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A problem on 0–1 matrices

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Abstract. We compute the maximal and the minimal value of $\|M^2\|$ over the class of 0–1 valued $N \times N$ matrices M with K entries equal to one for fixed K and N , where $\|\cdot\|$ denotes the sum of the entries. This result has applications to graph theory and probability theory.

1. Introduction

1.0. A despotic problem

A country has 38 airports. Between these airports exist 639 direct flights. The despot of this country wants to get more control over the population by diminishing the interlocal traffic. Because of the public opinion in the rest of the world, he can not change the number of airports or the number of direct flights.

How should the despot distribute the 639 direct flights over the (ordered) pairs of airports, such that the number of different flights with one transit is minimized?

This problem can be solved by applying Theorem 2 of this paper. The minimal number of flights with one transit is 6239.

1.1. The matrix problem

Let $\|M\|$ denote the sum of the absolute values of the entries of a matrix M . Let $\mathcal{M}_{N,K}$ be the set of 0–1 valued $N \times N$ matrices with $\|M\| = K$.

In this paper we compute the maximal and minimal value of $\|M^2\|$ over $\mathcal{M}_{N,K}$ for fixed N and K ($0 \leq K \leq N^2$). So we are looking for

$$\max(N, K) := \max \{ \|M^2\| : M \in \mathcal{M}_{N,K} \}$$

and

$$\min(N, K) := \min \{ \|M^2\| : M \in \mathcal{M}_{N,K} \}.$$

We give an application of this problem to graph theory and to stochastic processes.

1.2. The problem in terms of graphs

Let G be a directed graph consisting of N vertices and K edges. Solving the matrix problem is equivalent (as [F.] remarks) to solving the problem of finding for fixed N and K the maximal and minimal number of paths of length two, i.e. pairs of edges $a = (v, v')$, $b = (v', v'')$.

1.3. The problem in terms of two-correlations of stochastic processes

Let $(Y_n)_{n \in \mathbb{Z}}$ be an i.i.d. sequence of random variables. A *two-block factor* $(X_n)_n$ of this sequence is defined by

$$X_n := f(Y_n, Y_{n+1})$$

for some function f .

The process $(X_n)_n$ has the property of *one-dependence*, i.e. for each integer time t the future $(X_n)_{n > t}$ is independent of the past $(X_n)_{n < t}$, as is easily checked. [A.G.] and [A.G.K.V.] have shown that not all one-dependent two-state processes are two-block factors (this was conjectured for several years).

We return to our matrices by restricting our attention to two-block factors of an i.i.d. sequence $(D_n)_n$, each D_n uniformly distributed over a finite set $\{1, \dots, N\}$. A matrix $M \in \mathcal{M}_{N,K}$ yields a two-block factor as follows

$$X_n := M_{D_n, D_{n+1}}.$$

Define $H_j := \sum_{i=1}^N M_{ij}$ and $V_j := \sum_{i=1}^N M_{ji}$ ($i, j = 1, \dots, N$). We have

$$P[X_n = 1] = K/N^2$$

and for the two-correlation $P[X_n = X_{n+1} = 1]$ we have

$$\begin{aligned} N^3 \cdot P[X_n = X_{n+1} = 1] &= \sum_{i=1}^N \sum_{j=1}^N (M^2)_{i,j} = \sum_{i=1}^N \sum_{j=1}^N \left(\sum_{t=1}^N M_{it} M_{tj} \right) \\ &= \sum_{i=1}^N H_i V_i =: I_M. \end{aligned}$$

We conclude that the matrix problem above is equivalent to the problem of computing the maximal and minimal two-correlation, for fixed probability of a one, over the class of two-block factors of i.i.d. sequences $(D_n)_n$, where D_n is uniformly distributed over $\{1, \dots, N\}$.

Let $(Y_n)_n$ be an i.i.d. sequence, each Y_n uniformly distributed over the unit interval. Given a Lebesgue-measurable set A in the unit square we construct a two-block factor (the corresponding *indicator process*) $(X_n)_n$ by taking f equal to the indicator function of A (see [V.] for more details).

Let $\max(\alpha)$ and $\min(\alpha)$ be the maximal, minimal resp., two-correlation over the class of indicator processes for fixed probability α of a one. An approximation argument (approximation of the uniform distribution by discrete distributions) shows that the connection between $\max(\alpha)$ and $\max(N, K)$, $\min(\alpha)$ and $\min(N, K)$ resp., is

$$\max(\alpha) = \sup_{N, K} \left\{ \frac{\max(N, K)}{N^3} : \alpha \geq K/N^2 \right\}$$

and

$$\min(\alpha) = \inf_{N, K} \left\{ \frac{\min(N, K)}{N^3} : \alpha \leq K/N^2 \right\}.$$

The discretization of the variational problems $\max(\alpha)$ and $\min(\alpha)$ was the motivation for this research.

We associate to a matrix $M \in \mathcal{M}_{N, K}$ a subset A_M of $[0, N] \times [0, N]$ by setting

$$A_M := \bigcup_{\{(i, j): M_{i, j} = 1\}} \langle i - 1, i \rangle \times \langle j - 1, j \rangle.$$

We remark that the class of two-block factors of an i.i.d. sequence $(D_n)_n$ (each D_n uniformly distributed over $\{1, \dots, N\}$) is a subclass of the class of indicator processes, by taking $A = (1/N)A_M$ for the associated matrix $M \in \mathcal{M}_{N, K}$.

1.4. Previous results

For the class of two-block factors the problem of the maximal two-correlation ($\max(\alpha)$) was solved in [Ka.] and [F.] and the problem of the minimal two-correlation ($\min(\alpha)$) was solved in [V.] (α denotes the fixed probability of a one). The results are

$$\max(\alpha) = \begin{cases} 2\alpha - 1 + (1 - \alpha)^{3/2}, & 0 \leq \alpha \leq \frac{1}{2} \\ \alpha^{3/2}, & \frac{1}{2} \leq \alpha \leq 1 \end{cases}$$

and

$$\min(\alpha) = \begin{cases} \frac{m(m-1)}{6(m+1)^2}(1-2\delta)(1+\delta)^2, & 0 \leq \alpha < \frac{1}{2} \\ \frac{1}{6}, & \alpha = \frac{1}{2} \\ 2\alpha - 1 + \min(1 - \alpha), & \frac{1}{2} < \alpha \leq 1 \end{cases}$$

with $m := \text{int}(1/(1 - 2\alpha))$ and $\delta := \sqrt{1 - 2\alpha((m+1)/m)}$. (Here $\text{int}(x)$ is the integer part of x).

The upper bound $\max(\alpha)$ also holds for the wider class of one-dependent processes. For $\alpha \neq \frac{1}{2}$ there is a unique one-dependent process with two-correlation $\max(\alpha)$, and for $\alpha = \frac{1}{2}$ there are exactly two such processes. These processes are all two-block factors, determined by the sets

$$A = [0, 1 - \sqrt{1 - \alpha}] \times [0, 1] \cup [1 - \sqrt{1 - \alpha}, 1] \times [0, 1 - \sqrt{1 - \alpha}]$$

for $0 \leq \alpha \leq \frac{1}{2}$,

and

$$A = [0, \sqrt{\alpha}] \times [0, \sqrt{\alpha}] \quad \text{for } \frac{1}{2} \leq \alpha \leq 1.$$

For proofs see [G.K.V.].

1.5. Introductory remarks

Let l be the $N \times N$ matrix with all entries equal to one.

The following lemma shows that we may restrict our attention to the case $K \leq \frac{1}{2}N^2$ and that the maximum (c.q. minimum) is attained in M (for K) iff it is attained in $l - M$ (for $N^2 - K$).

We will use this observation in Theorem 2.

COMPLEMENT LEMMA. *For a matrix $M \in \mathcal{M}_{N,K}$ we have*

$$I_{l-M} = I_M - 2NK + N^3.$$

We omit the straightforward proof. (see also the Complement Lemma in [V.])

REFLECTION LEMMA. *Let $M \in \mathcal{M}_{N,K}$. Let $M', M'' \in \mathcal{M}_{N,K}$ be the matrices obtained by reflecting M with respect to the diagonal, the cross-diagonal resp., i.e., $M'_{i,j} = M_{j,i}$ and $M''_{i,j} = M_{N+1-j, N+1-i}$. Then $I_{M'} = I_{M''} = I_M$.*

We omit the straightforward proof.

2. The results

THEOREM 1 (Maximum). Let $\mathcal{M}_{N,K}$ be the class of 0-1 valued $N \times N$ matrices with K entries equal to one. Then $I_M = \|M^2\|$ attains its maximal value $\max(N, K)$ over $\mathcal{M}_{N,K}$ in (at least) one of the types I, II, III and IV.

THEOREM 2 (Minimum). Let $\mathcal{M}_{N,K}$ be the class of 0-1 valued $N \times N$ matrices with K entries equal to one. The following table gives the possible types where $I_M = \|M^2\|$ can attain its minimal value $\min(N, K)$ over $\mathcal{M}_{N,K}$ for the corresponding ranges of K .

