On k–sets, convex quadrilaterals, and the rectilinear crossing number of K_n

József Balogh* and Gelasio Salazar†

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Abstract

We use circular sequences to give an improved lower bound on the minimum number of $(\leq k)$–sets in a set of points in general position. We then use this to show that if S is a set of n points in general position, then the number $\square(S)$ of convex quadrilaterals determined by the points in S is at least $0.37533\binom{n}{4} + O(n^3)$. This in turn implies that the rectilinear crossing number $\overline{\mathrm{cr}}(K_n)$ of the complete graph K_n is at least $0.37533\binom{n}{4} + O(n^3)$, and that Sylvester's Four Point Problem Constant is at least 0.37533. These improved bounds refine results recently obtained by Ábrego and Fernández–Merchant, and by Lovász, Vesztergombi, Wagner and Welzl.

Keywords: Convex quadrilaterals, k–sets, crossing number, rectilinear crossing number, complete graph, circular sequence, allowable sequence

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1 Introduction

In an influential paper published in 1980, Goodman and Pollack [11] introduced the concept of circular sequences (see definition below) as a combinatorial encoding scheme for sets of points in the plane.

Recently, Ábrego and Fernández–Merchant [1], and independently Lovász, Vesztergombi, Wagner and Welzl [12] used circular sequences to establish new important results concerning the following classical problems in combinatorial geometry (Problems 1 and 2) and geometric probability (Problem 3):

Problem 1

Let S be a set of n points in general position in the plane. What is the number $\square(S)$ of convex quadrilaterals in S?

For the following problem, recall that the *rectilinear crossing number* $\overline{\mathrm{cr}}(G)$ of a graph G is the minimum number of pairwise intersections of edges in a drawing of G in the plane in which every edge is drawn as a straight segment.

Problem 2

What is the rectilinear crossing number $\overline{\mathrm{cr}}(K_n)$ of the complete graph K_n on n vertices?

*Department of Mathematics, The Ohio State University, Columbus OH 43210, USA. E–mail: jobal@math.ohio-state.edu.
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†IICO–UASLP, Av. Karakorum 1470, Lomas 4ta. Seccion, San Luis Potosi SLP, C.P. 78210, Mexico. E–mail: gsalazar@cactus.iico.uaslp.mx.
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The connection between Problems 1 and 2 is the observation that the crossings of edges in a (rectilinear) drawing of K_n are in one–to–one correspondence with the convex quadrilaterals formed by its set of vertices.

Observation 1 *For each positive integer n,*

$$\overline{\mathrm{cr}}(K_n) = \min_{|S|=n} \square(S),$$

where the minimum is taken over all the point sets S with n elements in general position.

Following [12], for a (Borel) probability distribution in the plane μ, let $\square(\mu)$ denote the probability that four independent μ–random points form a convex quadrilateral. The following is known as Sylvester's Four Point Problem, after Sylvester's paper from 1865 [16] (for a nicely written survey on the history and status of this problem until 1989, see [13]).

Problem 3 (Sylvester's Four Point Problem)

What is *Sylvester Four Point Problem's Constant* $q_* := \inf_\mu \square(\mu)$?

In [15], Scheinerman and Wilf proved the following striking connection between $\overline{\mathrm{cr}}(K_n)$ and Sylvester Four Point Problem's Constant q_*.

Theorem 2 (Scheinerman and Wilf)

$$q_* = \lim_{n\to\infty} \frac{\overline{\mathrm{cr}}(K_n)}{\binom{n}{4}}.$$

In this paper we follow the approach used by Ábrego and Fernández–Merchant and (independently) by Lovász, Vesztergombi, Wagner and Welzl, to these closely related questions, and refine their results to obtain improved bounds for these classical problems.

1.1 The relationship between $\square(S)$ and circular sequences

In [12], Lovász, Vesztergombi, Wagner and Welzl showed that $\square(S)$ is closely related to the number of $(\leq k)$–sets in S. We recall that a *k–set* is a subset T of S with $|T| = k$, and such that T can be separated from its complement $T \setminus S$ by a line. An i–set with $1 \leq i \leq k$ is a *$(\leq k)$–set*. We use $\eta_{\leq k}(S)$ to denote the number of $(\leq k)$–sets of S.

While the important problem of determining, for each k, the maximum number of k–sets remains tantalizingly open (the best current bounds are $O(nk^{1/3})$ and $ne^{\Omega(\log k)}$ (see [7] and [17], respectively), it is known that the maximum number of $(\leq k)$–sets of an n–point set S in the plane is nk (this is attained iff S is in convex position [3, 20]).

In [12, 20], it is shown that if S is a collection of points in general position, then $\square(S)$ is a linear combination of $\{\eta_{\leq j}(S)\}$. The following is a direct consequence of Lemma 9 in [12].

Theorem 3 (Lovász, Vesztergombi, Wagner and Welzl) *Let S be a set of n points in the plane in general position. Then*

$$\square(S) = \sum_{1\leq k<(n-2)/2} \big(n-2k-3\big)\eta_{\leq k+1}(S) + O(n^3),$$

where $\eta_{\leq j}(S)$ denotes the number of $(\leq j)$–sets of S.

This crucial observation is exploited in [12] by finding a nontrivial lower bound for $\eta_{\leq k}(S)$ for every $k < n/2$ and every set S of n points in general position (and using an even better bound for k close to $n/2$, which follows from the results in [19]). See Theorems 2 and 4 in [12]. To obtain the bound in their Theorem 2, they follow the approach of circular sequences.

We recall that a *circular sequence on n elements* Π is a sequence $(\pi_0, \pi_1, \ldots, \pi_{\binom{n}{2}})$ of permutation of the set $\{1, 2, \ldots, n\}$, where π_0 is the identity permutation $(1, 2, \ldots, n)$, $\pi_{\binom{n}{2}}$ is the reverse permutation $(n, n-1, \ldots, 1)$, and any two consecutive permutations differ by exactly one transposition of two elements in adjacent positions. A transposition that occurs between elements in positions i and $i+1$, or between elements in positions $n-i$ and $n-i+1$ is *i–critical.* A transposition is *$(\leq k)$–critical* if it is critical for some $i \leq k$. We denote the number of $(\leq k)$–critical transpositions in Π by $\chi_{\leq k}(\Pi)$), and use $\mathbf{X}_{\leq k}(n)$ to denote the minimum of $\chi_{\leq k}(\Pi)$ taken over all circular sequences Π on n elements.

Circular sequences can be used to encode any set S of points in general position as follows. Let L be a (directed) line that is not orthogonal to any of the lines defined by pairs of points in S. We label the points in S as $p_1, p_2, \ldots, p_n$, according to the order in which their orthogonal projections appear along L. As we rotate L (say counterclockwise), the ordering of the projections changes precisely at the positions where L passes through a position orthogonal to the line defined by some pair of points r, s in S. At the time the projection change occurs, r and s are adjacent in the ordering. and the ordering changes by transposing r and s. By keeping track of all permutations of the projections as L is rotated by 180^o, we obtain a circular sequence Π_S.

The crucial observation is that clearly $(\leq k)$–sets are in one–to–one correspondence with $(\leq k)$–critical transpositions of Π_S.

Observation 4 *Let S be a set of n points in the plane in general position, and let $k < n/2$. Then*

$$\eta_{\leq k}(S) = \chi_{\leq k}(\Pi_S).$$

Combining Theorem 3 and Observation 4 and recalling the definition of $\mathbf{X}_{\leq k}(n)$, one immediately obtains the following statement, obtained independently in [1] and [12].

Theorem 5 *Let S be a set of n points in the plane in general position. Then*

$$\begin{aligned}\square(S) &= \sum_{1 \leq k < (n-2)/2} \big(n - 2k - 3\big)\chi_{\leq k+1}(\Pi_S) + O(n^3) \\ &\geq \sum_{1 \leq k < (n-2)/2} \big(n - 2k - 3\big)\mathbf{X}_{\leq k+1}(n) + O(n^3).\end{aligned}$$

Having reduced the problem of bounding $\square(S)$ to the problem of bounding $\mathbf{X}_{\leq k}(n)$, Ábrego and Fernández–Merchant [1], and independently Lovász, Vesztergombi, Wagner and Welzl [12], then proceeded to the (combinatorial) problem of deriving good estimates for $\mathbf{X}_{\leq k}(n)$.

1.2 Previous estimates for $\mathbf{X}_{\leq k}(n)$ and their consequences

In [1] and [12], the following was proved:

$$\mathbf{X}_{\leq k}(n) \geq 3\binom{k+1}{2}, \quad \text{for every positive } n \text{ and every } k < n/2. \tag{1}$$

In [1], this result was applied, together with Theorem 5, to obtain the following.

Theorem 6 *If S is any set of n points in general position, then*

$$\Box(S) \;\geq\; \frac{1}{4}\left\lfloor\frac{n}{4}\right\rfloor \left\lfloor\frac{n-1}{4}\right\rfloor \left\lfloor\frac{n-2}{4}\right\rfloor \left\lfloor\frac{n-3}{4}\right\rfloor \;=\; 0.375\binom{n}{4} + O(n^3). \tag{2}$$

As a corollary, they obtain $\overline{\mathrm{cr}}(K_n) \geq 0.375\binom{n}{4} + O(n^3)$.

