$, so that Lemma 4.6.(3) yields $S_\square(\mathcal{P}) \leq 5$. □

Remark 4.8. *Note that the statements (2)-(4) are tight in the sense that $\mathcal{P}^1_{7,2}$, $\mathcal{P}^1_{4,1} \cup \mathcal{P}^1_{4,1}$, and $\mathcal{P}^1_{9,3}$ are reduced configurations that cannot be obtained by recursive 2-extension. Statement (1) is trivially tight and for statement (5) we do no know yet since e.g. $S_\square(10; \mathcal{P}^\star_{6,2}) \in \{4, 5\}$. In order to prove that each $(11, \geq 8)$-configuration can be obtained by recursive 2-extension, in the vein of the proof of Lemma 4.7, we would need to prove $S_{\llcorner -3\square}(5) = 5$.*

Proposition 4.9. *Each reduced $(11, \geq 7)$-configuration can be obtained by recursive 2-extension.*

Proof. Let $\mathcal{P}$ be an arbitrary reduced $(11, \geq 7)$-configuration and $\mathcal{P}'$ be a 2-extension maximal subconfiguration of $\mathcal{P}$. From $S_\square(n; \mathcal{P}^\star_{6,2}) \leq A(n, 6, 4)$ and the values in Table 4.6 we can conclude $\#\mathcal{P}' \geq 6$. If we can show $\#\mathcal{P}' = 11$ the statement is true.

If $\#\mathcal{P} - \#\mathcal{P}' \leq 2$, then Lemma 4.6.(1) yields $S_\square(\mathcal{P}) = S_\square(\mathcal{P}')$, which implies $\#\mathcal{P}' = \#\mathcal{P}$ since $\mathcal{P}$ is reduced. If $\#\mathcal{P} - \#\mathcal{P}' = 3$, then $\#\mathcal{P}' = 8$ and $S_\square(\mathcal{P}') \leq 4$, so that Lemma 4.6.(2) yields $S_\square(\mathcal{P}) \leq 5$. If $\#\mathcal{P} - \#\mathcal{P}' = 4$, then $\#\mathcal{P}' = 7$ and $S_\square(\mathcal{P}') \leq 3$, so that Lemma 4.6.(3) yields $S_\square(\mathcal{P}) \leq 6$.

It remains to consider the case $\#\mathcal{P}' = 6$, where $S_\square(\mathcal{P}') \leq 2$. If $S_\square(\mathcal{P}) \geq 7$, then the five points in $\mathcal{P} \backslash \mathcal{P}'$ have to be contained in at least five squares, each having at most one vertex in $\mathcal{P}'$. Choosing any three of these five squares and their vertices gives an $(n', 3)$-subconfiguration $\mathcal{P}''$ with $n' \leq 8$. Since $S_\square(6) < 3$, we have $n' \in \{7, 8\}$, so that Proposition 4.7 implies that $\mathcal{P}''$ can be obtained by recursive 2-extension, which contradicts the maximality of $\#\mathcal{P}'$. □

Corollary 4.10. *We have $S_\square(10) = 7$, $S_\square(11) = 8$, and the corresponding extremal configurations can be obtained by recursive 2-extension, i.e. are given in Appendix A.*

Proposition 4.11. *Each $(12, \geq 10)$-configuration can be obtained by recursive 2-extension and $S_\square(13) = 13$.*

Proof. Let $\mathcal{P}$ be a $(12, \geq 10)$-configuration. Lemma 4.1 yields the existence of a $(11, \geq 7)$-subconfiguration $\mathcal{P}_1$. Let $\mathcal{P}_2$ be a reduced $(n', \geq 7)$-subconfiguration of $\mathcal{P}_1$. Since $S_\square(9) < 7$ we have $n' \in \{10, 11\}$, so that $\mathcal{P}_2$ is a reduced $(\geq 10, \geq 7)$-subconfiguration of $\mathcal{P}$. Now let $\mathcal{P}'$ be a 2-extension maximal subconfiguration of $\mathcal{P}$. From the existence of $\mathcal{P}_2$ we conclude $\#\mathcal{P}' \geq 10$, so that we can apply Lemma 4.6.(1) to deduce the first statement.

Let $\mathcal{P}$ be a reduced $(13, \geq 14)$-configuration. Lemma 4.1 yields the existence of a $(11, \geq 7)$-subconfiguration $\mathcal{P}_1$. Let $\mathcal{P}_2$ be a reduced $(n', \geq 7)$-subconfiguration of $\mathcal{P}_1$. Since $S_\square(9) < 7$ we have $n' \in \{10, 11\}$, so that $\mathcal{P}_2$ is a reduced $(\geq 10, \geq 7)$-subconfiguration of $\mathcal{P}$. Now let $\mathcal{P}'$ be a 2-extension maximal subconfiguration of $\mathcal{P}$. From the existence of $\mathcal{P}_2$ we conclude $\#\mathcal{P}' \geq 10$, so that we can apply Lemma 4.6.(1) and Lemma 4.6.(2) to deduce $\#\mathcal{P}' = \#\mathcal{P}$. However, this contradicts Table 3.4, i.e., each 13-configuration obtained by recursive 2-extension contains at most 13 squares. □

Corollary 4.12. *We have* $S_\square(12) = 11$, $S_\square(13) = 13$, *and the extremal* $(12, 11)$*-configurations can be obtained by recursive* 2*-extension, i.e. are given in Appendix A.*

Corollary 4.13. *Conjecture 3.1 is true for* $n \le 12$.

Note that $A(13, 6, 4) = 13$, i.e., in order to prove Conjecture 3.1 for $n = 13$, we have to show $S_\square\big(13, \mathcal{P}^\star_{6,2}\big) < 13$, see Section 6.

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

Definition 4.14. *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* $1 \le i \le l$*, whose pairwise intersection equals* p *and the vertices of each square containing* p *are contained in one of the* $\mathcal{P}_i$*. The integer* $l \ge 1$ *is called the cardinality of the decomposition.*

We speak of a 2-extension maximal decomposition *if*

- *for each square* s *of* $\mathcal{P}$ *the intersection of the set of vertices of* s *with each* $\mathcal{P}_i$ *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 4.15. *Let* $\mathcal{P}$ *be the point set from Figure 6.15. 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 $\mathcal{P}'' = \mathcal{P} \backslash \{1\}$ *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.*

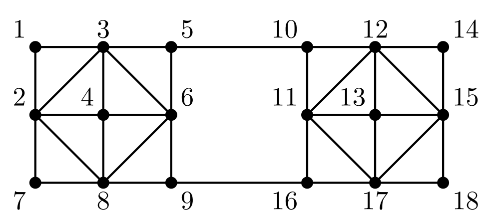

Figure 4.12: An example highlighting possible pitfalls for decompositions of point sets into components that can be obtained by recursive 2-extension.

Remark 4.16. *While the existence of a 2-extension maximal decomposition sounds quite natural we have to be a bit careful, see the 18-point set $\mathcal{P}$ in Figure 4.12. Assume that the smallest distance between two points is one and let $\mathcal{P}_1 \subset \mathcal{P}$ and $\mathcal{P}_2 \subset \mathcal{P}$ be the point sets consisting of the vertices with labels $1, \dots, 9$ and $10, \dots, 18$, respectively. Note that $\mathcal{P}_1$ as well as $\mathcal{P}_2$ can be obtained by recursive 2-extension starting from every square of side length at most $\sqrt{2}$ while this is not the case for the square of side length 2. The square $\{5, 9, 10, 16\}$ meets both disjoint subconfigurations in two vertices each. Nevertheless the largest subconfiguration of $\mathcal{P}$ that can be obtained by recursive 2-extension consists of 13 points.*

Definition 4.17. *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 4.18. *Let $\mathcal{P}$ be the point set from Figure 6.15. 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 $\{2, 3, 4, 5, 6, 7, 8, 9, 10\} = \mathcal{P}\backslash\{1\}$ 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 $\mathcal{P}\backslash\{p\}$ 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 $C_1, \dots, C_r$ be the connected components of $\mathcal{G}$. By $\mathcal{P}_1, \dots, \mathcal{P}_r$ 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 4.19. *Using the above notation, every $\mathcal{P}_i$ can be obtained by recursive 2-extension starting from every square containing vertex p. Moreover, $\mathcal{P}_1, \dots, \mathcal{P}_r$ is a decomposition of $\mathcal{P}$ at p.*

Proof. Let $y \in \mathcal{P}_i\backslash\{p\}$ 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 $(x_0, \dots, x_l)$ 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 4.14 are satisfied for $\mathcal{P}_1, \dots, \mathcal{P}_r$. □

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 $\mathcal{P}_1, \dots, \mathcal{P}_r$ be a decomposition of $\mathcal{P}'$ at p according to Lemma 4.19. The possible candidate for the $\mathcal{P}_i$ are enumerated in Table 4.7 including the information of the maximum possible degree of p in $\mathcal{P}_i$.