Range of K	Type
(a) $0 \leq K \leq \frac{1}{4}N^2$	V
(b) $\frac{1}{4}N^2 < K < \frac{1}{2}N(N-1)$	VI, VII or VIII
(c) $\frac{1}{2}N(N-1) \leq K \leq \frac{1}{2}N(N+1)$	IX
(d) $\frac{1}{2}N(N+1) < K < \frac{3}{4}N^2$	complement of VI, VII or VIII
(e) $\frac{3}{4}N^2 \leq K \leq N^2$	complement of V

In each matrix of these types $I_M = \min(N, K)$ and for each pair (N, K) there exists a matrix of these types. In case (c) there exists a unique matrix of the described type. In cases (b) and (d) there exists exactly one or exactly two matrices of the corresponding types.

The solution to the despotic problem is found by computing the corresponding parameters of the type VI, VII and VIII. It turns out that only type VIII is suitable for the despotic problem. We shall give the solution in the Appendix.

The types of matrices where I_M attains its maximal and minimal value

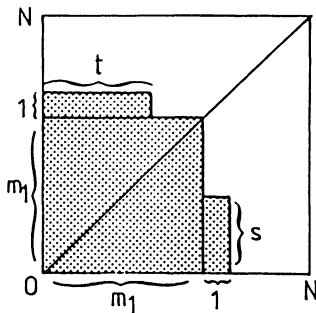


Figure I

Type I: (Maximum)

$$0 \leq s \leq t \leq m_1 \leq N,$$

$$t - s \leq 1,$$

$$K = m_1^2 + s + t,$$

$$I_M = m_1^3 + s(m_1 + 1) + tm_1 + st.$$

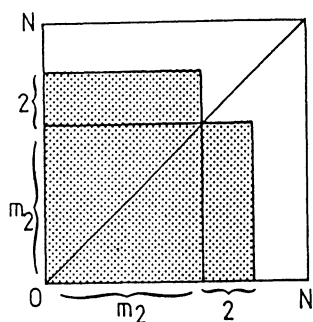


Figure II

Type II: (Maximum)

$$K = (m_2 + 2)^2 - 4,$$

$$I_M = m_2(m_2^2 + 6m_2 + 4).$$

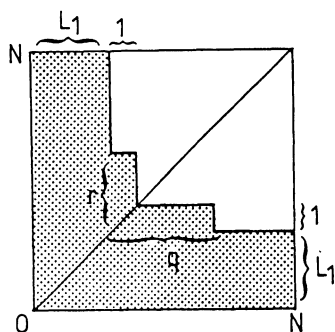


Figure III

Type III: (Maximum)

This type is the complement of type I reflected in the diagonal through $(0, N)$.

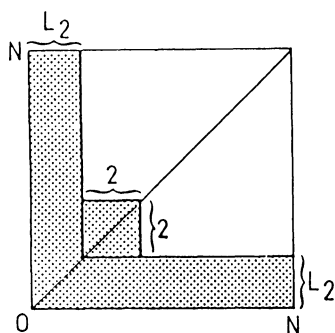


Figure IV

Type V: (Minimum)

This type is the complement of type II reflected in the diagonal through $(0, N)$.

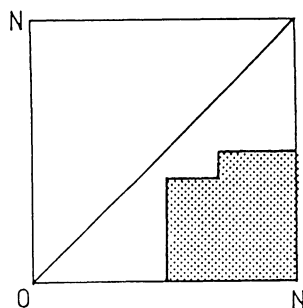


Figure V

Type V: (Minimum)

$$A_M \subset [\text{int}(\tfrac{1}{2}N), N] \times [0, \text{int}(\tfrac{1}{2}N)],$$

$$I_M = \min(N, K) = 0.$$

A_M is as in Figure V.

Type VI: (Minimum)

$$\exists d, 1 \leq d < N,$$

d divides N such that

$$\frac{1}{2}N(N-d) - K \in \{0, 1\}.$$

A_M is as in Figure VI.

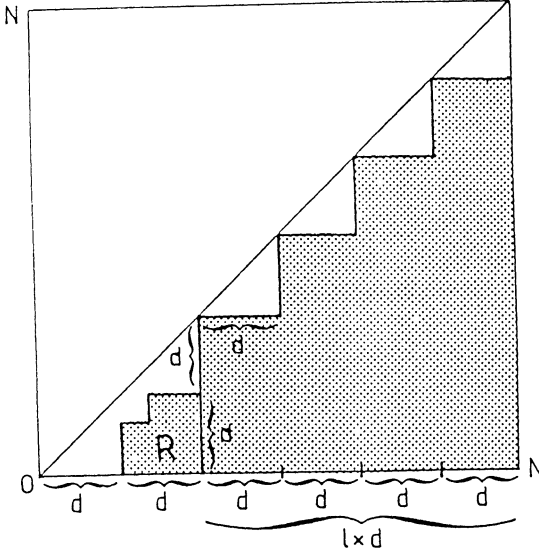


Figure VI

ℓ and R are defined by $N = (\ell + 2)d$ and $N^2 - 2K = (\ell + 4)d^2 - 2R$. This implies $R \in \{d^2 - 1, d^2\}$.

There are R ones within the $d \times d$ square with corners at $(d, 0)$ and $(2d, d)$.

Further $V_{jd+i} = jd$ for $2 \leq j \leq \ell + 1$ and $1 \leq i \leq d$.

$$I_M = \min(N, K) = R\ell d + \frac{d^3}{6}\ell(\ell-1)(\ell+4).$$

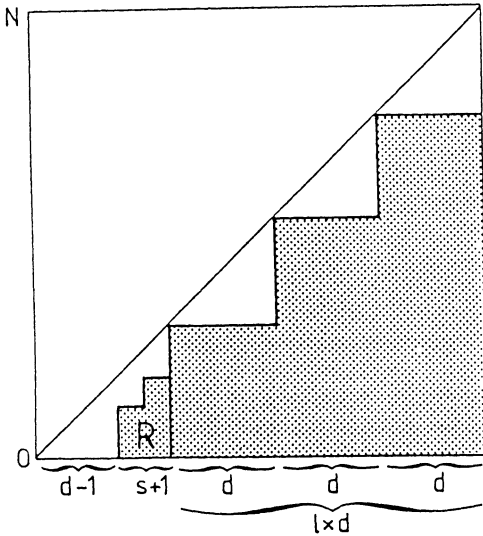


Figure VII

Type VII: (Minimum)

$$\exists d, 1 \leq d < N,$$

$$\exists s, 0 \leq s \leq d-1,$$

such that

$$N = (\ell + 1)d + s$$

for some integer ℓ and

$$\frac{1}{2}N(N-d) + \frac{1}{2}s(d-s) - K - 1 \in \{-d+s, \dots, \min(d-s, sd-2)\}.$$

A_M is as in Figure VII.

R is defined by $N^2 - 2K = \ell d^2 + (d + s)^2 - 2R$.

This implies $1 \leq R$ and $(s - 1)(d + 1) \leq R \leq (s + 1)(d - 1)$.

There are R ones within the $(s + 1) \times (d - 1)$ rectangle with corners at $(d - 1, 0)$ and $(d + s, d - 1)$.

Further $V_{s+jd+i} = s + jd$ for $1 \leq j \leq \ell$ and $1 \leq i \leq d$.

$$I_M = \min(N, K) = R\ell d + \frac{d^2}{6}\ell(\ell - 1)\{(\ell + 1)d + 3s\}.$$

Type VIII: (Minimum)

$$\exists d, 1 \leq d < N,$$

$$\exists s, 1 \leq s \leq d,$$

$$\exists p, q \geq 1,$$

such that

$$N = (p + 1)d + q(d + 1) + s$$

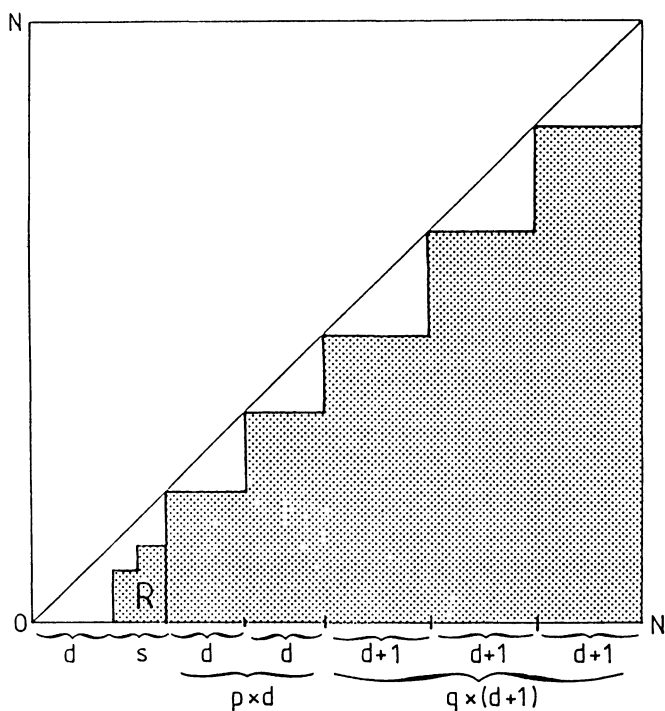


Figure VIII

and

$$\frac{1}{2}N(N-d) + \frac{1}{2}d(s-q) - \frac{1}{2}s^2 - \frac{1}{2}q - K - 1 \in \{-1, \dots, \min(d-s, sd-2)\}.$$

A_M is as in Figure VIII.

R is defined by $N^2 - 2K = q(d+1)^2 + pd^2 + (d+s)^2 - 2R$.

This implies $1 \leq R$ and $(s-1)(d+1) \leq R \leq sd$.