We observe that the bound $\mathbf{X}_{\leq k}(n) \geq 3\binom{k+1}{2}$ is sharp for $k \leq n/3$ (see Example 3 in [12]). Therefore, any improvement on $\Box(S)$ based on the approach of circular sequences must necessarily rely on bounds for $\mathbf{X}_{\leq k}(n)$ that are strictly better than $3\binom{k+1}{2}$ for (some subset of) the interval $n/3 < k < (n-2)/2$. Prior to the present paper, the only such bound reported is the following, which is derived in [12] using a result from [19]:

$$\mathbf{X}_{\leq k}(n) \geq \frac{n^2}{2} - n\sqrt{n^2 - 4k^2} + O(n). \tag{3}$$

Now (3) is strictly better than (1) for k sufficiently close to $n/2$, namely for $k > k_0(n) := \sqrt{(2\sqrt{13}-5)/9}n \approx 0.4956n + O(\sqrt{n})$. Combining (1) (which is also proved in [12] independently of [1]) and (3), and applying Theorem 5, the following was proved in [12].

Theorem 7 *If S is any set of n points in general position, then*

$$\Box(S) > 0.37501\binom{n}{4} \;+\; O(n^3).$$

Again, in view of Observation 1 this immediately yields an improved bound for $\overline{\mathrm{cr}}(K_n)$.

Although numerically the improvement (of roughly $1.088 \cdot 10^{-5}$) given in Theorem 7 over 0.375 may seem marginal, conceptually it is most relevant, since it shows that the rectilinear and the ordinary crossing number of K_n (which considers drawings in which the edges are not necessarily straight segments) are different on the asymptotically relevant term n^4. This last observation follows since there are (non–rectilinear) drawings of K_n with exactly $(1/4)\lfloor n/4\rfloor\lfloor (n-1)/4\rfloor\lfloor (n-2)/4\rfloor\lfloor (n-3)/4\rfloor = 0.375\binom{n}{4} + O(n^3)$ crossings. No better (non–rectilinear) drawings of K_n are known, and consequently the (non–rectilinear) crossing number of K_n has been long conjectured to be exactly $(1/4)\lfloor n/4\rfloor\lfloor (n-1)/4\rfloor\lfloor (n-2)/4\rfloor\lfloor (n-3)/4\rfloor$ (see for instance [9]).

1.3 Our results: an improved bound for $\mathbf{X}_{\leq k}(n)$ and its consequences

The core of this paper is an improved bound on the minimum number $\mathbf{X}_{\leq k}(n)$ of $(\leq k)$–critical transpositions in any circular sequence on n elements. Our bound is given in terms of two functions $F(k,n)$ and $s(k,n)$ defined as follows.

For all positive integers k, n such that $k < n$, let

$$F(k,n) := \left(2 - \frac{1}{s(k,n)}\right)k^2 - \left(\frac{(s(k,n)-1)^2}{s(k,n)}\right)k(n-2k-1)$$

$$+ \left(\frac{s(k,n)^4 - 7s(k,n)^2 + 12s(k,n) - 6}{12s(k,n)}\right)(n-2k-1)^2,$$

where

$$s(k,n) := \left\lfloor \frac{1}{2}\left(1 + \sqrt{\frac{1+6\left(\frac{k}{n}\right) - \left(\frac{9}{n}\right)}{1-2\left(\frac{k}{n}\right) - \left(\frac{1}{n}\right)}}\right)\right\rfloor.$$

Using this notation, our main result is the following.

Theorem 8 (Main result) *For every positive integer n and every $k < n/2$,*

$$\mathbf{X}_{\leq k}(n) \;\geq\; F(k,n) \;+\; O(n).$$

This bound is better than the bounds in (1) and (3) for $k > k_1(n) := (1/162)\left(-71 + 71n + \sqrt{19n^2 - 38n + 19}\right)$ $\approx 0.465178n + O(\sqrt{n})$ (see Appendix).

The bulk of this paper is the proof of Theorem 8, which is given in Section 2.

By Observation 4, the refined bound for $\mathbf{X}_{\leq k}(n)$ given in Theorem 8 immediately implies improved bounds for $\eta_{\leq k}(S)$, for $k \geq k_1(n)$.

Moreover, in view of Theorem 5, Theorem 8 also gives improved bounds for $\square(S)$, for any set S of n points in general position (and, in view of Observation 4 and Theorem 2, also for $\overline{\mathrm{cr}}(K_n)$, and for q_*).

The corresponding calculations (which are somewhat tedious but by no means difficult) are given in Section 3, where the following is proved.

Proposition 9 *For every positive integer n and every $k < n/2$,*

$$\sum_{1\leq k<(n-2)/2} (n-2k-3)\cdot \max\left\{3\binom{k+2}{2}, F(k+1,n)\right\} \geq 0.37553\binom{n}{4} + O(n^3).$$

By applying Theorem 8 and Proposition 9 to Theorem 5, we obtain the following.

Corollary 10 *If S is a set of n points in the plane in general position, then*

$$\square(S) \geq 0.37553\binom{n}{4} + O(n^3).$$

In view of Observation 1, we also have the following.

Corollary 11 *For each positive integer n,*

$$\overline{\mathrm{cr}}(K_n) \geq 0.37553\binom{n}{4} + O(n^3).$$

To put this improved lower bound on $\overline{\mathrm{cr}}(K_n)$ into context, first we should point out that the lower bounds on $\overline{\mathrm{cr}}(K_n)$ proved in [1] and [12] represent a remarkable improvement over the previous best general lower bounds. Previous to the successful use of the approach of circular sequences (Edelsbrunner et al. [8] also claimed to have proved that $\mathbf{X}_{\leq k}(n) \geq 3\binom{k+1}{2}$, but their argument seems to have a gap), the best lower bound known was $\overline{\mathrm{cr}}(K_n) \geq 0.3288\binom{n}{4}$ [18].

The improved lower bounds on $\overline{\text{cr}}(K_n)$ reported in [1] and [12] are particularly attractive since they are remarkably close to the best upper bound currently known, namely $\overline{\text{cr}}(K_n) \leq 0.3807\binom{n}{4}$ [2]. This bound was obtained using a computer–generated base case. The best known upper bound derived "by hand" (quoting [12]), namely $\overline{\text{cr}}(K_n) \leq 0.3838\binom{n}{4}$, was obtained by Brodsky, Durocher, and Gethner [5].

We also mention that the exact crossing number of K_n is known for $n \leq 16$. For all $n \leq 9$, the exact value of $\overline{\text{cr}}(K_n)$ can be found for instance in [21]. For $n = 10$ it was determined by Brodsky, Durocher, and Gethner [6], for $n = 11$ and 12 it was calculated by Aichholzer, Aurenhammer, and Krasser [2], and quite recently Aichholzer and Krasser determined it for $n = 13, 14, 15, 16$ (private communication). The most current information on the rectilinear crossing number of K_n for specific values of n is given in the the comprehensive web page `http://www.igi.tugraz.at/oaich/triangulations/crossing.html`, maintained by Aichholzer.

In view of Corollary 11, the best bounds currently known for $\overline{\text{cr}}(K_n)$ are as follows:

$$0.37553\binom{n}{4} + O(n^3) \leq \overline{\text{cr}}(K_n) \leq 0.3807\binom{n}{4} + O(n^3).$$

We finally note that Theorems 2 and 11 yield the following improved bound on Sylvester's Four Point Problem Constant.

Corollary 12

$$q_* \geq 0.37553.$$

2 Bounding the number of $(\leq k)$–critical transpositions: Proof of Theorem 8

Our strategy to prove Theorem 8 is as follows. First we show that the number of $(\leq k)$–critical transpositions in *any* circular sequence Π on n elements is bounded by below by a function that depends on the solution of a maximization problem over a certain family of digraphs. This is done in Section 2.1 (see Proposition 13). Then, in Section 2.2, we find an upper bound for the solution of the maximization problem over this set of digraphs (see Proposition 23).

We will conclude this section with the (by then obvious) observation that Theorem 8 follows from Propositions 13 and 23.

2.1 Bounding the number of $(\leq k)$–critical transpositions in terms of the solution of a digraph optimization problem

Our lower bound for the number of $(\leq k)$–critical transpositions in a circular sequence is given in terms of the maximum of an objective function taken over a certain set of digraphs which we now proceed to define. We use $\overrightarrow{uv}$ to denote the directed edge from vertex u to vertex v. The indegree and outdegree of vertex u in the digraph D are denoted $[u]^-_D$ and $[u]^+_D$, respectively.

Definition Let k, m be integers such that $2 \leq m < k$. A digraph D with vertex set $\{v_1, v_2, \ldots, v_k\}$ is a (k, m)–*digraph* if it satisfies the following conditions:

(i) There is some vertex v_i such that $[v_i]^-_D = 0$.

(ii) For every $i \in \{1, \ldots, k\}$, $[v_i]^+_D \leq [v_i]^-_D + (m - 1)$.

(iii) There is a one–to–one *ordering map* $f_D : \{1, 2, \ldots, k\} \to \{1, 2, \ldots, k\}$, such that, for all $i, j \in \{1, 2, \ldots, k\}$, if $\overrightarrow{v_i v_j}$ is in D then $f_D(i) < f_D(j)$.