Lemma 4.20. *Let $\emptyset \neq \mathcal{P} \subset \mathbb{R}^2$ be an arbitrary point set with maximum degree $\delta_{\max}$, $p \in \mathcal{P}$, $\mathcal{P}_1, \dots, \mathcal{P}_l$ be a decomposition of $\mathcal{P}$ at p, and $\mathcal{P}' := \cup_{i=1}^{l} \mathcal{P}_i$. If none of the $\mathcal{P}_i$ can be further extended by 2-extension and $l \leq 3$, then we have*

$$S_{\square}(\mathcal{P}) \leq \sum_{i=1}^{l} S_{\square}(\mathcal{P}_i) + \frac{\#(\mathcal{P}\backslash\mathcal{P}') \cdot \delta_{\max}}{4 - l}.$$

Proof. We have $S_{\square}(\mathcal{P}') = \sum_{i=1}^{l} S_{\square}(\mathcal{P}_i)$. Each square outside of $\mathcal{P}'$ can have at most l vertices in $\mathcal{P}'$, so that at least $4 - l$ vertices have to be contained in $\mathcal{P}\backslash\mathcal{P}'$. □

n	4	6	7	8	8	9	9	9	10	10	10	10	11	11	11	11	12	12
m	1	2	3	3	4	4	5	6	4	5	6	7	5	6	7	8	5	6
#	1	2	2	5	1	12	1	1	11	10	5	1	79	14	3	2	26	79
$\delta_{\max}$	1	2	3	3	3	4	4	4	4	5	5	5	5	5	6	6	5	6

n	12	12	12	13	13	13	13	13	13	14	14	14	14	14	14	14
m	7	8	9	6	7	8	9	10	11	6	7	8	9	10	11	12
#	18	10	2	398	159	41	11	4	2	64	533	251	131	42	4	4
$\delta_{\max}$	6	6	7	6	7	7	7	8	8	6	7	7	8	8	9	9

n	15	15	15	15	15	15	15	15	15	16	16	16	16
m	7	8	9	10	11	12	13	14	15	7	8	9	10
#	1594	1191	500	202	77	41	8	4	1	159	2812	2146	1204
$\delta_{\max}$	7	8	8	8	9	10	10	8	7	7	8	9	9

n	16	16	16	16	16	16	16	16	17	17	17	17	17
m	11	12	13	14	15	16	17	18	8	9	10	11	12
#	591	160	87	25	3	3	3	1	5539	6358	4130	2099	1107
$\delta_{\max}$	9	10	10	11	9	9	8	8	8	9	9	10	10

n	17	17	17	17	17	17	17	17	17	17	18	18	18
m	13	14	15	16	17	18	19	20	21	22	8	9	10
#	528	224	121	40	11	11	3	3	0	1	392	12293	12568
$\delta_{\max}$	11	11	12	12	10	10	7	8	0	8	8	9	10

n	18	18	18	18	18	18	18	18	18	18	18	18	18	18	18
m	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
#	8840	5276	2272	1223	480	227	102	63	29	19	7	5	2	0	1
$\delta_{\max}$	10	10	11	12	12	13	13	11	11	11	9	10	9	0	9

Table 4.7: 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 $m = S_{\square}(\mathcal{P})$.

Proposition 4.21. $S_{\square}(14) = 15$

Proof. Exhaustive 2-extension starting from the unit square yields at most 15 squares for 14 points. Assume that $\mathcal{P} \subset \mathbb{R}^2$ is a 14-point set with $S_{\square}(\mathcal{P}) \geq 16$. Let $\mathcal{M}$ be an arbitrary 2-extension maximal subconfiguration of $\mathcal{P}$. From Lemma 4.5 and Lemma 4.6 we conclude $\#\mathcal{M} \leq 7$. From Lemma 4.2 we conclude $\delta_{\max} \geq 5$ for the maximum degree of $\mathcal{P}$. Let $p \in \mathcal{P}$ be a vertex of maximum degree, $\mathcal{P}'$ be the neighborhood of p in $\mathcal{P}$, and $\mathcal{P}_1, \ldots, \mathcal{P}_l$ be a decomposition of $\mathcal{P}'$ at p as in Lemma 4.19. W.l.o.g. we assume $\#\mathcal{P}_1 \geq \#\mathcal{P}_2 \geq \cdots \geq \#\mathcal{P}_l$. Using the data in Table 4.7 we conclude that the only possible choices for $(\#\mathcal{P}_1, \#\mathcal{P}_2, \ldots, \#\mathcal{P}_l)$ with $1 + \sum_{i=1}^{l} (\#\mathcal{P}_i - 1) \leq 14$ and $\#\mathcal{P}_1 \leq 7$ that can attain a degree of at least 5 at vertex p are given by

(1) $(7, 7)$;

(2) $(7, 6)$; and

(3) $(6, 6, 4)$.

Thus, we have $\delta_{\max} \leq 6$. Now let $\tilde{\mathcal{P}}_1, \ldots, \tilde{\mathcal{P}}_t$ be an arbitrary decomposition of $\mathcal{P}$ at p. If $t = 2$ and $\left(\#\tilde{\mathcal{P}}_1, \#\tilde{\mathcal{P}}_2\right) = (7, 7)$, then, using $\#\mathcal{M} \leq 7$, we conclude that the $\tilde{\mathcal{P}}_i$ are 2-extension maximal. Applying Lemma 4.20 gives

$$S_{\square}(\mathcal{P}) \leq S_{\square}(\tilde{\mathcal{P}}_1) + S_{\square}(\tilde{\mathcal{P}}_2) + \frac{1}{\delta_{\max}} 2 \leq 3 + 3 + 3 = 9 < 16,$$

a contradiction. So, we have $(\#\mathcal{P}_1, \#\mathcal{P}_2) \neq (7, 7)$ and $\delta_{max} = 5$. If $t = 2$ and $\left(\#\tilde{\mathcal{P}}_1, \#\tilde{\mathcal{P}}_2\right) = (7, 6)$, then we conclude that the $\tilde{\mathcal{P}}_i$ are 2-extension maximal so that Lemma 4.20 yields a contradiction. In case (3) we have $\#\mathcal{P}' = 14$ and $S_{\square}(\mathcal{P}_1) + S_{\square}(\mathcal{P}_2) + S_{\square}(\mathcal{P}_3) \leq 5$. Now assume that there is an additional square s outside of the $\mathcal{P}_i$. So there exist indices $1 \leq j, h \leq 3$ such that the vertices of s meet $\mathcal{P}_j$ in at least two points and $\mathcal{P}_h$ in at least one point x. Thus we can apply 2-extension with the square s to $\mathcal{P}_j$. The resulting point set contains the pair $\{p, x\}$, so that also all points of $\mathcal{P}_h$ can be reached by 2-extension, see Lemma 4.19. Thus $\mathcal{M}' = \mathcal{P}_j \cup \mathcal{P}_h$ can be obtained by recursive 2-extension starting from the unit square. However, $\#\mathcal{M}' > 7$ – contradiction. $\square$

Proposition 4.22. $S_{\square}(15) = 17$

Proof. Exhaustive 2-extension starting from the unit square yields at most 17 squares for 15 points. Assume that $\mathcal{P} \subset \mathbb{R}^2$ is a 15-point set with $S_{\square}(\mathcal{P}) \geq 18$. Let $\mathcal{M}$ be an arbitrary 2-extension maximal subconfiguration of $\mathcal{P}$. From Lemma 4.5 and Lemma 4.6 we conclude $\#\mathcal{M} \leq 8$. From Lemma 4.2 we conclude $\delta_{\max} \geq 5$ for the maximum degree of $\mathcal{P}$. Let $p \in \mathcal{P}$ be a vertex of maximum degree, $\mathcal{P}'$ be the neighborhood of p in $\mathcal{P}$, and $\mathcal{P}_1, \ldots, \mathcal{P}_l$ be a decomposition of $\mathcal{P}'$ at p as in Lemma 4.19. W.l.o.g. we assume $\#\mathcal{P}_1 \geq \#\mathcal{P}_2 \geq \cdots \geq \#\mathcal{P}_l$. Using the data in Table 4.7 we conclude that the only possible choices for $(\#\mathcal{P}_1, \#\mathcal{P}_2, \ldots, \#\mathcal{P}_l)$ with $1 + \sum_{i=1}^{l} (\#\mathcal{P}_i - 1) \leq 15$ and $\#\mathcal{P}_1 \leq 8$ that can attain a degree of at least 5 at vertex p are given by

(1) $(8, 8)$;

(2) $(8, 7)$;

(3) $(8, 6)$;

(4) $(7,7)$;

(5) $(7,6)$;

(6) $(7,6,4)$; and

(7) $(6,6,4)$;

Thus, we have $\delta_{\max} \le 6$. Now let $\tilde{\mathcal{P}}_1, \ldots, \tilde{\mathcal{P}}_t$ be an arbitrary decomposition of $\mathcal{P}$ at p. If $t = 2$ and $\left(\#\tilde{\mathcal{P}}_1, \#\tilde{\mathcal{P}}_2\right) = (8,8)$, then, using $\#\mathcal{M} \le 8$, we conclude that the $\tilde{\mathcal{P}}_i$ are 2-extension maximal. Applying Lemma 4.20 gives

$$S_{\Box}(\mathcal{P}) \le S_{\Box}(\tilde{\mathcal{P}}_1) + S_{\Box}(\tilde{\mathcal{P}}_2) + \frac{1}{\delta_{\max}} 2 \le 4 + 4 + 3 = 11 < 18,$$

a contradiction. Similarly we exclude the cases (2)-(5).