There are R ones within the $s \times d$ rectangle with corners at $(d, 0)$ and $(d+s, d)$.

Further $V_{s+jd+i} = s+jd$ for $1 \leq j \leq p$ and $1 \leq i \leq d$, and $V_{s+(p+1)d+j(d+1)+i} = s+(p+1)d+j(d+1)$ for $0 \leq j \leq q-1$ and $1 \leq i \leq d+1$.

$$\begin{aligned} I_M = \min(N, K) &= R\{pd + q(d+1)\} + \frac{d^2}{6}p(p+1)\{(p-1)d + 3q(d+1) - 3s\} + \\ &+ sd p(pd + q(d+1)) + \frac{(d+1)^3}{6}q(q-1)(q+1) + \\ &+ \frac{(d+1)^2}{2}q(q-1)(pd + s - 1). \end{aligned}$$

Type IX: (Minimum)

$$V_i = i \quad \text{for } 1 \leq i \leq K - \frac{1}{2}N(N-1)$$

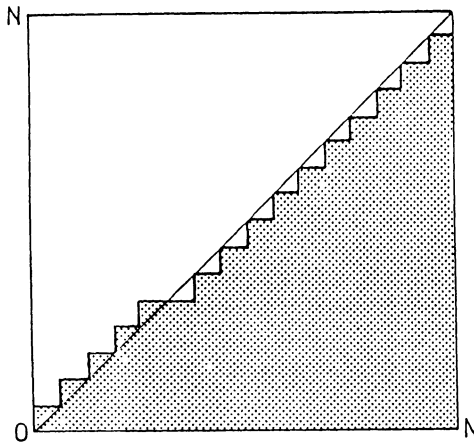


Figure IX

and

$$V_i = i - 1 \quad \text{for} \quad K - \frac{1}{2}N(N-1) < i \leq N.$$

A_M is as in Figure IX.

$$I_M = \min(N, K) = NK - \frac{1}{3}N(N-1)(N+1).$$

3. Proof of Theorem 1

Fix natural numbers N and K .

In several steps we will show that solutions to the problem belong to smaller and smaller subclasses of the class $\mathcal{M}_{N,K}$. To facilitate reading we refer to the appendix for technical details.

3.1. PERMUTATION LEMMA. *Let $M \in \mathcal{M}_{N,K}$, let T be a permutation of $\{1, \dots, N\}$. Then I_M is invariant under $T \times T$.*

We omit the easy proof.

Step 1. Permutation. By taking T such that $\{H_{T_i}\}_{i=1}^N$ is a non-increasing sequence, we may assume that M is such that $(H_i)_{i=1}^N$ is non-increasing.

3.2. STANDARDIZATION LEMMA. *Let $M \in \mathcal{M}_{N,K}$ be a matrix such that $(H_i)_{i=1}^N$ is non-increasing. Then there exists a matrix $M' \in \mathcal{M}_{N,K}$ in standard form, i.e.,*

$$M'_{i_0, j_0} = 1 \Rightarrow M'_{i,j} = 1 \quad \text{for all } i \leq i_0, j \leq j_0,$$

such that $I_{M'} \geq I_M$.

Proof. Let M be a matrix, M not in standard form, such that the horizontal sections are non-increasing. Then there exist indices $i_1 < i_2, j$ such that

$$M_{i_1, j} = 0, \quad M_{i_2, j} = 1.$$

Let M' be the matrix obtained by interchanging this 0 and 1. We claim that $I_{M'} \geq I_M$. We have

$$\begin{aligned} I_{M'} - I_M &= H_{i_1}(V_{i_1} + 1) + H_{i_2}(V_{i_2} - 1) - H_{i_1}V_{i_1} - H_{i_2}V_{i_2} \\ &= H_{i_1} - H_{i_2} \geq 0. \end{aligned}$$

By repeating this argument (moving squares horizontally to the left) we obtain a matrix in standard form, while I_M does not decrease. \square

Step 2. Standardization. We conclude that we may assume that $M \in \mathcal{M}_{N,K}$ is in standard form.

3.3. SYMMETRIZATION LEMMA. *Let $M \in \mathcal{M}_{N,K}$ be a matrix in standard form. Then there exists a matrix $M' \in \mathcal{M}_{N,K}$ in standard form that is symmetric or nearly-symmetric, i.e.,*

$$M'_{i,j} = M'_{j,i} \text{ for all } (i,j) \text{ except one pair } (i,j),$$

such that $I_{M'} \geq I_M$.

Proof. Assume that M is not of this kind. Then there exist a, b, c, d such that $M_{a,b} = M_{c,d} = 1$ and $M_{b,a} = M_{d,c} = 0$. Let M' be the matrix obtained by interchanging $M_{c,d}$ and $M_{b,a}$. We claim that $I_{M'} > I_M$. (See Appendix 1.) \square

Step 3. Symmetrization. We conclude that we may assume that $M \in \mathcal{M}_{N,K}$ is in standard form and symmetric or nearly-symmetric.

With a matrix M in standard form we associate a left-continuous function $f_M: [0, N] \rightarrow [0, N]$ given by

$$f_M(x) = V_i \text{ for } x \in \langle i-1, i].$$

This implies that

$$A_M = \{(x, y) \in [0, N] \times [0, N]: y \leq f_M(x)\}.$$

Assume $f_M(a) \geq d, f_M(b) \geq c, f_M(c) \geq b, f_M(d) \geq a, b \leq c$.

Let H^w and V^w be the sections corresponding to the set

$$A^w := A_M \cap (\langle a, b] \times \langle c, d] \cup \langle c, d] \times \langle a, b]).$$

So, $H^w = H - c$ on $\langle a, b]$, $H^w = H - a$ on $\langle c, d]$ and $H^w = 0$ else, the same holds for V^w .

$$\text{Let } I_{M^w} := \sum_i H_i^w V_i^w.$$

3.4. WINDOWING LEMMA. *When we rearrange ones (preserving K that is the total number of ones) within $\langle a, b] \times \langle c, d] \cup \langle c, d] \times \langle a, b]$ (obtaining M') then*

$$I_{M'} - I_M = I_{M'^w} - I_{M^w}.$$

Conclusion. So, when we compute the influence of this rearrangement on I_M , we can pass over from H and V to H^w and V^w . (*Proof:* see Appendix 2.)

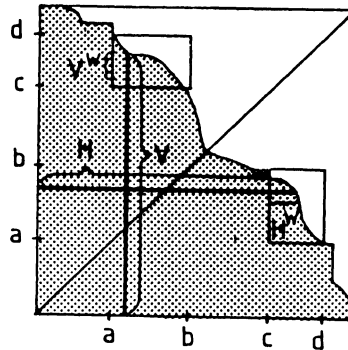


Figure X

3.5. LOCAL REFLECTION LEMMA. Assume that:

$$f_M(a) \geq d, f_M(b) \geq c, f_M(c) \geq b, f_M(d) \geq a, b \leq c$$

and also that $b - a = d - c$.

When we (obtaining M') reflect $A_M \cap \langle a, b] \times \langle c, d]$ with respect to the line $y = x + c - a$ and $A_M \cap \langle c, d] \times \langle a, b]$ with respect to the line $y = x + a - c$, then I_M is invariant. (See fig. XI). (Proof: see Appendix 3).

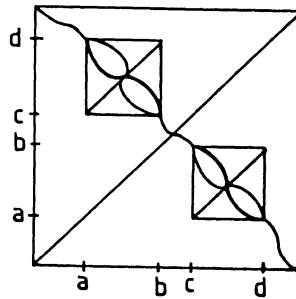


Figure XI

3.6. CONTRIBUTION OF A SQUARE LEMMA. Let $M \in \mathcal{M}_{N,K}$ be in standard form and symmetric or nearly-symmetric. Let $(a, b) (a, b \in \{1, \dots, N\})$ be a corner point of M , i.e., $f_M(a) = b$ and $f_M(a + 1) < b$ or $a = N$. Let M' be the matrix obtained from M by removing $(a, b) (M'_{i,j} = M_{i,j} - \delta_{a,i} \cdot \delta_{b,j})$. Then

$$I_M - I_{M'} = \begin{cases} a + b & \text{if } a \neq b, \quad M_{b,a} = 1 \\ a + b - 2 & \text{if } a \neq b, \quad M_{b,a} = 0 \\ a + a - 1 & \text{if } a = b. \end{cases}$$

Proof. See Appendix 4.

□

From now on all rearrangements of ones in M will be done such that M remains in standard form and (nearly-)symmetric. This means that a rearrangement of ones within $\langle a, b \rangle \times \langle c, d \rangle$ (above the diagonal) is attended with a (in some sense reflected) rearrangement within $\langle c, d \rangle \times \langle a, b \rangle$ (under the diagonal).

This will not lead to confusion.

Spreading out

We will consider quasi-blocks and we will decrease the number of these quasi-blocks and so we will diminish the class of matrices.

Let

$$f_M = \sum_{i=1}^m y_i \cdot 1_{\langle x_{i-1}, x_i \rangle}$$

be the function associated with M as defined in step 3 ($0 = x_0 < x_1 < \dots < x_m = N$). We call a rectangle $\langle x_{k-1}, x_k \rangle \times \langle y_{k+1}, y_k \rangle$ a *block* if it is disjoint with the diagonal. Note that the points (x_k, y_k) are corner points.