We let $\mathcal{D}_{k,m}$ denote the set of all (k,m)–digraphs.

Proposition 13 *Let Π be any circular sequence on n elements and let $k < n/2$. Define $m := n - 2k$. Then*

$$\chi_{\leq k}(\Pi) \;\geq\; 2k^2 + km \;-\; \max_{D \in \mathcal{D}_{k,m}} \left\{ 2\left(\sum_{1\leq i\leq k} [v_i]_D^- \right) + \left(\sum_{1\leq i\leq k} \min\left\{ [v_i]_D^- - [v_i]_D^+ + (m-1), m \right\} \right) \right\}.$$

Proof. For convenience we label the n points so that the starting permutation is

$$\pi_0 = (a_k, a_{k-1}, \ldots, a_1, b_1, b_2, \ldots, b_m, c_1, c_2, \ldots, c_k).$$

If the elements involved in a transposition are a_i, a_j for some i, j, then we call it an (a,a)*–transposition*. If the elements are a_i, b_j for some i, j, then it is an (a,b)*–transposition* (note that we call it an (a,b)–transposition regardless of the relative position of a_i and b_j at the moment the transposition occurs). We define (b,b)–, (c,c)–, (a,c)–, and (b,c)–transpositions similarly. Thus, every transposition is a (y,z)–transposition for some $(y,z) \in \{(a,a),(a,b),(a,c),(b,b),(b,c),(c,c)\}$.

Suppose that two elements transpose when they occupy positions i and $i+1$. If $i \leq k$ or $i \geq k+m$, then the transposition occurs *in the AC–zone.* If $k+1 \leq i \leq k+m-1$, then it occurs *in the B–zone.*

For all $(y,z) \in \{(a,a),(a,b),(a,c),(b,c),(c,c)\}$, we define

$$\begin{aligned} (AC)_{(y,z)} &:= \text{ number of } (y,z)\text{–transpositions in the AC–zone} \\ (B)_{(y,z)} &:= \text{ number of } (y,z)\text{–transpositions in the B–zone} \end{aligned}$$

In a transposition that transforms (x,y) into (y,x), we say that x *moves to the right*, and y *moves to the left.*

For each $x \in \{a_1, \ldots, a_k, c_1, \ldots, c_k\}$, let $R_{AC}(x)$ (respectively $L_{AC}(x)$) denote the total number of transpositions in the AC–zone in which x moves to the right (respectively left). Since at the start of the circular sequence each a_i is at position $k-i+1$, and at the end it is in position $k+m+i$, it follows that $R_{AC}(a_i) - L_{AC}(a_i) = (k+m+i) - (k-i+1) - (m-1) = 2i$ (note that the transpositions that involve a_i do not contribute to $R_{AC}(a_i)$ or $L_{AC}(a_i)$ if they occur in the B–Zone). A similar reasoning shows that $L_{AC}(c_i) - R_{AC}(c_i) = 2i$. Thus

$$\sum_{1\leq i\leq k} (R_{AC}(a_i) - L_{AC}(a_i)) = \sum_{1\leq i\leq k} (L_{AC}(c_i) - R_{AC}(c_i)) = 2\binom{k+1}{2}. \tag{4}$$

Now we note that every (a,b)–transposition in the AC–zone contributes 1 to $\sum_{1\leq i\leq k} R_{AC}(a_i)$ and in 0 to $\sum_{1\leq i\leq k} L_{AC}(a_i)$, since in every (a,b)–transposition an a_i moves to the right. Similarly, every (a,c)–transposition in the AC–zone contributes 1 to $\sum_{1\leq i\leq k} R_{AC}(a_i)$ and in 0 to $\sum_{1\leq i\leq k} L_{AC}(a_i)$. Finally, we note that every (a,a)–transposition in the AC–zone contributes 0 to $\sum_{1\leq i\leq k} (R_{AC}(a_i) - L_{AC}(a_i))$. Therefore

$$\sum_{1\leq i\leq k} (R_{AC}(a_i) - L_{AC}(a_i)) = (AC)_{(a,b)} + (AC)_{(a,c)}. \tag{5}$$

An analogous reasoning shows that

$$\sum_{1\leq i\leq k} (L_{AC}(c_i) - R_{AC}(c_i)) = (AC)_{(b,c)} + (AC)_{(a,c)}. \tag{6}$$

Combining (4), (5), and (6), we obtain

$$(AC)_{(a,b)} + (AC)_{(b,c)} + 2(AC)_{(a,c)} = 4\binom{k+1}{2}. \tag{7}$$

Now $\chi_{\leq k}(\Pi) = (AC)_{(a,a)} + (AC)_{(b,b)} + (AC)_{(c,c)} + (AC)_{(a,b)} + (AC)_{(b,c)} + (AC)_{(a,c)}$. Thus $\chi_{\leq k}(\Pi) \geq (AC)_{(a,a)} + (AC)_{(c,c)} + (AC)_{(a,b)} + (AC)_{(b,c)} + (AC)_{(a,c)}$, and so using (7) we obtain

$$\chi_{\leq n}(\Pi) \;\geq\; 2\binom{k+1}{2} + (AC)_{(a,a)} + (AC)_{(c,c)} + \frac{(AC)_{(a,b)} + (AC)_{(b,c)}}{2}. \tag{8}$$

Let D_a denote the digraph with (ordered) vertex set $\{a_k, a_{k-1}, \ldots, a_1\}$, such that $\overrightarrow{a_i a_j}$ is in D_a iff $i > j$ and the transposition $(a_i, a_j) \to (a_j, a_i)$ occurs in the B–zone. Our goal is to relate the parameters of D_a to $(AC)_{(a,a)}$ and $(AC)_{(a,b)}$ (see (11)).

The first obvious observation is that the total number of edges D_a, that is, $\sum_{1\leq i\leq k} [a_i]^-_{D_a}$, equals $(B)_{(a,a)}$. Since $(B)_{(a,a)} + (AC)_{(a,a)}$ equals the total number of (a,a)–transpositions, namely $\binom{k}{2}$, this implies

$$(AC)_{(a,a)} = \binom{k}{2} - \sum_{1\leq i\leq k} [a_i]^-_{D_a}. \tag{9}$$

For each fixed a_i, let $(B)_{(a_i,b)}$ denote the total number of transpositions that involve a_i and some b, and that occur in the B–Zone. We define $(B)_{(a_i,c)}$ analogously.

For each $x \in \{a_1, \ldots, a_k, c_1, \ldots, c_k\}$, let $R_B(x)$ (respectively $L_B(x)$) denote the total number of transpositions in the B–zone in which x moves to the right (respectively left). Since at the start of the circular sequence each a_i occupies one of the first k positions and at the end it occupies one of the last k positions (that is, it "traverses through the entire B-zone") it follows that $R_B(a_i) - L_B(a_i) = m - 1$. On the other hand, the definition of edges in D_a implies that $L_B(a_i) = [a_i]^-_{D_a}$. Therefore $R_B(a_i) = (m-1) + [a_i]^-_{D_a}$. Now every (a,b) or (a,c)–transposition that occurs in the B–Zone (actually, anywhere) involves an a_j that moves to the right. Combining this with the remark that $[a_i]^+_{D_a}$ is the total number of (a,a) moves in the B–zone in which a_i moves to the right, we get $R_B(a_i) = [a_i]^+_{D_a} + (B)_{(a_i,b)} + (B)_{(a_i,c)}$. Therefore $(B)_{(a_i,b)} + (B)_{(a_i,c)} = [a_i]^-_{D_a} - [a_i]^+_{D_a} + (m-1)$, and so $(B)_{(a_i,b)} \leq [a_i]^-_{D_a} - [a_i]^+_{D_a} + (m-1)$.

We also note that the total number of (a_i, b) transpositions is exactly m, and so $(B)_{(a_i,b)} \leq m$. Therefore, for each a_i, $(B)_{(a_i,b)} \leq \min\{[a_i]^-_{D_a} - [a_i]^+_{D_a} + (m-1), m\}$. Since $\sum_{1\leq i\leq k} (B)_{(a_i,b)} = (B)_{(a,b)}$ and $(B)_{(a,b)} + (AC)_{(a,b)} = km$, we finally obtain

$$(AC)_{(a,b)} \geq km - \sum_{1\leq i\leq k} \min\{[a_i]^-_{D_a} - [a_i]^+_{D_a} + (m-1), m\}. \tag{10}$$

Using (9) and (10), we obtain

$$(AC)_{(a,a)} + \frac{(AC)_{(a,b)}}{2} \geq \left(\binom{k}{2} - \sum_{1\leq i\leq k} [a_i]^-_{D_a}\right) + \frac{1}{2}\left(km - \sum_{1\leq i\leq k} \min\{[a_i]^-_{D_a} - [a_i]^+_{D_a} + (m-1), m\}\right). \tag{11}$$

If we now let D_c denote the digraph with (ordered) vertex set $\{c_1, c_2, \ldots, c_k\}$ such that there is an arc from c_i to c_j iff $i < j$ and the transposition $(c_j, c_i) \to (c_i, c_j)$ occurs in the B–zone, a totally analogous argument shows that

$$(AC)_{(c,c)} + \frac{(AC)_{(b,c)}}{2} \geq \left(\binom{k}{2} - \sum_{1\leq i\leq k} [c_i]^-_{D_c}\right) + \frac{1}{2}\left(km - \sum_{1\leq i\leq k} \min\{[c_i]^-_{D_c} - [c_i]^+_{D_c} + (m-1), m\}\right). \tag{12}$$

We claim that both D_a and D_c are (k,m)–digraphs. Define $f : \{1, 2, \ldots, k\} \to \{1, 2, \ldots, k\}$ by the rule $f(k - i + 1) = i$. We now show that D_a is a (k,m)–digraph with ordering map f. Condition (i) is satisfied since clearly $[a_k]^-_{D_a} = 0$. To check Condition (ii), we recall that we proved above that $(B)_{(a_i,b)} + (B)_{(a_i,c)} = [a_i]^-_{D_a} - [a_i]^+_{D_a} + (m-1)$, and so $[a_i]^-_{D_a} - [a_i]^+_{D_a} + (m-1) \geq 0$, as required. On the other hand, Condition (iii) follows at once from the definition of D_a. A totally analogous argument shows that D_c is a (k,m)–digraph, also with ordering map f.