For the remaining cases (6) and (7) assume that there is an additional square s outside of the $\mathcal{P}_i$. (Note that $S_{\Box}(\mathcal{P}_1) + S_{\Box}(\mathcal{P}_2) + S_{\Box}(\mathcal{P}_3) \le 6$.) Since $\#\mathcal{P}' \ge 14$, there exist indices $1 \le j, h \le 3$ such that the vertices of s meet $\mathcal{P}_j$ in at least two points and $\mathcal{P}_h$ in at least one point x. Thus we can apply 2-extension with the square s to $\mathcal{P}_j$. The resulting point set contains the pair $\{p, x\}$, so that also all points of $\mathcal{P}_h$ can be reached by 2-extension, see Lemma 4.19. Thus $\mathcal{M}' = \mathcal{P}_j \cup \mathcal{P}_h$ can be obtained by recursive 2-extension starting from the unit square. However, $\#\mathcal{M}' > 8$ – contradiction. $\Box$

Proposition 4.23. $S_{\Box}(16) = 20$

Proof. Exhaustive 2-extension starting from the unit square yields at most 20 squares for 16 points. Assume that $\mathcal{P} \subset \mathbb{R}^2$ is a 16-point set with $S_{\Box}(\mathcal{P}) \ge 21$. Let $\mathcal{M}$ be an arbitrary 2-extension maximal subconfiguration of $\mathcal{P}$. From Lemma 4.5 and Lemma 4.6 we conclude $\#\mathcal{M} \le 8$. From Lemma 4.2 we conclude $\delta_{\max} \ge 6$ for the maximum degree of $\mathcal{P}$. Let $p \in \mathcal{P}$ be a vertex of maximum degree, $\mathcal{P}'$ be the neighborhood of p in $\mathcal{P}$, and $\mathcal{P}_1, \ldots, \mathcal{P}_l$ be a decomposition of $\mathcal{P}'$ at p as in Lemma 4.19. W.l.o.g. we assume $\#\mathcal{P}_1 \ge \#\mathcal{P}_2 \ge \cdots \ge \#\mathcal{P}_l$. Using the data in Table 4.7 we conclude that the only possible choices for $(\#\mathcal{P}_1, \#\mathcal{P}_2, \ldots, \#\mathcal{P}_l)$ with $1 + \sum_{i=1}^{l} (\#\mathcal{P}_i - 1) \le 16$ and $\#\mathcal{P}_1 \le 8$ that can attain a degree of at least 6 at vertex p are given by

(1) $(8,8)$;

(2) $(8,7)$;

(3) $(7,7)$;

(4) $(7,7,4)$;

(5) $(8,6,4)$;

(6) $(7,6,4)$; and

(7) $(6,6,6)$.

Thus, we have $\delta_{\max} \le 7$. Now let $\tilde{\mathcal{P}}_1, \ldots, \tilde{\mathcal{P}}_t$ be an arbitrary decomposition of $\mathcal{P}$ at p. If $t = 2$ and $\left(\#\tilde{\mathcal{P}}_1, \#\tilde{\mathcal{P}}_2\right) = (8,8)$, then, using $\#\mathcal{M} \le 8$, we conclude that the $\tilde{\mathcal{P}}_i$ are 2-extension maximal. Applying Lemma 4.20 gives

$$S_{\Box}(\mathcal{P}) \le S_{\Box}(\tilde{\mathcal{P}}_1) + S_{\Box}(\tilde{\mathcal{P}}_2) + \frac{1}{\delta_{\max}} 2 \le 4 + 4 + 3.5 = 11.5 < 18,$$

a contradiction. Similarly we exclude the cases (2) and (3).

For the remaining cases (4)-(7) assume that there is an additional square s outside of the $\mathcal{P}_i$. (Note that $S_\square(\mathcal{P}_1) + S_\square(\mathcal{P}_2) + S_\square(\mathcal{P}_3) \le 7$.) Since $\#\mathcal{P}' \ge 15$, there exist indices $1 \le j, h \le 3$ such that the vertices of s meet $\mathcal{P}_j$ in at least two points and $\mathcal{P}_h$ in at least one point x. Thus we can apply 2-extension with the square s to $\mathcal{P}_j$. The resulting point set contains the pair $\{p, x\}$, so that also all points of $\mathcal{P}_h$ can be reached by 2-extension, see Lemma 4.19. Thus $\mathcal{M}' = \mathcal{P}_j \cup \mathcal{P}_h$ can be obtained by recursive 2-extension starting from the unit square. However, $\#\mathcal{M}' > 8$ – contradiction. $\square$

Presumably, the upper bounds in Lemma 4.6 are pretty weak and easy to improve if $S_{\triangleright-3\square}(n)$ is studied thoroughly.

Remark 4.24. *To sum up, the results obtained in this section are promising on the one hand. On the other hand, none of the used techniques is fine-tuned at all and even the essential constituents currently aren't worked out properly to yield streamlined proofs. So, currently it's merely a collection of approaches that may be used to determine exact values of $S_\square(n)$ (and similar values $S_{\mathcal{Q}}(n)$). Having the present methods at hand it should be possible to push the limits a bit further, but it seems very likely that additional ideas will be needed rather soon.*

4.1 Experiments with additional definitions and notation

Motivation: Let $\mathcal{P} \subset \mathbb{R}^2$ be an arbitrary n-point set and S its maximal oriented square set. If $\mathcal{P}$ can be obtained from the recursive application of 2-extension starting from the unit square, then all realizations of S are similar to $\mathcal{P}$. We may call such a point set "constructible" and ask for certain kinds of decompositions of a given point set into "constructible" parts that are maximal in a certain sense.

Definition 4.25. *Let $\mathcal{P} \subset \mathbb{R}^2$ be an n-point set and s be a square spanned by the points in $\mathcal{P}$. By $R(\mathcal{P}, s) \subseteq \mathcal{P}$ we denote the largest subset of $\mathcal{P}$ that can be obtained by repeated 2-extension starting from s.*

First we note that $R(\mathcal{P}, s)$ is well defined, i.e., if $\mathcal{P}' \subseteq \mathcal{P}$ and $\mathcal{P}'' \subseteq \mathcal{P}$ can be obtained by repeated 2-extension starting from s and both cannot be further extended, then we have $\mathcal{P}' = \mathcal{P}''$.

Definition 4.26. *Let $\mathcal{P} \subset \mathbb{R}^2$ be an arbitrary n-point set. For any two squares s, s' spanned by $\mathcal{P}$ we write $s \sim s'$ iff $R(\mathcal{P}, s) = R(\mathcal{P}, s')$.*

Lemma 4.27. *For each n-point set $\mathcal{P} \subset \mathbb{R}^2$ the relation $\sim$ is an equivalence relation on the set of squares spanned by $\mathcal{P}$, i.e., $\sim$ partitions the set of squares into equivalence classes $S_1, \dots, S_l$.*

Lemma 4.28. *Let $\mathcal{P} \subset \mathbb{R}^2$ be an arbitrary n-point set and $S_1, \dots, S_l$ its equivalence classes of squares. Let $1 \le i < j \le l$, $s \in S_i$, and $s' \in S_j$. Then we have that s and s' share at most one common vertex.*

Proof. Assume to the contrary that s and s' share at least two common vertices and satisfy $R(\mathcal{P}, s) \ne R(\mathcal{P}, s')$. First we note that all four vertices of s are contained in $R(\mathcal{P}, s')$ and that all four vertices of s' are contained in $R(\mathcal{P}, s)$. So, by definition, if $v \in R(\mathcal{P}, s)$, then we have $v \in R(\mathcal{P}, s')$ and vice versa – contradiction. $\square$

Example 4.29. *Consider the 9-point set $\mathcal{P}_{9,6}^1$ with labels as in Figure 4.10. Here we have two equivalence classes of squares:*

$$\begin{aligned} S_1 &= \big\{\{1,2,3,4\},\{3,4,5,6\},\{2,3,6,8\},\{2,4,7,8\},\{4,6,8,9\}\big\} \\ S_2 &= \big\{\{1,5,7,9\}\big\} \end{aligned}$$

For each $s \in S_1$ we have $R\big(\mathcal{P}^1_{9,6}, s\big) = \{1, \ldots, 9\}$, while $R\big(\mathcal{P}^1_{9,6}, \{1,5,7,9\}\big) = \{1,5,7,9\}$.