We call a set $\langle x_{k-1}, x_k \rangle \times \langle y_{k+2}, y_k \rangle \cup \langle x_k, x_{k+1} \rangle \times \langle y_{k+2}, y_{k+1} \rangle$ (disjoint with the diagonal) a *quasi-block* if $y_k - y_{k+1} = 1$ or $x_{k+1} - x_k = 1$. We call in these cases $x_k - x_{k-1}$ c.q. $y_{k+1} - y_{k+2}$ the *remainder* of the quasi-block.

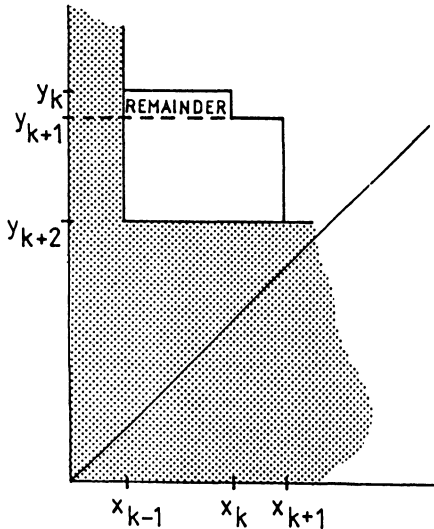


Figure XII. A quasi-block with $y_k - y_{k+1} = 1$.

We consider blocks as special quasi-blocks (with remainder equal to zero).

We shall spread out a quasi-block along the longest segment ($\langle x_{k-1}, x_{k+2} \rangle$ or $\langle y_{k+2}, y_{k-1} \rangle$), using the Local Reflection Lemma and the Contribution of a Square Lemma.

3.7. SPREADING-OUT LEMMA. Let $f_M = \sum_{i=1}^m y_i \cdot 1_{\langle x_{i-1}, x_i \rangle}$, assume that

$$\langle x_{K-1}, x_K \rangle \times \langle y_{K+2}, y_K \rangle \cup \langle x_K, x_{K+1} \rangle \times \langle y_{K+2}, y_{K+1} \rangle$$

is a quasi-block. Assume $y_{K+2} \geq x_{K+2}$. Then this quasi-block can be replaced by a quasi-block of the type

$$\langle x_{K-1}, t \rangle \times \langle y_{K+2}, r+1 \rangle \cup \langle t, x_{K+2} \rangle \times \langle y_{K+2}, r \rangle$$

or by a quasi-block of the type

$$\langle x_{K-1}, r \rangle \times \langle y_{K+2}, y_{K-1} \rangle \cup \langle r, r+1 \rangle \times \langle y_{K+2}, t \rangle$$

such that I_M does not decrease.

Proof. See Appendix 5. □

3.8. TWO QUASI-BLOCKS LEMMA. Let $f_M = \sum_{i=1}^m y_i \cdot 1_{\langle x_{i-1}, x_i \rangle}$, assume that

$$\langle x_{K-1}, x_K \rangle \times \langle y_{K+2}, y_K \rangle \cup \langle x_K, x_{K+1} \rangle \times \langle y_{K+2}, y_{K+1} \rangle$$

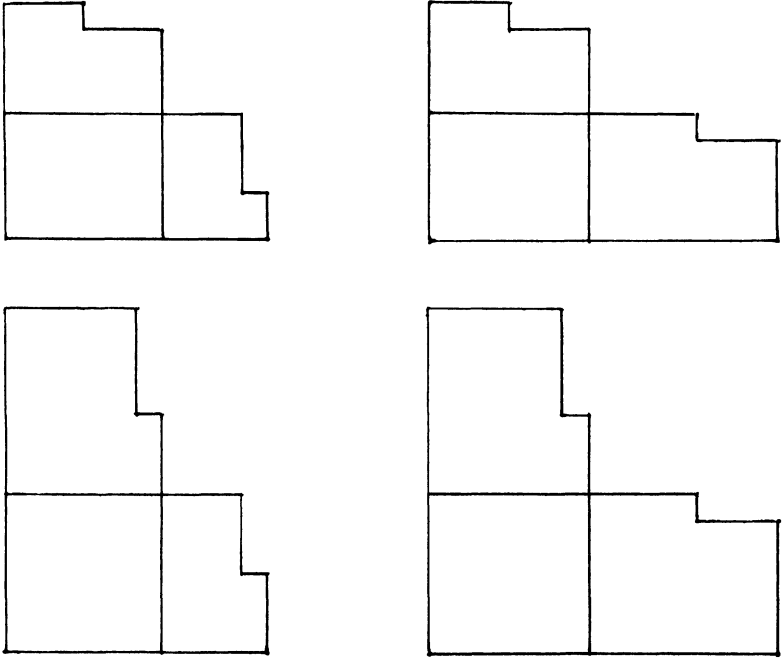


Figure XII a-d (4 cases)

and

$$\langle x_{K+1}, x_{K+2} \rangle \times \langle y_{K+4}, y_{K+2} \rangle \cup \langle x_{K+2}, x_{K+3} \rangle \times \langle y_{K+4}, y_{K+3} \rangle$$

are quasi-blocks. Assume $y_{K+4} \geq x_{K+4}$. Then these two quasi-blocks can be joined to one quasi-block, preserving standard form and (near-)symmetry, such that I_M does not decrease.

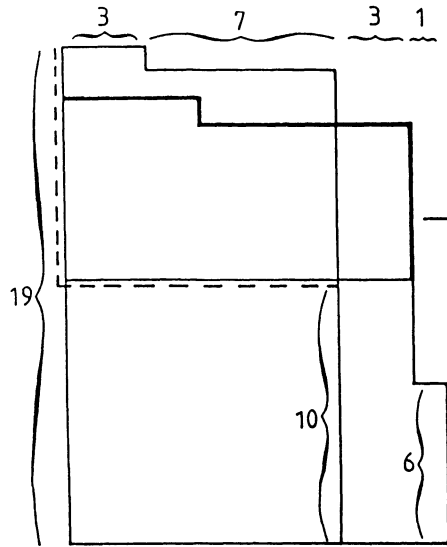


Figure XIII

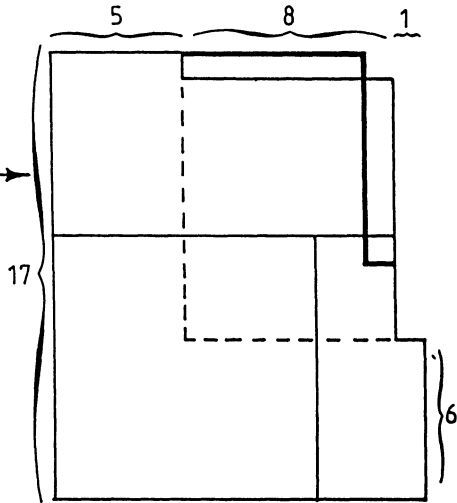


Figure XIV

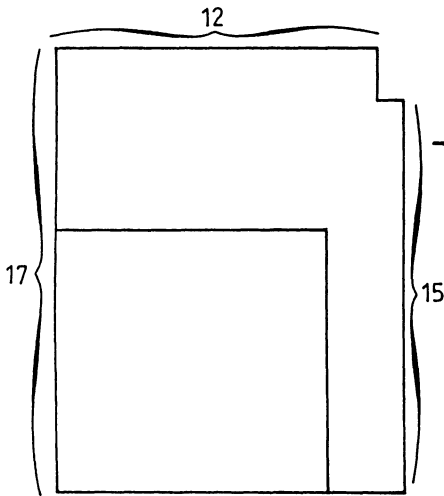


Figure XVI

(EXAMPLE)

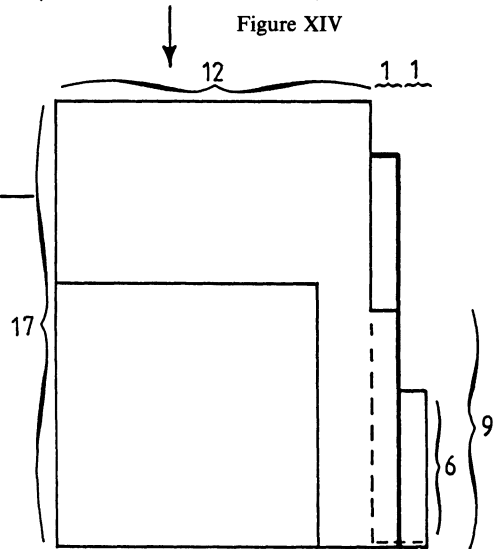


Figure XV

We use the Spreading-out Lemma and the Local Reflection Lemma. There are 4 cases (see Fig. XII), depending whether the two remainders are horizontal or vertical strips.

To avoid a long and detailed list of cases and subcases, we restrict ourselves to the case of a quasi-block with horizontal remainder with at its right lower side a quasi-block with vertical remainder.

The given example is typical for this case. Just as in Appendix 5 we may assume that the remainder of a quasi-block is a horizontal strip if $x_{K+1} - x_{K-1} \geq y_K - y_{K+2}$ and a vertical strip if $x_{K+1} - x_{K-1} < y_K - y_{K+2}$.

First we spread out horizontally the left upper quasi-block (Fig. XIII). Then, by a reflection, we obtain one quasi-block consisting of one strip and a remainder (Fig. XIV). We spread out this quasi-block and we are finished (Fig. XV).

We spread out the quasi-blocks marked with $\begin{smallmatrix} | \\ _ \\ _ \end{smallmatrix}$. (thin lines before the transformation, thick lines after the transformation) (Computation: see Appendix 6).