Thus both D_a and D_c are in $\mathcal{D}_{k,m}$, and so it follows from (8), (11), and (12) that

$$\chi_{\leq k}(\Pi) \geq 2\binom{k+1}{2} + \min_{D \in \mathcal{D}_{k,m}} \left\{ 2\left(\binom{k}{2} - \sum_{1\leq i\leq k} [v_i]^-_D\right) + \left(km - \sum_{1\leq i\leq k} \min\left\{[v_i]^-_D - [v_i]^+_D + (m-1), m\right\}\right)\right\}$$

$$= 2k^2 + km - \max_{D \in \mathcal{D}_{k,m}} \left\{ 2\left(\sum_{1\leq i\leq k} [v_i]^-_D\right) + \left(\sum_{1\leq i\leq k} \min\left\{[v_i]^-_D - [v_i]^+_D + (m-1), m\right\}\right)\right\}. \blacksquare$$

2.2 Bounding the solution of the digraph optimization problem

Our goal in this section is to find a (good) upper bound for the maximization problem in Proposition 13.

Define $f_{k,m}$ as follows:

$$f_{k,m}(D) := 2\sum_{1\leq i\leq k} [v_i]^-_D + \sum_{1\leq i\leq k} \min\left\{[v_i]^-_D - [v_i]^+_D + (m-1), m\right\}, \text{ for every } D \in \mathcal{D}_{k,m}. \tag{13}$$

Using this notation, our current goal is to find an upper bound for $\max_{D\in\mathcal{D}_{k,m}} \{f_{k,m}(D)\}$.

Our first step will be to find a (k,m)–digraph $D_0(k,m)$ that maximizes $f_{k,m}$.

2.2.1 Finding a digraph $D_0(k,m)$ that maximizes $f_{k,m}$

Let us define

$$\mathcal{M}_{k,m} := \left\{ D \in \mathcal{D}_{k,m} \;\middle|\; D \text{ maximizes } f_{k,m} \right\}.$$

Throughout this discussion, D is a fixed digraph in $\mathcal{M}_{k,m}$. Without any loss of generality, we assume D has vertex set $\{v_1, v_2, \ldots, v_k\}$, and if $\overrightarrow{v_iv_j}$ then $i < j$ (thus Property (ii) for (k,m)–digraphs is satisfied with the identity as ordering map). Since by assumption D is a (k,m)–digraph, it follows that, for every i, $[v_i]^-_D \leq [v_i]^+_D + (m-1)$.

Now let p, q, r be integers such that $1 \leq p < q < r \leq k$. We say that D has *the* (p,q,r)*–gap* if (i) for every j such that $p < j < q$, (v_p, v_j) is in D; (ii) for every j such that $q \leq j < r$, (v_p, v_j) is not in D; and (iii) (v_p, v_r) is in D.

If D has a gap, then the *order* of D is the lexicographically smallest vector $(p, q, -r)$ such that D has the (p,q,r)–gap. If D has no gaps, then the order of D is $(k-1, 1, 1)$ (note that no digraph can have a $(k-1, q, r)$–gap, since there are no integers q, r such that $k-1 < q < r \leq k$).

The crucial observation is the following.

Proposition 14 *Suppose that $D \in \mathcal{M}_{k,m}$ has some gap. Then there is a digraph D', also in $\mathcal{M}_{k,m}$, whose order is lexicographically greater than the order of D.*

The importance of Proposition 14 is that it implies that there is a digraph $D_0(k,m)$ in $\mathcal{M}_{k,m}$ that has no gaps (see Proposition 16). Furthermore, as we shall see later, the following observation, which will be used in the proof of Proposition 14, implies that having no gaps determines $D_0(k,m)$ uniquely inside $\mathcal{M}_{k,m}$.

Proposition 15 *For every $i \in \{1, \ldots, k\}$, $[v_i]^+_D = \min\{[v_i]^-_D + (m-1), k-i\}$.*

Proof. Suppose that for some i, $[v_i]^+_D \neq \min\{[v_i]^-_D + (m-1), k-i\}$. We note that since $[v_i]^+_D \leq \min\{[v_i]^-_D + (m-1), k-i\}$, we must then have $[v_i]^+_D < \min\{[v_i]^-_D + (m-1), k-i\}$. Thus in particular $[v_i]^+_D < k-i$, and so there is a $j > i$ such that $\overrightarrow{v_iv_j}$ is not in D. On the other hand, $[v_i]^+_D < [v_i]^-_D + (m-1)$ implies that the digraph $D + \overrightarrow{v_iv_j}$ is also in $\mathcal{D}_{k,m}$. It is readily checked that $f_{k,m}(D + \overrightarrow{v_iv_j}) > f_{k,m}(D)$, contradicting the maximality assumption for D. ∎

Proof of Proposition 14. Suppose that $D \in \mathcal{M}_{k,m}$ has a gap. Let (p, q, r) denote the order of D.

We need to analyze two cases separately.

Case 1 At least one of the following statements holds:

(A) There is a $j > r$ such that $\overrightarrow{v_rv_j}$ is in D, but $\overrightarrow{v_{r-1}v_j}$ is not in D.

(B) There is a j that satisfies $p < j < r-1$, such that $\overrightarrow{v_jv_{r-1}}$ is in D, but $\overrightarrow{v_jv_r}$ is not in D.

If (A) holds, then let $D' := D - \overrightarrow{v_pv_r} - \overrightarrow{v_rv_j} + \overrightarrow{v_pv_{r-1}} + \overrightarrow{v_{r-1}v_j}$ and if (B) holds, then let $D' := D - \overrightarrow{v_pv_r} - \overrightarrow{v_jv_{r-1}} + \overrightarrow{v_pv_{r-1}} + \overrightarrow{v_jv_r}$. Let (p', q', r') denote the order of D'. Since $[v_i]^-_{D'} - [v_i]^+_{D'} = [v_i]^-_D - [v_i]^-_D$ for every i, and D and D' have the same number of edges, it follows that $f_{k,m}(D') = f_{k,m}(D)$, and so D' is also in $\mathcal{M}_{k,m}$. Finally, it can be easily checked that in either case $(p', q', -r')$ is lexicographically greater than $(p, q, -r)$, as required.

Case 2 Neither (A) nor (B) holds.

Note that $\overrightarrow{v_{r-1}v_r}$ must be in D. Otherwise, the digraph $D_1 := D - \overrightarrow{v_pv_r} + \overrightarrow{v_pv_{r-1}} + \overrightarrow{v_{r-1}v_r}$ is also in $\mathcal{D}_{k,m}$, and $f_{k,m}(D_1) > f_{k,m}(D)$, contradicting that $D \in \mathcal{M}_{k,m}$. This observation, together with the assumption that (A) does not hold, implies the following:

$$[v_{r-1}]^+_D \geq [v_r]^+_D + 1. \tag{14}$$

Claim If $p > 1$, then the sequence $[v_1]^-_D, [v_2]^-_D, \ldots, [v_{p-1}]^-_D$ is non–decreasing.