Let $s_1, \ldots, s_l$ be an arbitrary representations system of the equivalence classes $S_1, \ldots, S_l$ of squares for a given point set $\mathcal{P} \subset \mathbb{R}^2$. Note that $R(\mathcal{P}, s_1), \ldots, R(\mathcal{P}, s_l)$ is a decomposition of $\mathcal{P}$ into "constructible" parts. As demonstrated in Example 4.29, it can happen that two of these parts share two points

n	4	6	7	8	8	9	9	9	10	10	10	10	11	11	11	11	12	12
m	1	2	3	3	4	4	5	6	4	5	6	7	5	6	7	8	5	6
#	1	2	2	5	1	13	1	1	24	11	1	1	88	14	3	2	205	161
$\delta_{\max}$	1	2	3	3	3	4	4	4	4	5	5	5	5	5	6	6	5	6

n	12	12	12	13	13	13	13	13	13	14	14	14	14	14	14	14
m	7	8	9	6	7	8	9	10	11	6	7	8	9	10	11	12
#	26	11	2	698	237	56	19	6	2	1657	1909	505	192	57	8	6
$\delta_{\max}$	6	6	7	6	7	7	7	8	8	6	7	7	8	8	9	9

Table 4.8: Number of non-similar choices for the $\mathcal{P}_i$ in a 2-extension maximal decomposition $\mathcal{P}_1, \ldots, \mathcal{P}_l$ of the neighborhood of p in $\mathcal{P}$ at p.

Out of the fifteen 8-point sets $\mathcal{P}$ with 3 squares that can be obtained by 2-extension there are five point sets that contain a vertex p whose neighborhood is $\mathcal{P}$ so that they are counted in Table 4.8:

```
                                        .xx.
xx.x     xxx.     xxx.     x.x.x       xxx.
xxx.     .xxx     xxxx     .x.x.       .x.x
.x.x     x.x.     ..x.     x.x.x       ..x.
```

The thirteen $(9,4)$-configurations counted in Table 4.8 are given by

```
                     .xx.  .xx.  x.x.  x.x.  xxx.  xxx.  xxx.  .xx..  .xx..  .xxx.
xxx.  xxxx  .xxx.  xxx.  xxxx  .xxx  .xxx  .x.x  xx.x  xxx.  xxx.x  xxx.x  x.x.x
xx.x  xxx.  xxx.x  .xxx  xx..  x.xx  xxx.  x.x.  x.x.  .x.x  .xx..  xx...  .x.x.
xxx.  .x.x  .x.x.  ..x.  ..x.  .x..  .x..  .xx.  .x..  .x..  ...x.  ...x.  .x...
```

The first point set on the left-hand side is the one that is not counted in Table 4.7, see Figure 4.13.

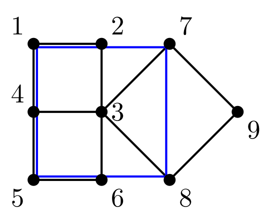

Figure 4.13: The $(9,4)$-configuration counted in table 4.8 but not in Table 4.7.

Lemma 4.30. *Let $\emptyset \neq \mathcal{P} \subset \mathbb{R}^2$ be an arbitrary point set with maximum degree $\delta_{\max}$, $p \in \mathcal{P}$, $\mathcal{P}_1, \ldots, \mathcal{P}_l$ be a 2-extension maximal decomposition of $\mathcal{P}$ at p, and $\mathcal{P}' := \cup_{i=1}^{l} \mathcal{P}_i$. It $l \leq 3$, then we have*

$$S_{\Box}(\mathcal{P}) \leq \sum_{i=1}^{l} S_{\Box}(\mathcal{P}_i) + \frac{\#(\mathcal{P} \backslash \mathcal{P}') \cdot \delta_{\max}}{4 - l}.$$

Proof. We have $S_{\Box}(\mathcal{P}') = \sum_{i=1}^{l} S_{\Box}(\mathcal{P}_i)$. Each square outside of $\mathcal{P}'$ can have at most l vertices in $\mathcal{P}'$, so that at least $4 - l$ vertices have to be contained in $\mathcal{P} \backslash \mathcal{P}'$. $\Box$

4.2 General upper bounds for $S_{\Box}(n)$

Let $\preceq$ 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 4.14.

Lemma 4.31. *Let $a = (0, 0)$, $b_1 = (u, v)$, and $b_2 = (v, -u)$.*

(1) For $0 \leq u < v$ 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 $0 \leq u < v$ 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 $0 < v \leq u$ 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 $0 < v \leq u$ 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.

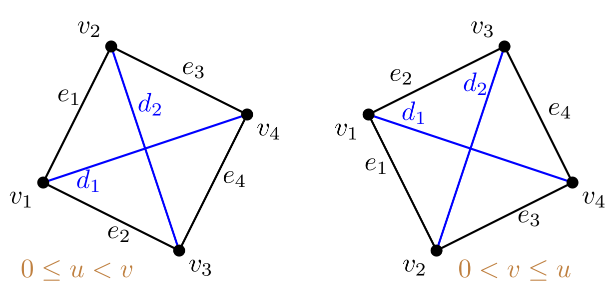

Figure 4.14: The lexicographical ordering of the vertices and the types of pairs of vertices of a square.

Corollary 4.32. *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 4.33. *For $n \geq 1$ we have $S_\square(n) \leq \frac{n^2-1}{8}$.*

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

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

so that

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

□

Remark 4.34. *It seems natural to also consider the x-axis and to decompose the Euclidean plane into four orthants. Potentially, a refined analysis considering the possible cases how the four vertices of a square distribute over the four orthants may yield an improved upper bound for $S_\square(n)$.*

Remark 4.35. *The underlying idea of the proof of Proposition 4.33 fits into the framework of a general method based on ordering relations as introduced in [1, 13].*

4.3 The set of squares sharing a common vertex

Here we want to study the structure of the neighborhood of a given vertex v in an n-point set $\mathcal{P}$ as defined in Definition 4.17. So, let $\mathcal{P}'$ be the neighborhood of v in $\mathcal{P}$, i.e., $\mathcal{P}' \subseteq \mathcal{P}$ is the subset that contains v and all vertices of those squares of $\mathcal{P}$ that contain v. With this, the *neighborhood graph* $\mathcal{G}$ (of v) consists of the vertices of $\mathcal{P}'$ except the "root vertex" v. Two vertices x, y in $\mathcal{G}$ form an edge $\{x, y\}$ (in the graph theory sense) iff v, 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 similar copies of the subsets of $\mathcal{P}$ (or $\mathcal{P}'$) such that the points in $\mathcal{P}_i$ are given by v and the vertices of C_i scaled in such a way such that the smallest distance between v and another point of $\mathcal{P}_i$ equals 1. So, every square of $\mathcal{P}'$ is contained in exactly one of the point sets $\mathcal{P}_i$ (possibly scaled by some factor).

Lemma 4.36. *Using the above notation and assumptions we state: For each point $z \in \mathcal{P}_i$ with $z \neq v$ there exists a non-negative integer j such that $d(z, v) = \sqrt{2}^j$ is the Euclidean distance between z and v in $\mathcal{P}_i$.*

Proof. Let $\mathcal{V}$ be the set of all vertices of C_i that are at the smallest possible distance 1 to v in $\mathcal{P}_i$. This starting set $\mathcal{V}$ is non-empty and the corresponding integer is $j = 0$ in all cases. Now we are recursively adding vertices y to $\mathcal{V}$ till $\mathcal{V}$ equals the vertex set of C_i. More precisely, iteratively choose $y \notin \mathcal{V}$ such that there exists an edge $\{x, y\}$ in $\mathcal{G}$ with $x \in \mathcal{V}$. Since C_i is connected, it is always possible to find such a y and x till all vertices of C_i are contained in $\mathcal{V}$.

By construction, the points v, x, and y form a square s in $\mathcal{P}_i$. If $\{v,x\}$ and $\{v,y\}$ both are edges of s, then we have $d(v,x)=d(v,y)$. If $\{v,x\}$ is an edge and $\{v,y\}$ is a diagonal of s, then we have $d(v,y)=\sqrt{2}\cdot d(v,x)$. If $\{v,x\}$ is a diagonal and $\{v,y\}$ is an edge of s, then we have $d(v,y)=d(v,x)/\sqrt{2}$.