COROLLARY. Let $M \in \mathcal{M}_{N,K}$ be a matrix in standard form and (nearly-)symmetric. Then there exists a matrix $M' \in \mathcal{M}_{N,K}$ of type A or B such that $I_{M'} \geq I_M$.

Proof. Apply Lemma 3.8 iteratively. \square

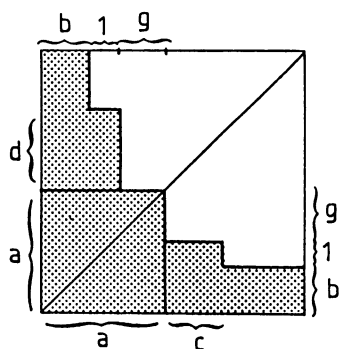


Figure XVIIC

Type A:

$$|c - d| \leq 1.$$

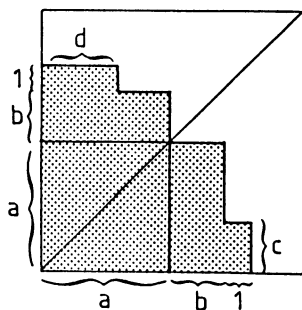


Figure XVIIIC

Type B:

$$|c - d| \leq 1.$$

3.9. *Last Step.* To complete the Proof of Theorem 1 we will reduce this class of matrices to the types I, II, III, IV. (see Appendix 7). \square

REMARK. If $K = m^2 > \frac{1}{2}N^2$ for some integer m , then the maximal value of I_M is attained when we take A_M equal to $m \times m$ square of ones, and if $K = N^2 - m^2 < \frac{1}{2}N^2$ for some integer m , then we obtain the maximal value of I_M by taking the complement of a $m \times m$ square. This directly follows from the fact that in these cases I_M assumes the value $N^3 \cdot \max(\alpha)$ (with $\alpha = K/N^2$).

In other cases I_M is strictly less than $N^3 \cdot \max(\alpha)$.

Generally, if $\alpha = K/N^2 > \frac{1}{2}$ the maximal value of I_M is attained in type I or II, and if $\alpha < \frac{1}{2}$ in type III or IV, because in these types $(1/N)A_M$ is an approximation of the corresponding $\sqrt{\alpha} \times \sqrt{\alpha}$ square (the solution of the continuous version for $\alpha > \frac{1}{2}$) c.q. the complement of a $\sqrt{1-\alpha} \times \sqrt{1-\alpha}$ square (the solution of the continuous version for $\alpha < \frac{1}{2}$). However, for $\alpha \approx \frac{1}{2}$ this can be different, as the following example shows. (See also the table at the end of this paper, before the appendix.)

EXAMPLE. Take $N = 10$ and $K = 49$, then $\alpha = 0.49 < \frac{1}{2}$. The maximal value of I_M is attained in type I (see Figure 1) where $I_M = 7 \times 7 \times 7 = 343$, and not in type III (see Figure 2) where $I_M = 339$.

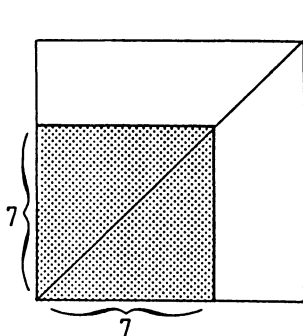


Figure 1

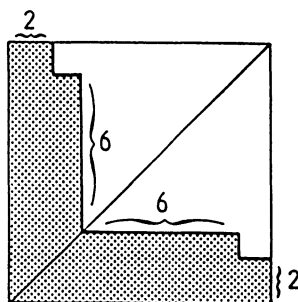


Figure 2

EXAMPLE. We show the existence of three sequences $(N_i)_{i=1}^\infty$, $(K_i)_{i=1}^\infty$, $(v_i)_{i=1}^\infty$ (each tending to infinity) such that

- (1) $K_i = \frac{1}{2}N_i^2 - v_i$ and
- (2) I_M attains its maximal value $\max(N_i, K_i)$ in type I and not in type III or IV.

From the theory of continued fractions follows the existence of increasing integer sequences $(p_i)_{i=1}^\infty$, $(q_i)_{i=1}^\infty$ such that

$$0 < \frac{1}{\sqrt{2}} - \frac{p_i}{q_i} < \frac{1}{q_i^2}, \quad \text{and all } q_i \text{ are odd.}$$

This implies

$$(3) \quad 0 < \frac{1}{2}q_i^2 - p_i^2 < \sqrt{2}.$$

Now (3) implies $\frac{1}{2}q_i^2 - p_i^2 = \frac{1}{2}$.

We define

$$N_i := q_i + 3 \quad \text{and} \quad K_i := (p_i + 2)^2.$$

Defining v_i by

$$K_i = \frac{1}{2}N_i^2 - v_i$$

we have

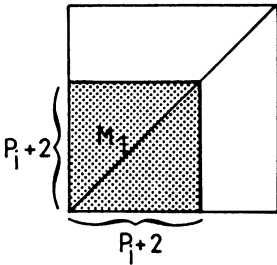
$$v_i = 3q_i - 4p_i + 1$$

So we have

$$(3\sqrt{2} - 4)p_i < v_i < (3\sqrt{2} - 4)p_i + 6.$$

So, for p_i sufficiently large we have

$$v_i < \frac{1}{2}p_i.$$

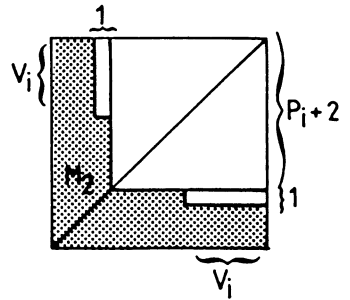


Taking M_1 of type I ($(p_i + 2) \times (p_i + 2)$ square of ones) we have

$$I_{M_1} = (p_i + 2)^3.$$

Taking M_2 of type III (see figure) we have
(by the Complement Lemma)

$$\begin{aligned} I_{M_2} &= v_i(p_i + 3)^2 + (p_i + 2 - v_i) \\ &\quad \times (p_i + 2)^2 + v_i^2 + 2(q_i + 3) \\ &\quad \times (p_i + 2)^2 - (q_i + 3)^3 \\ &= (p_i + 2)^3 - v_i(2p_i - q_i) < I_{M_1}. \end{aligned}$$



This proves the statement of the example.

4. Proof of Theorem 2

Fix natural numbers N and K . The case $K \leq \frac{1}{4}N^2$ is trivial because $I_M = 0$. In several steps we will show that solutions to the problem exist in smaller and smaller subclasses of $\mathcal{M}_{N,K}$. After the third step we will discriminate the cases $\frac{1}{4}N^2 < K < \frac{1}{2}N(N-1)$ and $\frac{1}{2}N(N-1) \leq K \leq \frac{1}{2}N^2$. To facilitate reading we refer to the Appendix for technical details.

4.1. STEP 1. PERMUTATION. Using Lemma 3.1 (Permutation Lemma) we may assume that (H_i) is a non-increasing sequence.

We define a new standard form; M is in *standard form* when

$$M_{i,j} = 1 \quad \text{if} \quad M_{i_0,j_0} = 1 \quad \text{for} \quad i \geq i_0, j \leq j_0.$$

4.2. STANDARDIZATION LEMMA. Let $M \in \mathcal{M}_{N,K}$ be a matrix such that $(H_i)_{i=1}^N$ is a non-increasing sequence. Then there exists a matrix $M' \in \mathcal{M}_{N,K}$ in standard form such that $I_{M'} \leq I_M$.

Proof. Analogous to the proof of Lemma 3.2 (Standardization Lemma). \square

Step 2. Standardization. We conclude that we may assume that $M \in \mathcal{M}_{N,K}$ is in standard form.

We associate with the matrix M in standard form a right-continuous function $f_M: [0, N] \rightarrow [0, N]$ given by

$$f_M(x) = V_i \quad \text{for} \quad x \in [i-1, i).$$

We redefine A_M equal to

$$A_M := \bigcup_{\{(i,j): M_{i,j}=1\}} [i-1, i) \times \langle j-1, j].$$

This implies that $A_M = \{(x, y) \in [0, N] \times [0, N]: y \leq f_M(x)\}$. Except the right-continuity, f_M is the same as in the proof of Theorem 1. We call (a, b) a *corner point* of M if $f_M(a-1) = b$ and $f_M(a-2) < b$.

4.3. UNDER THE DIAGONAL LEMMA. Let $M \in \mathcal{M}_{N,K}$ be a matrix in standard form. If $\frac{1}{4}N^2 < K < \frac{1}{2}N(N-1)$, then there exists a matrix $M' \in \mathcal{M}_{N,K}$ such that $I_{M'} \leq I_M$ and M' lies under the diagonal, i.e.,

$$M'_{i,j} = 0 \quad \text{if} \quad j \geq i.$$

If $\frac{1}{2}N(N-1) \leq K \leq \frac{1}{2}N^2$, then there exists a matrix $M' \in \mathcal{M}_{N,K}$ such that

$I_{M'} \leq I_M$ and

$$M'_{i,j} = 1 \quad \text{if } j < i.$$

Proof. Assume that M has some corner point (i, j) not lying under the diagonal ($j \geq i$), and assume that there exists a point (i_1, j_1) under the diagonal ($i_1 \geq j_1 + 1$) such that $M_{i_1, j_1} = 0$ and $f_M(i_1) \geq j_1 + 1$.