Proof of Claim. Seeking a contradiction, let i be smallest integer such that $i < p$ and $[v_i]^-_D < [v_{i-1}]^-_D$. Note that $i \geq 2$, since $[v_2]^-_D = 1$ (this follows since $p > 1$, and so $\overrightarrow{v_1v_2}$ is in D) and $[v_1]^-_D = 0$. Now since $[v_i]^-_D < [v_{i-1}]^-_D$, and $\overrightarrow{v_{i-1}v_i}$ is in D, (otherwise there would be an $(i-1, q'', r'')$–gap for some q'', r'', and since $i - 1 < p$ this would contradict the choice of p), there are distinct j, j', with $j < j' < i-1$, such that both $\overrightarrow{v_jv_{i-1}}$ and $\overrightarrow{v_{j'}v_{i-1}}$ are in D, but neither $\overrightarrow{v_jv_i}$ nor $\overrightarrow{v_{j'}v_i}$ is in D. Since $j < p$, D has no (j, p'', q'')–gaps, and therefore $\overrightarrow{v_jv_\ell}$ is in D iff $j < \ell \leq i-1$. A similar argument shows that $\overrightarrow{v_{j'}v_\ell}$ is in D iff $j' < \ell \leq i-1$. Therefore $[v_j]^+_D = i-1-j$ and $[v_{j'}]^+_D = i-1-j'$. These numbers are less than $k-j$ and $k-j'$, respectively (since neither $\overrightarrow{v_jv_i}$ nor $\overrightarrow{v_{j'}v_i}$ are in D), and so it follows from Proposition 15 that $[v_j]^-_D = [v_j]^+_D - (m-1)$ and $[v_{j'}]^-_D = [v_{j'}]^+_D - (m-1)$. Thus $[v_{j'}]^-_D < [v_j]^-_D$, contradicting the choice of i. ∎

This Claim readily implies that at most one vertex v_j with $j < p$ satisfies that both $\overrightarrow{v_jv_{r-1}}$ is in D and $\overrightarrow{v_jv_r}$ is not in D. Since $\overrightarrow{v_pv_r}$ and $\overrightarrow{v_{r-1}v_r}$ are both in D and $\overrightarrow{v_pv_{r-1}}$ is not in D, and (B) does not hold, we have the following:

$$[v_{r-1}]^-_D \leq [v_r]^-_D - 1. \tag{15}$$

By Claim 15, $[v_r]^+_D$ equals either $[v_r]^-_D + (m-1)$ or $k-r$. Now if $[v_r]^+_D = [v_r]^-_D + (m-1)$, then it follows from (14) and (15) that $[v_{r-1}]^+_D \geq [v_{r-1}]^-_D + (m-1) + 2$, which contradicts the assumption that $D \in \mathcal{D}_{k,m}$. Therefore $[v_r]^+_D = k-r$. Now since (A) does not hold and $\overrightarrow{v_{r-1}v_r}$ is in D, it follows that $[v_{r-1}]^+_D = k-(r-1)$.

We define $D' := D - \overrightarrow{v_p v_r} + \overrightarrow{v_p v_{r-1}}$. It is straightforward to check that the order of D' is lexicographically greater than $(p, q, -r)$. Thus to conclude the proof it suffices to show that $D' \in \mathcal{M}_{k,m}$.

First we have to show that $D' \in \mathcal{D}_{k,m}$. We note that $[v_1]^-_{D'} = [v_1]^-_D = 0$, so Condition (i) holds. Condition (iii) also clearly holds. Since $[v_\ell]^-_{D'} \geq [v_\ell]^-_D$ for every $\ell \neq r$, it follows that in order to check that Condition (ii) holds we only need to verify that $[v_r]^-_{D'} + (m-1) \geq [v_r]^+_{D'}$. First we note that $[v_r]^+_{D'} = [v_r]^+_D = k - r$ and $[v_r]^-_{D'} = [v_r]^-_D - 1$. Thus it suffices to show $[v_r]^-_D + (m-1) - 1 \geq k - r$. Since $[v_{r-1}]^+_D = k - (r-1)$, it follows that $[v_{r-1}]^-_D + (m-1) \geq k - (r-1)$. Combined with (15), this implies $[v_r]^-_D + (m-1) - 1 \geq k - (r-1) > k - r$, as required.

We now show that $D' \in \mathcal{M}_{k,m}$. The construction of D' implies that (a) $\sum_{1 \leq i \leq k} [v_i]^-_{D'} = \sum_{1 \leq i \leq k} [v_i]^-_D$; (b) $[v_i]^+_{D'} = [v_i]^+_D$ for all i; (c) $[v_{r-1}]^-_{D'} = [v_{r-1}]^-_D + 1$; (d) $[v_r]^-_{D'} = [v_r]^-_D - 1$; and (e) $[v_i]^-_D = [v_i]^-_{D'}$ for all $i \notin \{r-1, r\}$. Given the definition of $f_{k,m}$, these statements imply that $f_{k,m}(D') - f_{k,m}(D) = \Delta_{r-1} + \Delta_r$, where $\Delta_{r-1} = \min\{[v_{r-1}]^-_{D'} - [v_{r-1}]^+_{D'}, 1\} - \min\{[v_{r-1}]^-_D - [v_{r-1}]^+_D, 1\}$, and $\Delta_r = \min\{[v_r]^-_{D'} - [v_r]^+_{D'}, 1\} - \min\{[v_r]^-_D - [v_r]^+_D, 1\}$. With this notation, $D' \in \mathcal{M}_{k,m}$ iff $\Delta_{r-1} + \Delta_r \geq 0$. Thus we conclude the proof by showing this last inequality. We observe that since $[v_{r-1}]^-_{D'} = [v_{r-1}]^-_D + 1$ and $[v_{r-1}]^+_{D'} = [v_{r-1}]^+_D$, it follows that $\Delta_{r-1} \geq 0$. Similarly, since $[v_r]^-_{D'} = [v_r]^-_D - 1$ and $[v_r]^+_{D'} = [v_r]^+_D$, then $\Delta_r \geq -1$.

First we deal with the case in which $[v_r]^-_D - [v_r]^+_D > 1$ (so that $[v_r]^-_{D'} - [v_r]^+_{D'} > 0$). In this case, $\min\{[v_r]^-_D - [v_r]^+_D, 1\} = \min\{[v_r]^-_{D'} - [v_r]^+_{D'}, 1\} = 1$, and so $\Delta_r = 0$. Since $\Delta_{r-1} \geq 0$, the required inequality follows.

Finally, suppose that $[v_r]^-_D - [v_r]^+_D \leq 1$. Using (14) and (15) we obtain $[v_{r-1}]^-_D - [v_{r-1}]^+_D \leq -1$ (and therefore $[v_{r-1}]^-_{D'} - [v_{r-1}]^+_{D'} \leq 0$). Thus, in this case $\min\{[v_{r-1}]^-_D - [v_{r-1}]^+_D, 1\} = [v_{r-1}]^-_D - [v_{r-1}]^+_D$ and $\min\{[v_{r-1}]^-_{D'} - [v_{r-1}]^+_{D'}, 1\} = [v_{r-1}]^-_{D'} - [v_{r-1}]^+_{D'}$. Since $[v_{r-1}]^-_{D'} = [v_{r-1}]^-_D + 1$ and $[v_{r-1}]^+_D = [v_{r-1}]^+_{D'}$, this gives $\Delta_{r-1} = 1$. Recalling that $\Delta_r \geq -1$, we obtain $\Delta_{r-1} + \Delta_r \geq 0$, as required. ∎

We are finally ready to define the graph $D_0(k, m)$.

Proposition 16 *Let $D_0(k, m)$ be the digraph with vertex set $\{v_1, v_2, \ldots, v_k\}$, defined as follows:*

(1) $[v_1]^-_{D_0(k,m)} = 0$;

(2) $[v_i]^+_{D_0(k,m)} = \min\{[v_i]^-_{D_0(k,m)} + (m-1), k - i\}$, for every $i \geq 1$; and

(3) For all i, j such that $1 \leq i < j \leq k$, the directed edge $\overrightarrow{v_i v_j}$ is in $D_0(k, m)$ if and only if $i + 1 \leq j \leq i + [v_i]^+_{D_0(k,m)}$.

Then $D_0(k, m) \in \mathcal{M}_{k,m}$. That is, $D_0(k, m)$ maximizes $f_{k,m}$ over $\mathcal{D}_{k,m}$.

Proof. By Proposition 14, there is a digraph in $\mathcal{M}_{k,m}$ with no gaps. By performing a relabeling if necessary, we may assume that its vertex set is $\{v_1, v_2, \ldots, v_k\}$, and that the identity is an ordering map for this digraph so that, in particular, the indegree of v_1 in this digraph is 0. Now Proposition 15 and the fact that the digraph has no gaps imply that this digraph is precisely the digraph $D_0(k, m)$. ∎

Before we proceed to estimate a lower bound for $f_{k,m}(D_0(k, m))$, we establish some basic properties of $D_0(k, m)$.

Proposition 17 *The digraph $D_0 = D_0(k, m)$ satisfies the following properties.*

(a) The sequence $\{[v_i]^-_{D_0}\}_{i=1}^k$ is non–decreasing.

(b) If i' is an integer such that $i := i' + [v_{i'}]^-_{D_0} + (m-1) \leq k$, then $[v_i]^-_{D_0} = [v_{i'}]^-_{D_0} + (m-1)$.

(c) If i' is an integer such that $i := i' + [v_{i'}]^-_{D_0} + (m-1) + 1 \leq k$, then $[v_i]^-_{D_0} = [v_{i'}]^-_{D_0} + (m-1)$.