Since $1=\sqrt{2}^0$ is the smallest occurring distance between v and another point in $\mathcal{P}_i$, the claim is proven. $\square$

Let us call the integer j for vertex z in $\mathcal{P}_i$, as in Lemma 4.36, the *level* of z (in $\mathcal{P}_i$). Denote the maximum possible level in $\mathcal{P}_i$ by $d^{(i)}$ and the number of points in $\mathcal{P}_i$ with level j by $l_j^{(i)}$. We may say that v is at level -1 in all $\mathcal{P}_i$. Directly from the construction we conclude:

Lemma 4.37. *Let $1\le i\le r$ be arbitrary. Then, we have $d^{(i)}\ge 1$, $l_{d^{(i)}}^{(i)}\ge 1$, and $l_j^{(i)}\ge 2$ for all $0\le j<d^{(i)}$. The number of vertices of C_i equals $\sum\limits_{j\ge 0} l_j^{(i)}$.*

Now let us upper bound the number of squares in $\mathcal{P}_i$ that contain v as a vertex. Each square s in $\mathcal{P}_i$ that contains v as a vertex uses two vertices x_1,x_2 at some level j and one vertex y at level $j+1$, for some integer $0\le j<d^{(i)}$. The pairs $\{v,x_1\}$ and $\{v,x_2\}$ form edges of the square with vertices $\{v,x_1,x_2,y\}$ while the pair $\{v,y\}$ (as well as $\{x_1,x_2\}$) forms a diagonal. Since each pair of points can be an edge of at most two squares and the diagonal of a most one square we obtain:

Lemma 4.38. *The number of squares in $\mathcal{P}_i$ that contain v as a vertex is at most*

$$\sum_{j=0}^{d^{(i)}-1}\min\left\{l_j^{(i)},l_{j+1}^{(i)}\right\}.$$

Note that we have $l_j^{(i)}\le 4$ for all j due to the inner angles of $\pi/2$. For some special vertices we can further improve this upper bound:

Lemma 4.39. *Let $\mathcal{P}$ be an arbitrary n-point set an v be a vertex on its convex hull with an inner angle ((on the outer k-gon) of strictly less than π. For the neighborhood of v we have $l_{d^{(i)}}^{(i)}=1$ and $l_j^{(i)}=2$ for all $0\le j<d^{(i)}$. Moreover, the number of squares in $\mathcal{P}_i$ that contain v as a vertex equals $d^{(i)}$.*

Corollary 4.40. *Let $\mathcal{P}$ be an arbitrary n-point set an v be a vertex on its convex hull with an inner obtuse angle. If its neighborhood graph $\mathcal{G}$ is connected, i.e., $r=1$, then the degree of v is at most $\lfloor n/2\rfloor-1$.*

Remark 4.41. *Corollary 4.40 implies an upper bound of $S_\square(n)\le\frac{n^2}{4}+O(n)$. However, note that the upper bound of Corollary 4.40 is attained for a connected neighborhood graph $\mathcal{G}$, i.e., $r=1$, with $d^{(1)}=\lfloor n/2\rfloor-1$, where the point set contains distances between points that are an exponential factor apart. One might conjecture that the (normalized) diameter of of point set with many squares should be relatively small.*

Even if we assume $d^{(i)}=1$ for all $1\le i\le r$ we can reach a degree of $\lfloor (n-1)/3\rfloor$, see the subsequent example. The corresponding upper bound would be only $S_\square(n)\le\frac{n^2}{6}+O(n)$, which is still weaker than the one in Proposition 4.33.

Example 4.42. *For $k\ge 1$ consider the point set $\mathcal{P}=\{(i,i)\mid 0\le i\le k\}\cup\{(0,i),(i,0)\mid 1\le i\le k\}$. We have $\#\mathcal{P}=3k+1$ and vertex $(0,0)$ is contained in k squares of $\mathcal{P}$.*

Remark 4.43. *Note that we have $\Omega(\#\mathcal{P})$ points on the x- as well as the y-axis in Example 4.42. One might conjecture that point sets with many points on a line cannot have too many squares. To this end we mention that the maximum number of incidences between m lines and n points in the Euclidean plane is at most $m^{2/3}n^{2/3} + m + n$. In [20, Lemma 1] it was shown that for each set $\mathcal{P}$ of n distinct points in the plane there exists an axis-parallel line that contains at least one and at most $\sqrt{n}$ points of $\mathcal{P}$. Note that there exist at least two vertices satisfying the conditions of Lemma 4.39.*

5 Constructions for point sets attaining `blbk` for $S_\square(n)$

Sets of grid points enclosed by circles are considered in sequences A192493 and A192494. Here we consider circles spanned by three integer grid points $(x_1, y_1) = (0, 0)$, (x_2, y_2), and (x_3, y_3). If the three points are non-collinear the the corresponding radius and center of the circle are uniquely determined. As a corresponding point set we choose all grid points inside such a circle. Up to $n = 100$ points $S_\square(n)$ almost always is attained this way. In a few instance we have to remove 1 or 2 points (occurs for $n = 50$ only) from the circumference. We present the corresponding data in Table 5.9 and Table 5.9.

n	(x_2, y_2)	(x_3, y_3)	radius	center	removed points
4	$(1, -1)$	$(0, -1)$	0.707107	$(0.5, 0.5)$	
5	$(1, -1)$	$(0, -2)$	1	$(1, 1)$	
6	$(1, 2)$	$(2, 1)$	1.17851	$(0.833333, 0.833333)$	
7	$(2, -1)$	$(0, -2)$	1.25	$(0.75, 1)$	
8	$(2, -2)$	$(0, -2)$	1.41421	$(1, 1)$	1
9	$(2, -2)$	$(0, -2)$	1.41421	$(1, 1)$	
10	$(2, 0)$	$(1, 3)$	1.66667	$(1, 1.33333)$	
11	$(1, 3)$	$(3, 1)$	1.76777	$(1.25, 1.25)$	
12	$(1, -3)$	$(0, -3)$	1.58114	$(1.5, 1.5)$	
13	$(-3, -2)$	$(-1, 1)$	1.83848	$(1.3, 1.3)$	
14	$(3, 2)$	$(3, 1)$	1.90029	$(1.16667, 1.5)$	
15	$(2, -1)$	$(1, -4)$	2.08248	$(1.21429, 1.92857)$	
16	$(3, -3)$	$(0, -3)$	2.12132	$(1.5, 1.5)$	
17	$(3, -2)$	$(0, -4)$	2.16667	$(1.83333, 2)$	
18	$(2, 4)$	$(4, 2)$	2.35702	$(1.66667, 1.66667)$	
19	$(4, 2)$	$(1, 4)$	2.3744	$(1.64286, 1.71429)$	
20	$(1, -3)$	$(0, -4)$	2.23607	$(2, 2)$	1
21	$(1, -3)$	$(0, -4)$	2.23607	$(2, 2)$	
22	$(-4, -3)$	$(-1, 1)$	2.52538	$(1.78571, 1.78571)$	
23	$(4, 3)$	$(4, 1)$	2.57694	$(1.625, 2)$	
24	$(2, -1)$	$(1, -5)$	2.6117	$(1.94444, 2.38889)$	
25	$(-3, 1)$	$(-1, -4)$	2.70054	$(1.80769, 2.42308)$	
26	$(2, -5)$	$(0, -5)$	2.69258	$(2, 2.5)$	
27	$(1, -4)$	$(5, -1)$	2.76629	$(2.28947, 2.44737)$	
28	$(-4, 3)$	$(0, 1)$	2.79508	$(2.25, 2.5)$	
29	$(-4, 2)$	$(-1, -3)$	2.94508	$(2.14286, 2.28571)$	
30	$(1, 5)$	$(5, 1)$	3.06413	$(2.16667, 2.16667)$	1
31	$(1, -4)$	$(0, -5)$	2.91548	$(2.5, 2.5)$	1
32	$(1, -4)$	$(0, -5)$	2.91548	$(2.5, 2.5)$	
33	$(-5, -4)$	$(-1, 1)$	3.22126	$(2.27778, 2.27778)$	
34	$(-4, 5)$	$(-2, 6)$	3.23407	$(2.35714, 2.78571)$	
35	$(-4, 5)$	$(-1, 6)$	3.24123	$(2.39474, 2.81579)$	
36	$(5, 3)$	$(1, 6)$	3.2841	$(2.72222, 2.7963)$	
37	$(2, -6)$	$(0, -6)$	3.16228	$(3, 3)$	
38	$(5, 4)$	$(-1, 1)$	3.37474	$(2.83333, 2.83333)$	1
39	$(5, 4)$	$(-1, 1)$	3.37474	$(2.83333, 2.83333)$	
40	$(1, -5)$	$(6, -1)$	3.42414	$(2.74138, 2.94828)$	
41	$(5, 4)$	$(5, 2)$	3.44819	$(2.7, 3)$	
42	$(2, 0)$	$(1, 7)$	3.57143	$(3, 3.42857)$	
43	$(2, 5)$	$(-4, 1)$	3.63892	$(2.72727, 3.40909)$	
44	$(2, -7)$	$(0, -7)$	3.64005	$(3, 3.5)$	
45	$(1, -5)$	$(0, -6)$	3.60555	$(3, 3)$	
46	$(4, 0)$	$(2, 7)$	3.78571	$(3, 3.21429)$	
47	$(5, -4)$	$(4, -1)$	3.79484	$(3.22727, 3.40909)$	
48	$(-5, 4)$	$(0, 1)$	3.73363	$(3.3, 3.5)$	
49	$(5, -3)$	$(4, -1)$	3.83991	$(3.21429, 3.35714)$	
50	$(2, -5)$	$(0, -7)$	3.80789	$(3.5, 3.5)$	2

Table 5.9: Circle constructions for point sets attaining `blbk` for $S_\square(n)$ – $4 \le n \le 50$

If the `blbk` for $S_\square(n)$ would be tight for $n \le 100$, then our findings would imply Conjecture 2.2 for $n \le 100$. There is also the following stronger variant:

Conjecture 5.1. *For each integer n there exists a circle with center $(x, y) \in \mathbb{R}^2$ and radius*

$r \in \mathbb{R}$ such that the point set $\mathcal{P}$ given by the integer grid points strictly inside the circle and a suitable subset of those on the circumference satisfies $\#\mathcal{P} = n$ and $S_\square(\mathcal{P}) = S_\square(n)$.