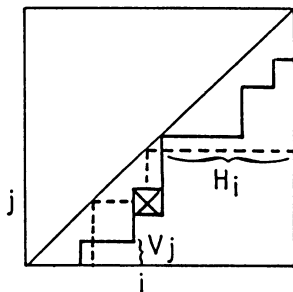
We move the one from (i, j) to (i_1, j_1) and we consider two cases. In both cases I_M will decrease (see Appendix 8).

Step 3. Under the diagonal. We conclude that we may assume that in the case $\frac{1}{4}N^2 < K < \frac{1}{2}N(N-1)$, M lies under the diagonal and that in the case $\frac{1}{2}N(N-1) \leq K \leq \frac{1}{2}N^2$, $M_{i,j} = 1$ if $j < i$.

Now we consider the CASE $\frac{1}{4}N^2 < K < \frac{1}{2}N(N-1)$.

4.4. REMARK: Changing of I_M by a corner point. We consider the influence on I_M of removing a square from a corner point (i, j) of M to obtain a matrix M' . We have

$$I_M - I_{M'} = H_i V_i + H_j V_j - H_i(V_i - 1) - (H_j - 1)V_j = H_i + V_j.$$



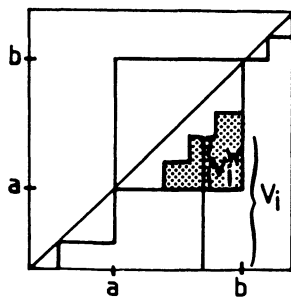
We say that the corner point (i, j) changes I_M by the sections H_i and V_j .

4.5. WINDOWING LEMMA. Assume $f_M(a) = a, f_M(b) = b$ for some $0 \leq a < b \leq N$.

Let H^w and V^w be the sections of $A_M \cap [a, b] \times [a, b]$, and let

$$I_{M^w} := \sum_i H_i^w V_i^w.$$

When we rearrange ones (preserving K that is the total number of ones) within



$[a, b] \times [a, b]$ (obtaining M') we have

$$I_M - I_{M'} = I_{M^w} - I_{M'^w}$$

The proof is analogous to the proof of Lemma 3.4. So, when we rearrange within $[a, b] \times [a, b]$, we can compute the influence on I_M by passing over from H_i and V_i to H_i^w and V_i^w .

4.6. LOCAL REFLECTION LEMMA. Assume again $f_M(a) = a, f_M(b) = b$ ($a < b$). Then I_M is invariant under reflecting $A_M \cap [a, b] \times [a, b]$ with respect to the line $y = -x + a + b$.

We leave the straightforward proof to the reader (use the Windowing Lemma).

We say that a corner (i, j) lies *strictly under the diagonal* resp. *on the diagonal* if

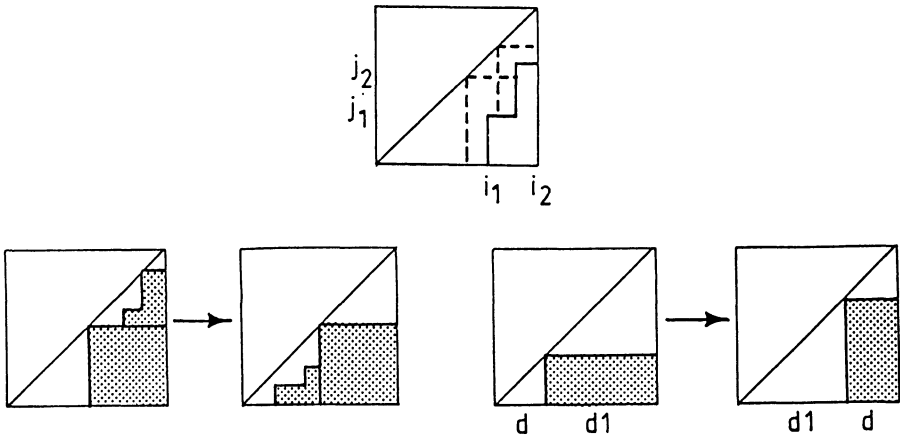
$$i \geq j + 2 \text{ resp. } i = j + 1.$$

4.7. MOVING TO THE DIAGONAL LEMMA. Let $M \in \mathcal{M}_{N,K}$ (for $\frac{1}{4}N^2 < K < \frac{1}{2}N(N-1)$) be a matrix in standard form, lying under the diagonal. Then there exists a matrix $M' \in \mathcal{M}_{N,K}$ in standard form, lying under the diagonal, such that $I_{M'} \leq I_M$, and such that M' has at most two corners (i_1, j_1) and (i_2, j_2) ($i_1 < i_2$ and $j_2 < i_1$) strictly under the diagonal.

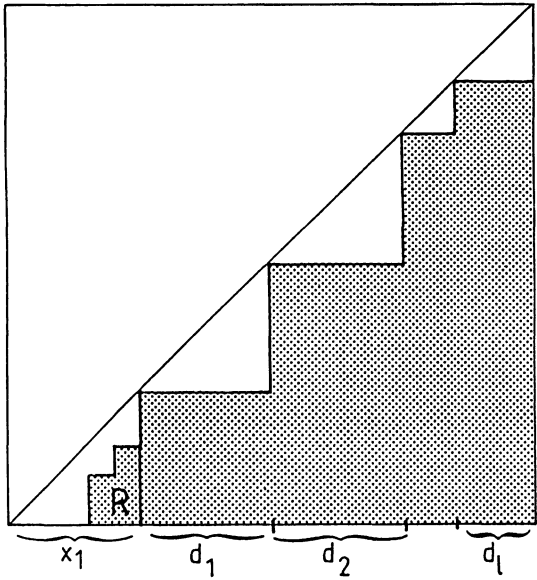
Proof. See Appendix 9. □

Note that $j_2 < i_1$ means that the corner point (i_1, j_1) changes I_M by horizontal sections at a higher level than j_2 and that (i_2, j_2) changes I_M by vertical sections lying more to the left than i_1 (see picture below).

Step 4. Moving to the diagonal. We conclude that we may assume that in the case $\frac{1}{4}N^2 < K < \frac{1}{2}N(N-1)$, M has at most two corner points $(i_1, j_1), (i_2, j_2)$ ($i_1 < i_2$ and $j_2 < i_1$) lying strictly under the diagonal.



Using some local reflections (shown above), that leave I_M invariant, we can assume that M is the following type:



$$0 < x_1 < \dots < x_{\ell+1} = N, d_i = x_{i+1} - x_i.$$

$$V_j = x_i \quad \text{if} \quad x_i < j \leq x_{i+1}$$

and there are R ones ($1 \leq R \leq \frac{1}{4} x_1^2$) within some rectangle which is a subset of

$$\{(i, j): 1 \leq i \leq x_1, j < i\}.$$

$$N = x_1 + \sum_{i=1}^{\ell} d_i,$$

$$N^2 - 2K = \sum_{i=1}^{\ell} d_i^2 + x_1^2 - 2R.$$

We call R the *remainder*.

Note that we can interchange the d_i 's by the Local Reflection Lemma.

4.8. LESS INEQUALITY BETWEEN DIFFERENCES. With various rearrangements we will prove that we may assume that

- (8a) $x_1 \geq d_i \quad \forall i$
- (8b) $x_1 \leq 2d_i \quad \forall i$,
- (8c) $R \geq (s-1)(d+1) \quad (d := \min\{d_i: i \geq 1\}, \quad s := x_1 - d)$,
- (8d) $d \leq d_i \leq d+1 \quad \forall i$,
- (8e) $R \leq sd$ if $d_i = d+1$ for some i ,
- (8f) $R \leq (s+1)(d-1)$ or $R = d^2$.

See Appendix 10.

We have now reached the class of matrices of the types VI, VII, VIII.

We will prove that in each of these types I_M attains its minimal value $\min(N, K)$, and that for each pair (N, K) there exist at most two matrices of these types.

Our method is a lexicographical ordering \ll on the class of matrices of the types VI, VII, VIII. We will prove that if $M_1 \ll M_2$ then $K_1 < K_2$ or $K_1 = K_2$ and $I_{M_1} = I_{M_2}$. Further we prove that if $M_1 \ll M_2 \ll M_3$ then $K_1 < K_3$. These facts imply the theorem for the case $\frac{1}{4}N^2 < K < \frac{1}{2}N(N-1)$ (See Appendix 11).

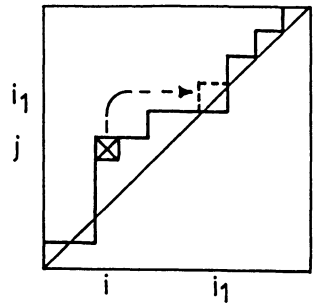
CASE $\frac{1}{2}N(N-1) \leq K \leq \frac{1}{2}N^2$.

Assume that M is not of type IX. Then, by Step 3, we can move a one from a corner point (i, j) above the diagonal ($j > i$) to a place (i_1, i_1) at the diagonal. We obtain a matrix M' .