Proof. Suppose that the sequence $[v_1]^-_{D_0}, [v_2]^-_{D_0}, \ldots, [v_k]^-_{D_0}$ is *not* non–decreasing and let i_0 be the smallest integer such that $[v_{i_0}]^-_{D_0} < [v_{i_0-1}]^-_{D_0}$. Note that $i \geq 3$, since $[v_2]^-_{D_0} = 1$ and $[v_1]^-_{D_0} = 0$. Now since $[v_{i_0}]^-_{D_0} < [v_{i_0-1}]^-_{D_0}$, and $\overrightarrow{v_{i_0-1}v_{i_0}}$ is in D_0 (since D_0 has no gaps), then there are distinct j, j', with $j < j' < i_0 - 1$, such that both $\overrightarrow{v_j v_{i_0-1}}$ and $\overrightarrow{v_{j'} v_{i_0-1}}$ are in D_0, but neither $\overrightarrow{v_j v_{i_0}}$ nor $\overrightarrow{v_{j'} v_{i_0}}$ is in D_0. Since D_0 has no gaps, it follows that $\overrightarrow{v_j v_\ell}$ is in D_0 iff $\ell \in \{j+1, j+2, \ldots, i_0 - 1\}$, and $\overrightarrow{v_{j'} v_\ell}$ is in D_0 iff $\ell \in \{j'+1, j'+2, \ldots, i_0 - 1\}$. Therefore $[v_{j'}]^-_{D_0} < [v_j]^-_{D_0}$ (see Proposition 15). Since this contradicts the minimality of i_0, it follows that $\{[v_i]^-_{D_0}\}$ is non–decreasing.

Now suppose that $i := i' + [v_{i'}]^-_{D_0} + (m-1) \leq k$. Note that it follows that $[v_{i'}]^+_{D_0} = [v_{i'}]^-_{D_0} + (m-1)$. Then $\overrightarrow{v_{i'} v_i}$ is in D_0. Moreover, using (a) and the fact that D_0 has no gaps, it follows that $\overrightarrow{v_j v_i}$ is in D_0 iff $i' \leq j \leq i' + [v_{i'}]^+_{D_0} - 1$. Thus $[v_i]^-_{D_0} = i' + [v_{i'}]^+_{D_0} - 1 - i' + 1 = [v_{i'}]^+_{D_0}$. This proves (b).

Finally, suppose that $i := i' + [v_{i'}]^-_{D_0} + (m-1) + 1 \leq k$. Note that it follows that $[v_{i'}]^+_{D_0} = [v_{i'}]^-_{D_0} + (m-1)$. Then $\overrightarrow{v_{i'} v_i}$ is not in D_0. Moreover, using (a) and the fact that D_0 has no gaps, it follows that $\overrightarrow{v_j v_i}$ is in D_0 iff $i' + 1 \leq j \leq i' + [v_{i'}]^+_{D_0}$. Thus $[v_i]^-_{D_0} = i' + [v_{i'}]^+_{D_0} - i' = [v_{i'}]^+_{D_0}$. This proves (c). ∎

2.2.2 Estimating $f_{k,m}(D_0(k,m))$

In order to bound $f_{k,m}(D_0(k,m))$, we will separately estimate upper bounds for the two expressions whose sum equals $f_{k,m}(D_0(k,m))$. These upper bounds are given in Propositions 20 and 22. In Proposition 23 we combine these statements to obtain the required upper bound for $f_{k,m}(D_0(k,m))$.

For the rest of the section, for convenience we denote $D_0(k,m)$ simply by D_0.

Step 1: Bounding the first summand of $f_{k,m}(D_0)$

Definition 18 *For each real number $x \geq 1$, we let $S_m(x)$ denote the (unique) positive integer such that*

$$1 + \frac{(S_m(x)-1)S_m(x)}{2}(m-1) \leq x < \frac{S_m(x)(S_m(x)+1)}{2}(m-1).$$

If $i \geq 1$ is an integer, then we let $T_m(i), U_m(i)$ denote the (unique) integers that satisfy $0 \leq T_m(i) \leq m-2$, $0 \leq U_m(i) \leq S_m(i) - 1$, and such that

$$i = 1 + \frac{(S_m(i)-1)S_m(i)}{2}(m-1) + S_m(i)T_m(i) + U_m(i). \tag{16}$$

Proposition 19 *For each integer i such that $1 \leq i \leq k$, we have $[v_i]^-_{D_0} = (S_m(i)-1)(m-1) + T_m(i)$.*

Proof. We proceed by induction on i. First suppose that $1 \leq i \leq m-1$. Then $S_m(i) = 1$ and $T_m(i) = i - 1$. Since $[v_1]^-_{D_0} = 0$, an iterated application of Property (1) in Proposition 17 shows that $[v_i]^-_{D_0} = i - 1 = T_m(i)$, as required.

To deal with the inductive step we fix $j \geq m$, assume that the statement holds for all $i < j$, and show that then it also holds for $i = j$.

Suppose first that $U_m(j) < S_m(j) - 1$. Define $j' := 1 + (1/2)(S_m(j)-1)(S_m(j)-2)(m-1) + (S_m(j)-1)T_m(j) + U_m(j)$. We note that it follows from (the uniqueness part of) Definition 18 that $S_m(j') = S_m(j) - 1, T_m(j') = T_m(j)$, and $U_m(j') = U_m(j)$. Now by the induction hypothesis, $[v_{j'}]^-_{D_0} = (S_m(j')-1)(m-1) + T_m(j') = (S_m(j)-2)(m-1) + T_m(j)$. An elementary calculation then shows that $j' + [v_{j'}]^-_{D_0} + (m-1) = j$. Applying Proposition 17(b), we obtain $[v_j]^-_{D_0} = [v_{j'}]^-_{D_0} + (m-1) = (S_m(j)-1)(m-1) + T_m(j)$, as required.

Finally, suppose that $U_m(j) = S_m(j) - 1$. Define $j' := 1 + (1/2)(S_m(j) - 1)(S_m(j) - 2)(m - 1) + (S_m(j) - 1)T_m(j) + (U_m(j) - 1)$. As in the previous case, the uniqueness guaranteed by Definition 18 yields that $S_m(j') = S_m(j) - 1, T_m(j') = T_m(j)$, and $U_m(j') = U_m(j) - 1$. By the induction hypothesis, $[v_{j'}]^-_{D_0} = (S_m(j') - 1)(m - 1) + T_m(j') = (S_m(j) - 2)(m - 1) + T_m(j)$, and so in this case an elementary calculation shows that $j' + [v_{j'}]^-_{D_0} + (m - 1) + 1 = j$. Applying Proposition 17(c), we obtain $[v_j]^-_{D_0} = [v_{j'}]^-_{D_0} + (m - 1) = (S_m(j) - 1)(m - 1) + T_m(j)$, as required. ∎

Before we proceed to bound the first summand of $f_{k,m}$, we note that (16) gives that, for all integers i,

$$T_m(i) = \left\lfloor \frac{i - 1 - S_m(i)(S_m(i) - 1)(m - 1)/2}{S_m(i)} \right\rfloor. \tag{17}$$

Proposition 20

$$\sum_{1 \le i \le k} [v_i]^-_{D_0} \le \left(\frac{1}{2S_m(k)}\right) k^2 + \left(\frac{1}{2}(S_m(k) - 1)\right) k(m - 1) + \frac{1}{24}\left(S_m(k) - S_m(k)^3\right)(m - 1)^2 + O(k),$$

where $O(k)$ is independent of m.

Proof. Let $B_m : [1, \infty] \to \mathbb{R}$ be function defined by

$$B_m(x) := (S_m(x) - 1)(m - 1) + \frac{x - 1 - S_m(x)(S_m(x) - 1)(m - 1)/2}{S_m(x)}. \tag{18}$$

It follows from Proposition 19 and (17) that $[v_i]^-_{D_0} \le B_m(i)$ for every $i \ge 1$. Therefore

$$\sum_{1 \le i \le k} [v_i]^-_{D_0} \le \int_1^k B_m(x)dx + O(k).$$

An elementary calculation shows that this last integral equals the right hand side (without the $O(k)$ term) of the inequality stated in Proposition 20. ∎

Step 2: Bounding the second summand of $f_{k,m}(D_0)$

Let

$$i_0 = i_0(k, m) := \max\{j \mid [v_j]^-_{D_0} + (m - 1) \le k - j\}. \tag{19}$$

Thus, informally, i_0 is the largest integer i such that $[v_i]^+_{D_0}$ is determined by $[v_i]^-_{D_0}$, and not by $k - i$: if $i \le i_0$, then $[v_i]^+_{D_0} = [v_i]^-_{D_0} + (m - 1)$; and if $i > i_0$, then $[v_i]^+_{D_0} = k - i$.

Now define the function $C_{k,m} : [1, k] \to \mathbb{R}$ as follows:

$$C_{k,m}(x) := \begin{cases} 0, & x \le i_0, \\ 1 + \dfrac{S_m(i_0) + 1}{S_m(i_0)}(x - i_0), & i_0 < x \le i_0 + \dfrac{S_m(i_0)}{S_m(i_0) + 1}(m - 1), \\ m, & i_0 + \dfrac{S_m(i_0)}{S_m(i_0) + 1}(m - 1) < x \le k. \end{cases}$$

Proposition 21 *For every integer $i \geq 1$,*

$$\min\left\{[v_i]^-_{D_0} - [v_i]^+_{D_0} + (m-1), m\right\} \leq C_{k,m}(i).$$

Proof. First we show that if $i \leq i_0$, then $\min\left\{[v_i]^-_{D_0} - [v_i]^+_{D_0} + (m-1), m\right\} = C_{k,m}(i) = 0$. Since by Proposition 19 $[v_j]^-_{D_0}$ is non–decreasing, it follows that $[v_i]^-_{D_0} + (m-1) \leq [v_{i_0}]^-_{D_0} + (m-1) \leq k - i_0 \leq k - i$. Thus, by Proposition 15, $[v_i]^+_{D_0} = [v_i]^-_{D_0} + (m-1)$, and so $\min\{[v_i]^-_{D_0} - [v_i]^+_{D_0} + (m-1), m\} = 0$.