Conjecture 5.2. *(Peter Munn)*
The asymptotic density of the numbers n such that there is no maximal arrangement formed by all the grid points within a suitably chosen circle, is 0.

We remark that allowing circles without three grid points on its circumference also gives a direct optimal construction for the case $n = 8$ without the necessity to remove a point from the circumference, cf. `https://oeis.org/A192493/a192493.pdf`.

n	(x_2, y_2)	(x_3, y_3)	radius	center	removed points
51	$(2, -5)$	$(0, -7)$	3.80789	$(3.5, 3.5)$	1
52	$(2, -5)$	$(0, -7)$	3.80789	$(3.5, 3.5)$	
53	$(6, 5)$	$(-1, 1)$	4.04775	$(3.31818, 3.31818)$	1
54	$(6, 5)$	$(-1, 1)$	4.04775	$(3.31818, 3.31818)$	
55	$(1, -6)$	$(7, -1)$	4.09673	$(3.20732, 3.45122)$	
56	$(6, 5)$	$(6, 2)$	4.11636	$(3.16667, 3.5)$	
57	$(5, 6)$	$(2, 8)$	4.1467	$(3.42857, 3.89286)$	
58	$(3, -2)$	$(1, -8)$	4.17836	$(3.40909, 3.86364)$	
59	$(3, -8)$	$(0, -8)$	4.272	$(3.5, 4)$	1
60	$(3, -8)$	$(0, -8)$	4.272	$(3.5, 4)$	
61	$(6, -4)$	$(0, -8)$	4.33333	$(3.66667, 4)$	
62	$(2, -6)$	$(8, -1)$	4.32876	$(3.80435, 3.93478)$	
63	$(5, 7)$	$(-2, 2)$	4.36049	$(3.91667, 3.91667)$	
64	$(-5, -7)$	$(-7, -1)$	4.37168	$(3.86364, 3.95455)$	
65	$(-7, -1)$	$(-1, -7)$	4.41942	$(3.875, 3.875)$	
66	$(-5, 1)$	$(-1, -7)$	4.47903	$(3.77778, 3.88889)$	
67	$(-6, 6)$	$(-1, 5)$	4.59619	$(3.75, 3.75)$	
68	$(2, -6)$	$(0, -8)$	4.47214	$(4, 4)$	1
69	$(2, -6)$	$(0, -8)$	4.47214	$(4, 4)$	
70	$(4, 0)$	$(2, 9)$	4.72222	$(4, 4.27778)$	
71	$(7, 6)$	$(-1, 1)$	4.73093	$(3.80769, 3.80769)$	
72	$(-6, 7)$	$(-2, 9)$	4.75164	$(3.875, 4.25)$	
73	$(4, 8)$	$(8, 4)$	4.71405	$(4.33333, 4.33333)$	
74	$(-8, 5)$	$(-8, 0)$	4.71699	$(4, 4.5)$	
75	$(7, 5)$	$(-2, 2)$	4.80885	$(4.25, 4.25)$	
76	$(3, -9)$	$(0, -9)$	4.74342	$(4.5, 4.5)$	
77	$(-8, -5)$	$(-3, 3)$	4.84096	$(4.42308, 4.42308)$	
78	$(8, 5)$	$(8, 2)$	4.86216	$(4.375, 4.5)$	
79	$(-1, -6)$	$(8, -2)$	4.94016	$(4.34, 4.36)$	
80	$(7, -7)$	$(0, -7)$	4.94975	$(4.5, 4.5)$	
81	$(2, -7)$	$(9, -1)$	4.98189	$(4.27049, 4.43443)$	
82	$(6, 8)$	$(-2, 2)$	5.05076	$(4.42857, 4.42857)$	
83	$(-6, -8)$	$(-8, -1)$	5.05984	$(4.37931, 4.46552)$	
84	$(-8, -1)$	$(-1, -8)$	5.10688	$(4.38889, 4.38889)$	
85	$(-6, 1)$	$(-1, -8)$	5.1521	$(4.31633, 4.39796)$	
86	$(-7, 7)$	$(-1, 6)$	5.23259	$(4.3, 4.3)$	
87	$(2, -7)$	$(0, -9)$	5.14782	$(4.5, 4.5)$	1
88	$(2, -7)$	$(0, -9)$	5.14782	$(4.5, 4.5)$	
89	$(8, 5)$	$(-2, 2)$	5.35735	$(4.65385, 4.65385)$	1
90	$(8, 5)$	$(-2, 2)$	5.35735	$(4.65385, 4.65385)$	
91	$(-6, -7)$	$(-3, -10)$	5.23557	$(4.88462, 4.88462)$	
92	$(3, -7)$	$(10, -1)$	5.26598	$(4.84328, 4.93284)$	
93	$(-7, 6)$	$(0, 2)$	5.30931	$(4.78571, 5)$	
94	$(3, 6)$	$(-6, 1)$	5.38599	$(4.73077, 4.88462)$	
95	$(6, -1)$	$(2, 9)$	5.39289	$(4.73214, 4.89286)$	
96	$(3, -7)$	$(0, -10)$	5.38516	$(5, 5)$	1
97	$(3, -7)$	$(0, -10)$	5.38516	$(5, 5)$	
98	$(-9, -6)$	$(-3, 3)$	5.51543	$(4.9, 4.9)$	
99	$(9, 6)$	$(9, 2)$	5.54026	$(4.83333, 5)$	
100	$(-1, -7)$	$(9, -2)$	5.60668	$(4.80769, 4.88462)$	

Table 5.10: Circle constructions for point sets attaining `blbk` for $S_\square(n) - 51 \le n \le 100$

While the mentioned circle construction gives a nice description of at least one similarity type of point sets attaining `blbk` for $S_\square(n)$ for $n \le 100$, it still remains interesting to determine other constructions that yield point sets with many squares. First we observe that the point set $\mathcal{P}$ obtained by the integer points in the circle centred at $(0.5, 0.5)$ with radius r is similar to the the points of the form $(2x+1, 2y+1)$ within a circle centred at $(0,0)$ with radius $2r$, where $x, y \in \mathbb{Z}$. The special point set $\mathcal{S}_{47}$, mentioned Section 2 can be described as the set of points of the form $(3x+1, 3y+1)$ in a circle centred at $(0,0)$ with radius $\sqrt{125}$:

```
.........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......
```

For $n \in \{12, 21, 32, 37, 45, 52, 69, 76, 88\}$ we may replace the description of set of integer points within a suitable circle by speaking of an octagon:

```
                                                     ...xxxx... ..xxxxxx..
                                           ..xxxxx.. ..xxxxxx.. .xxxxxxxx.
                                  ..xxxx.. .xxxxxxx. .xxxxxxxx. xxxxxxxxxx
                  ..xxx.. .xxxxx. .xxxxxx. xxxxxxxxx xxxxxxxxxx xxxxxxxxxx
           .xxxx. .xxxxx. xxxxxxx xxxxxxxx xxxxxxxxx xxxxxxxxxx xxxxxxxxxx
     .xxx. xxxxxx xxxxxxx xxxxxxx xxxxxxxx xxxxxxxxx xxxxxxxxxx xxxxxxxxxx
.xx. xxxxx xxxxxx xxxxxxx xxxxxxx xxxxxxxx xxxxxxxxx xxxxxxxxxx xxxxxxxxxx
xxxx xxxxx xxxxxx xxxxxxx xxxxxxx xxxxxxxx xxxxxxxxx .xxxxxxxx. xxxxxxxxxx
xxxx xxxxx xxxxxx .xxxxx. xxxxxxx .xxxxxx. .xxxxxxx. ..xxxxxx.. .xxxxxxxx.
.xx. .xxx. .xxxx. ..xxx.. .xxxxx. ..xxxx.. ..xxxxx.. ...xxxx... ..xxxxxx..
```

The circle construction can also be used to obtain an asymptotic lower bound.