This transformation yields

$$\begin{aligned} I_M - I_{M'} &= H_i V_i + H_j V_j + H_{i_1} V_{i_1} - H_i(V_i - 1) - (H_j - 1)V_j - \\ &\quad - (H_{i_1} + 1)(V_{i_1} + 1) = H_i + V_j - H_{i_1} - V_{i_1} - 1 \geq (N - i + 1) + \\ &\quad + j - (i_1 - 1) - (N - i_1) - 1 = j - i + 1 \geq 2. \end{aligned}$$

These last considerations prove Theorem 2. □



REMARK. The two-correlation in the discrete case attains the infimum of the continuous case ($\min(\alpha)$) only in the following cases:

- case $\alpha \leq \frac{1}{4}$ (type V),
- case $\frac{1}{4} < \alpha < \frac{1}{2} \cdot \frac{N-1}{N}$ and $R = d^2$ (type VI),
- case $\frac{1}{4} < \alpha < \frac{1}{2} \cdot \frac{N-1}{N}$ and $R = ds$ (type VII),

and of course (by the Complement Lemma) in the complements of these configurations. In the other cases the (discrete) two-correlation will be strictly greater than $\min(\alpha)$.

EXAMPLE

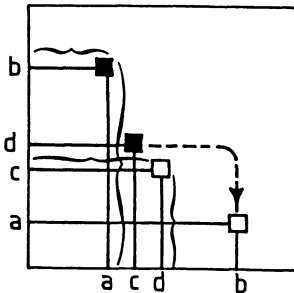
We give in a table the solutions of the minimality and maximality problem for $N = 10$ and $26 \leq K \leq 55$.

MINIMUM						MAXIMUM	
K	Type	d	p	R	min(10, K)	Type	max(10, K)
26	VII	5	1	1	5	III	142
27	VII	5	1	2	10	III	148
28	VII	5	1	3	15	III	156
29	VII	5	1	4	20	III	163
29	VII	4	1	5	20		
30	VII	4	1	6	24	III	172
31	VII	4	1	7	28	III	180
32	VII	4	1	8	32	III	190
33	VII	4	1	9	36	III	199
34	VII	3	2	1	42	III	210
35	VII	3	2	2	48	III	220

MINIMUM						MAXIMUM	
<i>K</i>	Type	<i>d</i>	<i>p</i>	<i>R</i>	min(10, <i>K</i>)	Type	max(10, <i>K</i>)
36	VII	3	2	3	54	III	232
37	VII	3	2	4	60	III	237
38	VIII	2	2	1	67	III	242
39	VIII	2	2	2	74	III	249
39	VI	2	3	3	74		
40	VI	2	3	4	80	IV	256
41	VII	2	4	1	88	III	263
42	VIII	1	2	1	96	III	270
43	VIII	1	4	1	104	III	279
44	VIII	1	6	1	112	III	287
45	IX				120	III	297
46	IX				130	III	306
46						I	306
47	IX				140	III	317
47						I	317
48	IX				150	I	330
49	IX				160	I	343
50	IX				170	III	350
50						I	350
51	IX				180	III	363
52	IX				190	III	370
53	IX				200	III	377
53						I	377
54	IX				210	III	386
54						I	386
55	IX				220	I	397

Appendix 1. (3.3. Symmetrization Lemma, Theorem 1)

We consider two cases:

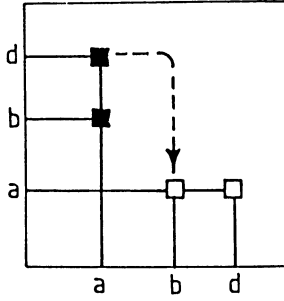


Case 1. a, b, c, d are all different. By permuting a, b, c, d it is no restriction to assume that

$$V_a + H_b \geq V_c + H_d.$$

We have:

$$\begin{aligned}
 I_{M'} - I_M &= (H_a + 1)V_a + H_b(V_b + 1) + H_c(V_c - 1) + \\
 &\quad + (H_d - 1)V_d - H_aV_a - H_bV_b - H_cV_c - H_dV_d \\
 &= V_a + H_b - H_c - V_d \geq V_a + H_b - (V_c - 1) - \\
 &\quad - (H_d - 1) \geq 2.
 \end{aligned}$$



Case 2. $a = c$ (case $b = d$ analogously). We have:

$$\begin{aligned} I_{M'} - I_M &= (H_a + 1)(V_a - 1) + H_b(V_b + 1) + \\ &\quad + (H_d - 1)V_d - H_a V_a - H_b V_b - H_d V_d \\ &= V_a - H_a - 1 + H_b - V_d \geq \\ &\geq d - (b - 1) - 1 + a - (a - 1) \geq 2. \end{aligned}$$

Clearly this symmetrization can be done such that standard form is preserved.

Appendix 2. (3.4. Windowing Lemma, Theorem 1)

Proof.

$$\begin{aligned} I_{M'} - I_M &= \sum_{\substack{i=a+1, \dots, b \\ i=c+1, \dots, d}} (H'_i V'_i - H_i V_i) \\ &= \sum_{i=a+1, \dots, b} \{(H_i^w + c)(V_i^w + c) - (H_i^w + c)(V_i^w + c)\} + \\ &\quad + \sum_{i=c+1, \dots, d} \{(H_i^w + a)(V_i^w + a) - (H_i^w + a)(V_i^w + a)\} \\ &= \sum_{\substack{i=a+1, \dots, b \\ i=c+1, \dots, d}} (H_i^w V_i^w - H_i^w V_i^w) + c \cdot \sum_{i=a+1, \dots, b} (H_i^w + V_i^w - H_i^w - V_i^w) + \\ &\quad + a \cdot \sum_{i=c+1, \dots, d} (H_i^w + V_i^w - H_i^w - V_i^w) = I_{M^w} - I_{M^w}. \end{aligned}$$

The last equality holds because the rearrangement preserves the number of ones ($=K$).

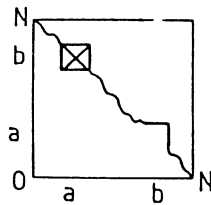
Appendix 3. (3.5. Local Reflection Lemma, Theorem 1).

Using the windowing principle we have

$$\begin{aligned} I_{M'} - I_M &= \sum_{i=a+1, \dots, b} (H_i^w V_i^w - H_i^w V_i^w) + \sum_{i=c+1, \dots, d} (H_i^w V_i^w - H_i^w V_i^w) = \\ &= \sum_{i=c+1, \dots, d} V_i^w H_i^w - \sum_{i=a+1, \dots, b} H_i^w V_i^w + \sum_{i=a+1, \dots, b} V_i^w H_i^w - \sum_{i=c+1, \dots, d} H_i^w V_i^w = 0. \end{aligned}$$

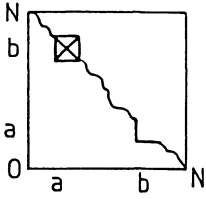
Appendix 4. (3.6. Contribution of a Square Lemma, Theorem 1)

We consider three cases in the (nearly-)symmetric situation:



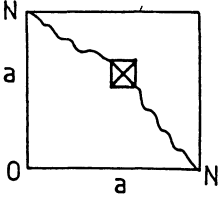
Case 1. $a \neq b, M_{b,a} = 1$.

$$\begin{aligned} I_M - I_{M'} &= b^2 + a^2 - \{b(b-1) + a(a-1)\} \\ &= a + b. \end{aligned}$$



Case 2. $a \neq b, M_{b,a} = 0$.

$$\begin{aligned} I_M - I_{M'} &= b(b-1) + a(a-1) - \{(b-1)^2 + (a-1)^2\} \\ &= a + b - 2. \end{aligned}$$



Case 3. $a = b$.

$$I_M - I_{M'} = a^2 - (a-1)^2 = a + a - 1.$$

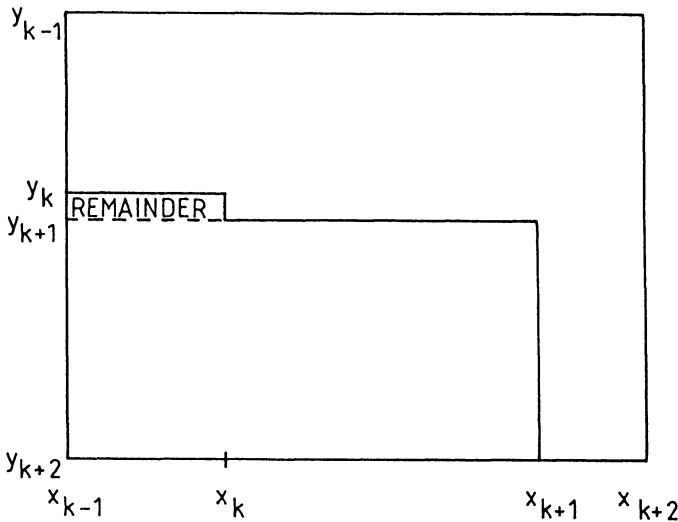
Note that removing both (a, b) and (b, a) leads to a decreasing of I_M by $2(a + b - 1)$. So, the average decreasing of I_M per square is the sum of the coordinates minus 1, just as in case 3.

Appendix 5. (3.7. Spreading-out Lemma, Theorem 1)

First we rearrange M such that the quasi-block lays with its longest side along the longest segment, i.e. if $x_{k+2} - x_{k-1} > y_{k-1} - y_{k+2}$ and $y_k - y_{k+2} > x_{k+1} - x_{k-1}$ or if $x_{k+2} - x_{k-1} < y_{k-1} - y_{k+2}$ and $y_k - y_{k+2} < x_{k+1} - x_{k-1}$, then we reflect the quasi-block with respect to the line $y = x - x_{k-1} + y_{k+2}$.