Now we analyze the case $i > i_0$. Since $\{[v_j]^-_{D_0}\}$ is non–decreasing, then $[v_i]^-_{D_0} + (m-1) \geq [v_{i_0}]^-_{D_0} + (m-1) = k - i_0 > k - i$. Thus Proposition 15 implies that $[v_i]^+_{D_0} = k - i$. Since $[v_{i_0}]^+_{D_0} = k - i_0$, then $[v_{i_0}]^+_{D_0} - [v_i]^+_{D_0} = i - i_0$. Therefore $([v_i]^-_{D_0} - [v_i]^+_{D_0}) + ([v_{i_0}]^+_{D_0} - [v_{i_0}]^-_{D_0}) = (i - i_0) + ([v_i]^-_{D_0} - [v_{i_0}]^-_{D_0})$.

We also observe that it follows easily from Proposition 19 that if $j < j'$, then $[v_{j'}]^-_{D_0} < [v_j]^-_{D_0} + 1 + (j' - j)/S_m(j)$. Thus $[v_i]^-_{D_0} - [v_{i_0}]^-_{D_0} < 1 + (i - i_0)/S_m(i_0)$.

Now since $[v_{i_0}]^+_{D_0} - [v_{i_0}]^-_{D_0} = m - 1$, we finally obtain

$$[v_i]^-_{D_0} - [v_i]^+_{D_0} + (m-1) < 1 + \frac{S_m(i_0)+1}{S_m(i_0)}(i - i_0), \text{ for all } i > i_0.$$

This last inequality immediately implies that $\min\{[v_i]^-_{D_0} - [v_i]^+_{D_0} + (m-1), m\} \leq C_{k,m}(i)$ for all $i > i_0$. ∎

Proposition 22

$$\sum_{1 \leq i \leq k} \min\left\{[v_i]^-_{D_0} - [v_i]^+_{D_0} + (m-1), m\right\} \leq \frac{k(m-1)}{S_m(k)} + \left(\frac{(S_m(k)-1)^2}{2S_m(k)}\right)(m-1)^2 + O(k). \quad ∎$$

Proof. First we observe that Proposition 21 implies that

$$\sum_{1 \leq i \leq k} \min\left\{[v_i]^-_{D_0} - [v_i]^+_{D_0} + (m-1), m\right\} \leq \int_1^k C_{k,m}(x)dx + O(k), \tag{20}$$

and an elementary calculation shows that

$$\int_1^k C_{k,m}(x)dx = (k - i_0)m - \frac{1}{2}\left(\frac{S_m(i_0)}{S_m(i_0)+1}\right)(m-1)^2. \tag{21}$$

Our aim now is to express $S_m(i_0)$ and (an estimate of) i_0 in terms of $S_m(k)$. First we show that $S_m(i_0) = S_m(k) - 1$.

Seeking a contradiction, suppose that $S_m(i_0) < S_m(k) - 1$ (that is, $S_m(i_0) \leq S_m(k) - 2$). Then, by Proposition 19, $[v_{i_0}]^-_{D_0} = (S_m(i_0) - 1)(m-1) + T_m(i_0) < (S_m(k) - 2)(m-1)$. Also note that $i_0 < \binom{S_m(k)-1}{2}(m-1) + 1$, and since $k \geq \binom{S_m(k)}{2}(m-1) + 1$, it follows that $k - i_0 > (S_m(k) - 1)(m-1)$. Therefore $[v_{i_0}]^-_{D_0} + (m-1) < (S_m(k) - 1)(m-1) < k - i_0$, and since both inequalities are strict we have $[v_{i_0}]^-_{D_0} + (m-1) \leq k - i_0 - 2$. Since D_0 has no gap, it follows that $[v_{i+1}]^-_{D_0} \leq [v_i]^-_{D_0} + 1$ for every i. Thus $[v_{i_0+1}]^-_{D_0} \leq [v_{i_0}]^-_{D_0} + 1$, and so $[v_{i_0+1}]^-_{D_0} + (m-1) \leq k - (i_0 + 1)$, contradicting the definition of i_0. Therefore $S_m(i_0) \geq S_m(k) - 1$.

Now suppose, again for sake of contradiction, that $S_m(i_0) \geq S_m(k)$. Since $S_m(i) \leq S_m(k)$ for every $i \in \{1, 2, \ldots, k\}$, it follows that $S_m(i_0) = S_m(k)$. Then $\binom{S_m(k)}{2}(m-1) + 1 \leq i_0$, and since $k < \binom{S_m(k)+1}{2}(m-1)$, it follows that $k - i_0 < S_m(k)(m-1) - 1$. Now since $S_m(i_0) = S_m(k)$, it follows from Proposition 19 that

$[v_{i_0}]^-_{D_0} \geq (S_m(k)-1)(m-1)$, and so using the definition of i_0 we obtain $k - i_0 \geq S_m(k)(m-1)$. The contradiction between these two inequalities for $k - i_0$ shows that $S_m(i_0) \leq S_m(k) - 1$. Thus $S_m(i_0) = S_m(k) - 1$, as claimed.

Let x_0 denote the solution of $B_m(x) + (m-1) = k - x$. Since $0 \leq B_m(i) - [v_i]^-_{D_0} < 1$ for every integer i, and the slope of $B_m(i)$ (note that $B_m(i)$ is piecewise linear) is never greater than one, it follows that (i) if $U_m(i_0) = 0$, then $i_0 \leq x_0 < i_0 + 1$; and (ii) if $1 \leq U_m(i_0) \leq S_m(i_0) - 1$, then $i_0 - 1 < x_0 < i_0 + 1$. These observations imply that $S_m(x_0) = S_m(i_0) = S_m(k) - 1$. Therefore, by (18),

$$B_m(x_0) = (S_m(k)-2)(m-1) + \frac{x_0 - 1 - (1/2)(S_m(k)-1)(S_m(k)-2)(m-1)}{S_m(k)-1}.$$

Solving $B_m(x_0) + (m-1) = k - x_0$, we obtain

$$x_0 = \left(\frac{S_m(k)-1}{S_m(k)}\right) k - \left(\frac{S_m(k)-1}{2}\right)(m-1) + \frac{1}{S_m(k)}.$$

Now since $|i_0 - x_0| < 1$ and $m, x_0 < k$, then $(k-i_0)m = (k-x_0)(m-1) + O(k)$. Therefore

$$\begin{aligned}(k-i_0)m - \frac{1}{2}\left(\frac{S_m(i_0)}{S_m(i_0)+1}\right)(m-1)^2 &= (k-x_0)(m-1) - \frac{1}{2}\left(\frac{S_m(k)-1}{S_m(k)}\right)(m-1)^2 + O(k) \\ &= \frac{k(m-1)}{S_m(k)} + \left(\frac{(S_m(k)-1)^2}{2S_m(k)}\right)(m-1)^2 - \frac{m-1}{S_m(k)} + O(k).\end{aligned}$$

We note that since $S_m(k) \geq 1$ and $m < k$, then $(m-1)/S_m(k)$ is $O(k)$. Thus the proposition follows using this last equality and (20) and (21). ∎

Proposition 23

$$\max_{D \in \mathcal{D}_{k,m}} \left\{ 2 \sum_{1 \leq i \leq k} [v_i]^-_D + \sum_{1 \leq i \leq k} \min\left\{[v_i]^-_D - [v_i]^+_D + (m-1), m\right\} \right\} \quad \leq$$

$$\left(\frac{1}{S_m(k)}\right) k^2 + \left(\frac{S_m(k)^2 - S_m(k) + 1}{S_m(k)}\right) k(m-1) - \left(\frac{S_m(k)^4 - 7S_m(k)^2 + 12S_m(k) - 6}{12S_m(k)}\right)(m-1)^2 + O(k),$$

where

$$S_m(k) = \left\lfloor \frac{1 + \sqrt{1 + \frac{8(k-1)}{m-1}}}{2} \right\rfloor.$$

Proof. First we note that an elementary calculation shows that the expression for $S_m(k)$ given in this statement indeed agrees with the value of $S_m(k)$ according to Definition 18.

Finally, we recall from Proposition 16 that D_0 maximizes $f_{k,m}$ over $\mathcal{D}_{k,m}$. This observation, together with Propositions 20 and 22, and a routine algebraic manipulation, implies Proposition 23. ∎

2.3 Proof of Theorem 8

We recall that $m = n - 2k$, and so $s(k,n) = S_m(k)$. Therefore Theorem 8 is an immediate consequence of Propositions 13 and 23 (note that we also used the obvious inequality $km \geq k(m-1)$). ∎

3 Proof of Proposition 9

Our first observation is that, for sufficiently large n, it follows from Claim 24 in the Appendix that $F(k,n) > 3\binom{k+1}{2}$ for every $k > k_1(n)$. We also note that if we define

$$\widetilde{s}\,(x) := \left\lfloor \frac{1}{2}\left(1 + \sqrt{\frac{1+6x}{1-2x}}\right) \right\rfloor,$$

then it is easy to check that $\widetilde{s}(k/n) = s(k,n)$ (and, moreover, $\widetilde{s}(k/n) = s(k+1,n)$) for all but at most $O(\sqrt{n})$ values of k.