Theorem 5.3. *(Peter Munn, with thanks to Benoît Jubin for the version used here)*

$$\liminf_{n\to\infty} \frac{S_\square(n)}{n^2} \geq \frac{1-\frac{2}{\pi}}{4} > \frac{1}{11.008}$$

Proof. *(Sketch)* For $r \geq 0$, denote by $D(r)$ the disc centered at the origin with radius r. If A is a point on the boundary of $D(r)$, then the set of points B such that the square with diagonal AB is included in $D(r)$ is a lens-shaped region. If A is the point $(-r, 0)$ at the left of the disc, the lens-shaped region is the intersection of the discs of radius $\sqrt{2}r$ centered at the points $(0, -r)$ and $(0, r)$, which pass through A and the point $(r, 0)$. The area of this region is $(\pi - 2)r^2$ (as a proportion of the disc area, this is twice A258146). Therefore, the number S of grid-squares included in $D(R)$ can be estimated as follows: since the set of squares with at least two vertices equidistant from the origin is negligible, we can assume that every square has a unique vertex furthest from the origin, say at distance r, which corresponds to the A above. The possible opposite vertices B are those in the region computed above that have even L^1 (aka rectilinear, or Manhattan) distance from A (being opposite vertices, they are two equal sides apart). So we divide the number of points in the lens-shaped region by 2. There are approximately $2\pi r$ grid points at a distance from the origin in $[r, r+1]$, so at first order,

$$S \simeq \int_0^R \pi r(\pi-2)r^2 \,\mathrm{d}\, r = \frac{\pi(\pi-2)}{4} \cdot R^4.$$

Since the disc $D(R)$ contains approximately πR^2 points, the statement follows. □

Remark 5.4. *In [2]* $\liminf\limits_{n\to\infty} \frac{S_{\triangle}(n)}{n^2} \geq \frac{3}{4} - \frac{1}{\pi} > 0.43169$ *was shown via the circle construction and an integration argument cf. [2, Theorem 2]. In [2, Theorem 4] this lower bound was improved to* $\liminf\limits_{n\to\infty} \frac{S_{\triangle}(n)}{n^2} \geq 0.433064$ *based on a configuration with two more or less concentric discs, the smaller one with double density (namely, points on the grid and points on the face-centered grid), see [2, Figure 1]. Interestingly enough, a similar construction will not improve upon Theorem 5.3. To this end, partition the grid into blue and green subgrids of half the density. Nearest neighbours of any grid point have the alternate colour, and any (blue, green) pair has odd rectilinear distance. (So diagonals of grid squares connect points of the same colour.) From a full disc configuration, remove green points outside the inner of the concentric discs.*

The asymptotic lower bound calculation from the proof of Theorem 5.3 is affected w.r.t. the proportion of configured points, B, that form a square's diagonal, AB, with A, where A is a (necessarily blue) point on the outer circumference. Considering all-blue squares, we already get the same proportion of qualifying blue points as in the proof of Theorem 5.3. But no green points qualify, and the qualifying blue points from blue-green squares do not compensate: they lie in a lens-shaped region that does not reach the inner disc's circumference. So the dual density configurations are not optimal.

To conclude, we remark that the comparison calculation is qualitatively different for similarly defined blue-green right triangles, which can have 2 *of* 3 *vertices outside the inner disc, whereas a blue-green square has at most* 1 *of* 4*. This may be part of the explanation for the difference in construction of the best-known solutions for squares as compared with isosceles right triangles.*

We conjecture that the "full discs" form asymptotically optimal grid-configurations. We can make this conjecture precise in a few different ways. For instance, let d be a distance on the space of (finite) grid configurations. Denote by D_n the set of grid-points at distance at most $\sqrt{n/\pi}$ of the origin, for $n \in \mathbb{N}$. Then the conjecture may take the following form, where $F\colon \mathbb{N} \to \mathbb{R}$.

Conjecture 5.5. *For all n, there exists an optimal configuration P_n such that $d(P_n, D_n) = O(F(n))$.*

For instance, we can take d to be the cardinality of the symmetric difference of the two configurations (that is, the number of points in exactly one of them), and take $F(n) = O(\#(D_n) - n)$. This error term is linked to the Gauss circle problem. It is known that $\#(D_n) - n = O(n^{131/416})$ and it is conjectured to be $O(n^{1/4+\epsilon})$.

We can also define $d(P, Q) \coloneqq d_{Haus}(P, Q) + d_{Haus}(\mathbb{Z}^2 \setminus P, \mathbb{Z}^2 \setminus Q)$ where d_{Haus} is the Hausdorff distance, and take $F(n) = 1$, or even conjecture that $d(P_n, D_n) \leq 2\sqrt{2}$.

5.1 A continuous variant of the maximization of $S_\square(n)$

For a planar domain D with area 1 define

$$S_\square(D) := \int_{\left\{(x,y,r,\theta)\;\middle|\; r>0, 0\le\theta<\pi/2, \begin{pmatrix} x\pm r\cos(\theta)\\ y\pm r\sin(\theta)\end{pmatrix}\in D, \begin{pmatrix} x\pm r\sin(\theta)\\ y\mp r\cos(\theta)\end{pmatrix}\in D\right\}} \mathrm{d}\,x\,\mathrm{d}\,y\,\mathrm{d}\,r\,\mathrm{d}\,\theta$$

as the "number of squares" generated by D. Here (x,y) is the center and $\sqrt{2}r$ the side length of the counted squares. The computations in the proof of Theorem 5.3 also yield $S_\square(D)=\frac{1}{4}-\frac{1}{2\pi}$ for a circular disk D of radius $1/\sqrt{\pi}$.

Conjecture 5.6. $S_\square(D)\le\frac{1}{4}-\frac{1}{2\pi}$*, i.e., the circular disk is optimal.*

If $\mathcal{P}\subset\mathbb{Z}^2$ is defined as $\lambda D\cap\mathbb{Z}^2$, i.e., the set of grid points in scaled version of D, then we have $S_\square(\mathcal{P})=S_\square(D)\cdot|\mathcal{P}|^2+o\big(|\mathcal{P}|^2\big)$. In light of the point set consisting of two different grids considered in Remark 5.4 we may consider a density $f\colon D\to\mathbb{R}_{\ge 0}$ such that $\int_{(x,y)\in D} f(x,y)\,\mathrm{d}\,x\,\mathrm{d}\,y=1$. In the modified version of $S_\square(D)$ we integrate

$$\min\{f(x\pm r\cos(\theta),y\pm r\sin(\theta)),f(x\pm r\sin(\theta),y\mp r\cos(\theta))\},$$

i.e., the minimum density over the four vertices of the square. One might conjecture that the maximum is obtained for the uniform density. Applying Steiner symmetrization might be an approach proving Conjecture 5.6. Techniques used in e.g. [11, 12] might also be useful.

6 Determination of exact values of $S_\square\big(n,\mathcal{P}^\star_{6,2}\big)$ for small n

Starting from the upper bound $S_\square\big(n,\mathcal{P}^\star_{6,2}\big)\le A(n,6,4)$, we remark that $S_\square\big(n,\mathcal{P}^\star_{6,2}\big)$ 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.

So far we know $S_\square\big(n,\mathcal{P}^\star_{6,2}\big)=0$ for $n\le 3$, $S_\square\big(n,\mathcal{P}^\star_{6,2}\big)=1$ for $4\le n\le 6$, $S_\square\big(7,\mathcal{P}^\star_{6,2}\big)=S_\square\big(8,\mathcal{P}^\star_{6,2}\big)=2$, and $S_\square\big(9,\mathcal{P}^\star_{6,2}\big)=3$, where we indeed have $S_\square\big(n,\mathcal{P}^\star_{6,2}\big)=A(n,6,4)$. Besides the relation to binary codes with minimum Hamming distance 6 and constant weight 4, the determination of $S_\square\big(n,\mathcal{P}^\star_{6,2}\big)$ is an interesting challenge, since for $n\ge 7$ the extremal examples cannot be obtained by recursive 2-extension starting from the unit square.

In the remaining part of this subsection we will always assume that the occurring oriented square sets do not contain two different squares that share at least two common vertices. Our aim is the determination of $S_\square\big(n,\mathcal{P}^\star_{6,2}\big)$ for small values of n. For $n\ge 7$ if suffices to consider point sets with maximum degree at least 2, i.e., $\mathcal{P}^1_{7,2}$ is a subconfiguration. Starting from the corresponding realizable oriented square set $\big\{(1,2,3,4),(1,5,6,7)\big\}$ the application of i-extension with $0\le i\le 3$ yields

- 54 realizable oriented square sets of order 9 and cardinality 3 for 2-extension and
- 42 realizable oriented square sets of order 10 and cardinality 3 for 3-extension

Currently no isomorphism check for oriented square sets is implemented, so that the stated numbers, very likely, are too large. Applying i-extension, with $i\le 3$, recursively, we subsequently verify the following statements. There are exactly 11 pairwise non-isomorphic rigid realizable oriented square sets of order 10 and cardinality 4:

```
                                                  x.xx..                  .x.x..
              .xxx.         .xx..  .xx..  x..x.   ....x.  xxxx..  x.x..   ......
x.xx.  xx.x.  x.xx.  .x.x.  .xx..  x.x..  .x...   .x...x  ....x.  .xx.x   xx.x..
..xx.  xxx..  .x...  xx.x.  x.x.x  .x.xx  ...xx   x..x..  .x...x  xxx..   xx...x
x.x.x  ....x  ....x  xx.xx  .x...  .x...  x.xxx   ...x..  x..x..  ...x.   ....x.
x..x.  x.xx.  .xx..  ..x..  ..xx.  .x.x.  ..x..   ...x..  ...x..  .x...   ..x...
```

Further realizable oriented square sets of order 10 and cardinality 4 that are non-rigid also exist. No realizable oriented square set of order 10 and cardinality 5 exists, i.e., $S_\Box\big(10, \mathcal{P}^\star_{6,2}\big) = 4$.

Example 6.1. *Consider the (realizable) oriented square set*

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

of order 10 *and cardinality* 4*. It can be obtained by* 1*-extension from the (realizable) oriented square set* $\big\{(1,2,3,4),(4,5,6,7),(3,8,9,7)\big\}$ *of order* 9 *and cardinality* 3*. The, up to similarity, unique representation of* S *is depicted in Figure 6.15. 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.*

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 3.14, so that we can check the existence of solutions algorithmically.

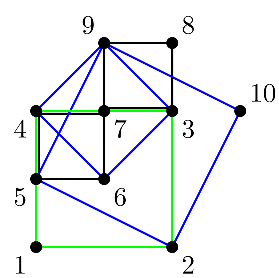

Figure 6.15: Four squares implying a fifth square.

Examples showing $S_\Box\big(11, \mathcal{P}^\star_{6,2}\big) \geq 5$ are given by:

```
       xxxx..   .x.xx..
x.xx.  ....x.   .....x.   x.x..
..xx.  .x...x   ..x...x   .xx.x
x.x.x  x..x..   .x..x..   xxx..
x..x.  ...x..   x...x..   ...x.
.x...  ...x..   ....x..   .x..x
```

Examples showing $S_\Box\big(12, \mathcal{P}^\star_{6,2}\big) \geq 6$ are given by:

```
.xxxx..
.....x.   .xx..
..x...x   .xxx.
.x..x..   x...x
x...x..   .xxx.
....x..   .xx..
```

Via exhaustive enumeration we have verified $S_{\square}(11, \mathcal{P}^{\star}_{6,2}) = 5$ and $S_{\square}(12, \mathcal{P}^{\star}_{6,2}) = 6$, so that Lemma 4.1 implies $S_{\square}(13, \mathcal{P}^{\star}_{6,2}) \le 9$ and $S_{\square}(14, \mathcal{P}^{\star}_{6,2}) \le 13$.

An example showing $S_{\square}(13, \mathcal{P}^{\star}_{6,2}) \ge 7$ is given by:

```
.xxxx..
.....x.
..x...x
.x..x..
x...x..
....x..
....x..
```

Conjecture 6.2.

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

Lemma 6.3.

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

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 $2 \le i \le 13$ 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 $S_{\square}(12, \mathcal{P}^{\star}_{6,2}) = 6$, we have $s_i \le 4$ for $2 \le i \le 10$ and $s_i \le 3$ for $11 \le i \le 13$. Since the vertices of each square are contained in at least 8 of the C_i, we have

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

□

With this, we can conclude $S_{\square}(14, \mathcal{P}^{\star}_{6,2}) \le \lfloor 14 \cdot 8/10 \rfloor = 11$ from Lemma 4.1.

Conjecture 6.4.

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

Acknowledgments

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A Dissimilar point sets attaining blbk for $S_{\square}(n)$

Here we list the known equivalence classes of n-point sets attaining blbk for $S_{\square}(n)$ mentioned in Table 3.5 for $n \leq 100$. Here the numbers just state the numbers of points and we separate different number of points by "|".

```
   |         |         |          |     |      | .xx. xxx.      xxx.
   |     xx. | xxx xx. | .xx. xxx | xxx | xxx. | xxxx xxxx xxxx xxxx .xxx.
xx | xxx xxx | xxx xxx | xxxx xxx | xxx | xxxx | xxxx xxx. xxxx xxx. xxxxx
xx | xxx .x. | .x. .xx | .xx. xx. | xxx | xxx. | .x.. .x.. xxx. ..x. .xxx.
4  | 6       | 7       | 8        | 9   | 10   | 11

     |      |           |            |            | .xxx. .xxx.
.xx. | xxx. | xxx. xxxx | .xxx. xxxx | .xxx. xxxx | xxxx. xxxxx xxxx. xxxx.
xxxx | xxxx | xxxx xxxx | xxxxx xxxx | xxxxx xxxx | xxxxx xxxxx xxxxx xxxxx
xxxx | xxxx | xxxx xxxx | xxxx. xxxx | xxxxx xxxx | xxxx. .xxx. xxxxx xxxx.
.xx. | .xx. | .xxx .xx. | .xxx. xxx. | .xxx. xxxx | ..x.. ..x.. .xxx. xxxx.
12   | 13   | 14        | 15         | 16         | 17

.xxx. xxxx.       | .xxx. .xxx. .xxx. .xxx. xxxx. | .xxx. | .xxx. | xxxx.
xxxxx xxxx. xxxx. | xxxxx xxxxx xxxxx xxxx. xxxxx | xxxxx | xxxxx | xxxxx
xxxxx xxxxx xxxxx | xxxxx xxxxx xxxxx xxxxx xxxxx | xxxxx | xxxxx | xxxxx
xxxx. xxxx. xxxxx | xxxx. xxxx. xxxxx .xxxx xxxx. | xxxxx | xxxxx | xxxxx
..x.. ..x.. xxxx. | ..xx. .xx.. ..x.. .xxx. ..x.. | .xx.. | .xxx. | .xxx.
18                | 19                            | 20    | 21    | 22

                   |        |        |        | .xxxx. .xxxx. | .xxxx. .xxxx.
.xxxx. xxxx. xxxxx | .xxxx. | .xxxx. | .xxxx. | xxxxxx xxxxx. | xxxxx. xxxxxx
xxxxx. xxxxx xxxxx | xxxxx. | xxxxxx | xxxxxx | xxxxxx xxxxxx | xxxxxx xxxxxx
xxxxxx xxxxx xxxxx | xxxxxx | xxxxxx | xxxxxx | xxxxxx xxxxxx | xxxxxx xxxxxx
xxxxx. xxxxx xxxxx | xxxxx. | xxxxx. | xxxxxx | .xxxx. .xxxx. | xxxxx. .xxxx.
.xxx.. .xxxx .xxx. | .xxxx. | .xxxx. | .xxxx. | ..x... ..xx.. | ..xx.. ..xx..
23                 | 24     | 25     | 26     | 27            | 28

.xxxx. | .xxxx. .xxxx. .xxxx. .xxxx. | .xxxx. | .xxxx. | .xxxx.. xxxxx.
xxxxxx | xxxxxx xxxxxx xxxxxx xxxxx. | xxxxxx | xxxxxx | xxxxxx. xxxxxx
xxxxxx | xxxxxx xxxxxx xxxxxx xxxxxx | xxxxxx | xxxxxx | xxxxxxx xxxxxx
xxxxxx | xxxxxx xxxxxx xxxxxx xxxxxx | xxxxxx | xxxxxx | xxxxxx. xxxxxx
xxxxx. | xxxxx. xxxxxx xxxxx. .xxxxx | xxxxxx | xxxxxx | xxxxxx. xxxxxx
..xx.. | ..xxx. ..xx.. .xxx.. .xxxx. | .xxx.. | .xxxx. | .xxxx.. .xxxx.
29     | 30                          | 31     | 32     | 33

        .xxxx..                 |         .xxxx.. |         .xxxx.. ..xxx..
.xxxxx. xxxxxx. .xxxxx. .xxxx.. | .xxxxx. xxxxxx. | .xxxxx. xxxxxx. .xxxxx.
xxxxxx. xxxxxx. xxxxxx. xxxxxx. | xxxxxx. xxxxxx. | xxxxxx. xxxxxxx xxxxxxx
xxxxxx. xxxxxxx xxxxxxx xxxxxxx | xxxxxxx xxxxxxx | xxxxxxx xxxxxxx xxxxxxx
xxxxxxx xxxxxx. xxxxxx. xxxxxxx | xxxxxxx xxxxxx. | xxxxxxx xxxxxx. xxxxxxx
xxxxxx. .xxxx.. xxxxxx. xxxxxx. | xxxxxx. .xxxxx. | xxxxxx. .xxxxx. .xxxxx.
.xxxx.. ...x... .xxxx.. .xxxx.. | .xxxx.. ...x... | .xxxxx. ...x... ..xx...
34                              | 35              | 36
```

```
..xxx.. | .xxxx.. | .xxxxx. .xxxx.. | .xxxxx. | .xxxxx. .xxxxx. | .xxxxx. ..xxxx..
.xxxxx. | .xxxxx. | .xxxxx. xxxxxx. | xxxxxx. | xxxxxxx xxxxxx. | xxxxxxx .xxxxxx.
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37      | 38      | 39              | 40      | 41              | 42

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43                                                | 44               | 45

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48                | 49       | 50                                  | 51

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52       | 53       | 54                | 55       | 56


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56                           | 57                            | 58

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59        | 60        | 61        | 62

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62                                                 | 63

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63        | 64                  | 65                  | 66        | 67
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67                            | 68        | 69        | 70

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71                                        | 72                    | 73

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74         | 75                               | 76
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77         | 78                               | 79

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79         | 80                    | 81

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82                               | 83                    | 84

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85         | 86                                          | 87         | 88
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89          | 90                      | 91                      | 92

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93                      | 94                      | 95

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95                                  | 96          | 97          | 98
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