These observations imply that

$$\sum_{k=1}^{(n-2)/2-1} \big(n-2k-3\big) \cdot \max\left\{3\binom{k+2}{2}, F(k+1,n)\right\}$$

$$\geq\ 3 \sum_{k=1}^{\lfloor k_1(n)\rfloor} \big(n-2k-3\big)\binom{k+2}{2} + \sum_{k=\lfloor k_1(n)\rfloor+1}^{(n-2)/2-1} \big(n-2k-3\big)F(k+1,n)$$

$$\geq\ \frac{3}{2}n^3 \cdot \left(\sum_{k=1}^{\lfloor k_1(n)\rfloor} \left(1 - 2\left(\frac{k}{n}\right)\right)\left(\frac{k}{n}\right)^2\right) + n^3 \cdot \left(\sum_{k=\lfloor k_1(n)\rfloor+1}^{(n-2)/2-1} \left(1-2\left(\frac{k}{n}\right)\right)\frac{F(k+1,n)}{n^2}\right) \ +\ O(n^3)$$

$$\geq\ \frac{3}{2}n^4 \cdot \left(\int_0^{c_1} (1-2x)x^2\ dx\right) + n^4 \cdot \left(\int_{c_1}^{1/2} (1-2x)\widetilde{f}(x)\ dx\right) + O(n^3),$$

where $c_1 := 0.465178$ (recall that $k_1(n) \approx 0.465178n + O(\sqrt{n})$), and

$$\widetilde{f}(x) := \left(2 - \frac{1}{\widetilde{s}(x)}\right)x^2 - \left(\frac{(\widetilde{s}(x)-1)^2}{\widetilde{s}(x)}\right)x(1-2x) + \left(\frac{\widetilde{s}(x)^4 - 7\widetilde{s}(x)^2 + 12\widetilde{s}(x) - 6}{12\widetilde{s}(x)}\right)(1-2x)^2.$$

To complete the proof, we note that a numerical evaluation of the integrals in the previous inequality yields

$$\frac{3}{2}\int_0^{c_1} (1-2x)x^2\ dx + \int_{c_1}^{1/2} (1-2x)\widetilde{f}(x)\ dx \approx \frac{0.37553}{24}. \ ∎$$

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Appendix: Analysis of our improved bound for $\mathbf{X}_{\leq k}(n)$

Previous to this paper, the best bounds known for $\mathbf{X}_{\leq k}(n)$ were those given by (1), which is tight for $k \leq n/3$, and (3), which is better than (1) for $k > k_0(n) = \sqrt{(2\sqrt{13}-5)/9n} \approx 0.4956n + O(\sqrt{n})$.

We claimed in several places that the bound we give in Theorem 8 is indeed better that the bounds in (1) and (3) for $k \geq k_1(n) = (1/162)\left(-71 + 71n + \sqrt{19n^2 - 38n + 19}\right) \approx 0.465178n + O(\sqrt{n})$.

Our aim in this Appendix is to prove this claim.

We note that since (3) is better than (1) iff $k > k_0(n)$, it follows that it suffices to prove the claims below.

Claim 24 *For all n sufficiently large, and every $k > k_1(n)$, the bound in Theorem 8 is better than the bound in (1).*

Proof. Since $3\binom{k+1}{2} = (3/2)k^2 + O(k) = (3/2)k^2 + O(n)$, it suffices to show that $F(k,n) > (3/2)k^2$ for $k > k_1(n)$.

Let $k > k_1(n)$. It follows from the definition of $s(k,n)$ that if $k \geq 6n/13 - 5/13 \approx 0.462n$, then $s(k,n) \geq 4$. Since (for n sufficiently large) $k_1(n) > 0.462n$, it follows that $s(k,n) \geq 4$.

We need to analyze three possibilities separately.

Case 1 : $s(k,n) = 4$.

In this case, by the definition of $s(k,n)$, $(6/13)n - (5/13) \leq k < (10/21)n - (10/21)$, and the definition of $F(k,n)$ gives $F(k,n) = \frac{7}{4}k^2 - \frac{9}{4}k(n-2k-1) + \frac{31}{8}(n-2k-1)^2$. We note that, for n sufficiently large, $(6/13)n - (5/13) < k_1(n) < (10/21)n - (10/21)$.

Solving $F(k,n) - (3/2)k^2 = 0$ for k in terms of n, we obtain the roots $(1/162)(-71+71n \pm \sqrt{19n^2 - 38n + 19})$ (one of which is $k_1(n)$). Now (for fixed n) $F(k,n) - (3/2)k^2$ is increasing for $k > k_1(n)$. Thus it follows that, if $s(k,n) = 4$ and $k > k_1(n)$, then $F(k,n) > (3/2)k^2$, as required.

Case 2 : $s(k,n) = 5$ or 6.

Suppose that $s(k,n) = 5$. Then $F(k,n) = \frac{9}{5}k^2 - \frac{16}{5}k(n-2k-1) + \frac{42}{5}(n-2k-1)^2$. On the other hand, the definition of $s(k,n)$ gives that $(10/21)n - (9/21) \leq k < (15/31)n - (15/31)$. Now solving the equation $F(k,n) - (3/2)k^2 = 0$ for k in terms of n, one finds that both roots are smaller than $(10/21)n - (9/21)$. As (for each fixed n) $F(k,n) - (3/2)k^2$ is an increasing function of k for all k larger than the largest root, it follows that within the given range for k, $F(k,n)$ is always greater than $(3/2)k^2$, as claimed.

Now suppose that $s(k,n) = 6$. Then $F(k,n) = \frac{11}{6}k^2 - \frac{25}{6}k(n-2k-1) + \frac{185}{12}(n-2k-1)^2$. Solving $F(k,n) - (3/2)k^2 = 0$ for k in terms of n yields imaginary roots. A direct evaluation at any k for which $s(k,n) = 6$ yields that $F(k,n) - (3/2)k^2 > 0$. Therefore in this case also $F(k,n) > (3/2)k^2$, as required.

Case 3 $s(k,n) \geq 7$. First we note that the definition of $s(k,n)$ gives that $k \geq (21/43)n - (20/43)$. A direct calculation can be used to verify the Claim in case $k = (21/43)n - (20/43)$. Thus, as n is arbitrarily large, we can assume $k/n \geq 21/43$.

Define

$$\overline{s}(k,n) := \frac{1}{2}\left(1+\sqrt{\frac{1+6\left(\frac{k}{n}\right)-\left(\frac{9}{n}\right)}{1-2\left(\frac{k}{n}\right)-\left(\frac{1}{n}\right)}}\right), \quad \text{and } \underline{s}(k,n) := \overline{s}(k,n)-1.$$

Clearly, for all values of k and n, $\underline{s}(k,n) < s(k,n) \leq \overline{s}(k,n)$.

Now we let

$$\underline{F}(k,n) := \left(2-\frac{1}{\underline{s}(k,n)}\right)k^2 - \left(\frac{(\overline{s}(k,n)-1)^2}{\underline{s}(k,n)}\right)k(n-2k-1)$$

$$+\left(\frac{\underline{s}(k,n)^4-7\overline{s}(k,n)^2+12\underline{s}(k,n)-6}{12\overline{s}(k,n)}\right)(n-2k-1)^2.$$

It follows immediately that, for all k and n, $F(k,n) > \underline{F}(k,n)$.

Finally, define

$$\overline{z}(x) := \frac{1}{2}\left(1+\sqrt{\frac{1+6x}{1-2x}}\right), \quad \text{and } \underline{z}(x) := \overline{z}(x)-1,$$

and

$$G(x) := \left(2-\frac{1}{\underline{z}(x)}\right)x^2 - \left(\frac{(\overline{z}(x)-1)^2}{\underline{z}(x)}\right)x(1-2x) + \left(\frac{\underline{z}(x)^4-7\overline{z}(x)^2+12\underline{z}(x)-6}{12\overline{z}(x)}\right)(1-2x)^2.$$

By making n sufficiently large, we can make $\left(n^2\cdot G(k/n)\right)/\underline{F}(k,n)$ arbitrarily close to 1. Since $F(k,n) > \underline{F}(k,n)$, it follows that it suffices to show that $n^2\cdot G(k/n) > (3/2)k^2$ if $k/n \geq 21/43$. Letting $x := k/n$, it suffices to show that $G(x) > (3/2)x^2$ if $x \geq 21/43$. This can be proved by a tedious but straightforward calculus argument, as $G(21/43) > 3(21/43)^2/2$ and $G(x)-(3/2)x^2$ is a smooth, strictly increasing in the the interval $(21/43, 1/2)$. ∎

Claim 25 *For all n sufficiently large, and every $k > k_0(n)$, the bound in Theorem 8 is better than the bound in (3).*

Proof. Invoking the discussion at the end of the proof of Claim 24, in this case it suffices to show that $n^2\cdot G(k/n) > n^2(1/2-\sqrt{1-4(k/n)^2})+O(n)$ if $k > k_0(n)$. Thus it suffices to show that $G(x) > 1/2-\sqrt{1-4x^2}$ if $0.4956 < x < 1/2$. As in the proof of Claim 24, this is proved with a long and tedious, but elementary, calculus argument. ∎