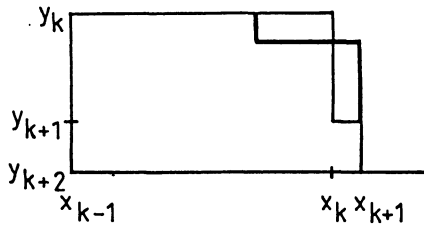
By the Local Reflection Lemma I_M is then invariant.

We consider the case $x_{k+2} - x_{k-1} \geq y_{k-1} - y_{k+2}$ (the other case goes analogously). We spread out the quasi-block from $\langle x_{k-1}, x_{k+1} \rangle$ over $\langle x_{k-1}, x_{k+1} + 1 \rangle$.



If $x_{k+1} - x_k = 1$, we add the ones from $\langle x_{k+1} - y_k + y_{k+1}, x_k \rangle \times \langle y_k - 1, y_k \rangle$ to the remainder

$\langle x_k, x_{k+1} \rangle \times \langle y_{k+1}, y_k - 1 \rangle$. So we obtain $y_k - y_{k+1} = 1$, while I_M is invariant by the Local Reflection Lemma.

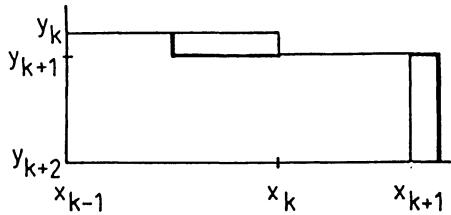


So we may assume that

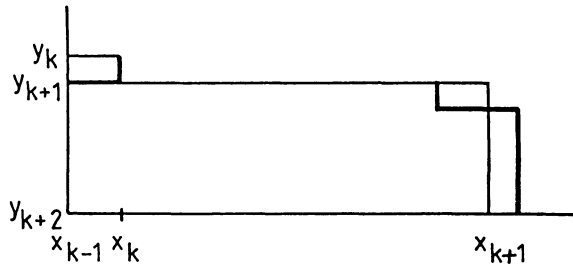
$$y_k - y_{k+1} = 1.$$

Now we have two cases:

Case 1. If the remainder $x_k - x_{k-1}$ is larger than (or equal to) $y_{k+1} - y_{k+2}$, then we spread out by moving $\langle x_k - y_{k+1} + y_{k+2}, x_k \rangle \times \langle y_{k+1}, y_k \rangle$ to $\langle x_{k+1}, x_{k+1} + 1 \rangle \times \langle y_{k+2}, y_{k+1} \rangle$.



Case 2. If $x_k - x_{k-1} < y_{k+1} - y_{k+2}$, then we move $\langle x_{k-1}, x_k \rangle \times \langle y_{k+1}, y_k \rangle$ and $\langle x_{k+1} - y_{k+1} + 1 + y_{k+2} + x_k - x_{k-1}, x_{k+1} \rangle \times \langle y_{k+1} - 1, y_{k+1} \rangle$ to $\langle x_{k+1}, x_{k+1} + 1 \rangle \times \langle y_{k+2}, y_{k+1} - 1 \rangle$.



Considering the contributions of the various squares it is easy to see that in both cases I_M does not decrease.

Iterating this procedure we obtain a quasi-block of the form $\langle x_{k-1}, t \rangle \times \langle y_{k+2}, r+1 \rangle \cup \langle t, x_{k+2} \rangle \times \langle y_{k+2}, r \rangle$ (for some r and t). In the case $x_{k+2} - x_{k-1} < y_{k+1} - y_{k+2}$ we spread out the quasi-block vertically from $\langle y_{k+2}, y_k \rangle$ over $\langle y_{k+2}, y_{k-1} \rangle$.

Appendix 6. (3.8. Two Quasi-Blocks Lemma, Theorem 1)

In the symmetric case I_M^w is in these four cases

$$3 \cdot 19^2 + 7 \cdot 18^2 + 3 \cdot 10^2 + 1 \cdot 6^2 + 6 \cdot 14^2 + 4 \cdot 13^2 + 8 \cdot 10^2 + 3^2 = 6348,$$

$$5 \cdot 17^2 + 8 \cdot 16^2 + 1 \cdot 6^2 + 6 \cdot 14^2 + 10 \cdot 13^2 + 1 \cdot 5^2 = 6420,$$

$$12 \cdot 17^2 + 1 \cdot 9^2 + 1 \cdot 6^2 + 6 \cdot 14^2 + 3 \cdot 13^2 + 8 \cdot 12^2 = 6420, \text{ and}$$

$$12 \cdot 17^2 + 1 \cdot 15^2 + 15 \cdot 13^2 + 2 \cdot 12^2 = 6516.$$

So first I_M increases by 72, then I_M is constant, and finally I_M increases by 96.

Appendix 7. (3.9. Last Step, Theorem 1)

Assume that M is of type A or B, but not of type I, II, III, IV.

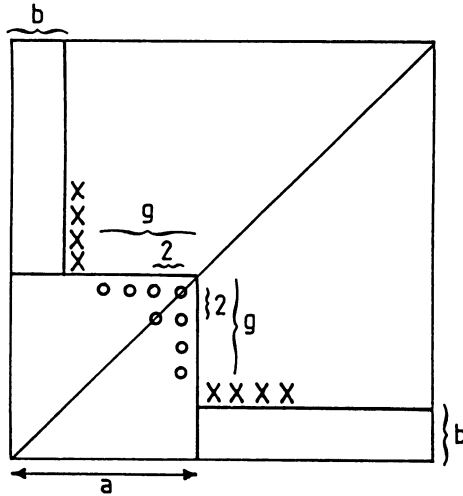
We consider several cases and subcases.

Type A

Case 1. $a \leq N/2$ and $d = c = 0$.

We move $2g$ ones from $\langle a - g, a \rangle \times \langle a - 1, a \rangle \cup \langle a - 2, a \rangle \times \langle a - 2, a - 1 \rangle \cup \langle a - 1, a \rangle \times \langle a - g, a - 2 \rangle$ to $\langle b, b + 1 \rangle \times \langle a, a + g \rangle \cup \langle a, a + g \rangle \times \langle b, b + 1 \rangle$.

CASE 1.

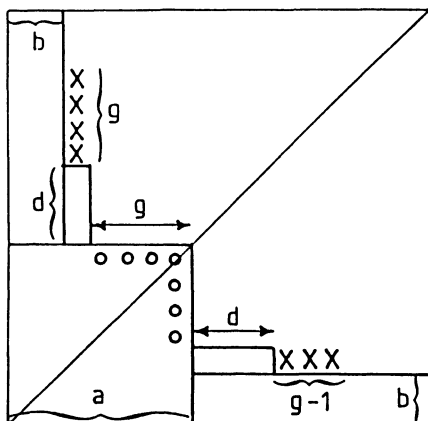


With the principle of the contribution of a square it is easy to see that I_M increases.

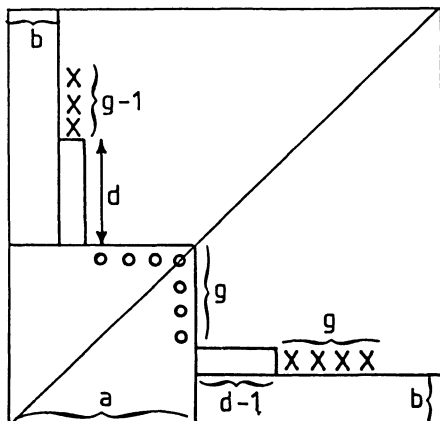
Case 2. $a \leq N/2$ and $(d > 0$ or $c > 0)$.

We move ones from the a th row and the a th column to the $b + 1$ th row and the $b + 1$ th column and (when there is no place enough in the $b + 1$ th row and the $b + 1$ th column) also to the $b + 2$ th row and the $b + 2$ th column.

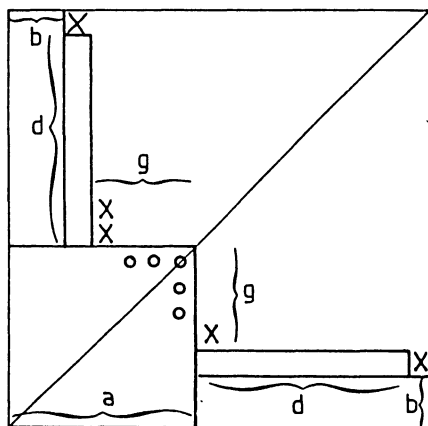
In detail we have 4 subcases (whether or not the matrix is symmetric or nearly-symmetric and whether the $b + 2$ th row and column are needed).



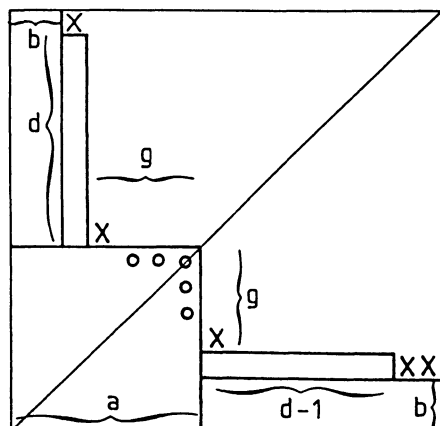
Subcase 2-1. M is symmetric and
 $a + d + g \leq N$.



Subcase 2-2. M is nearly-symmetric and
 $a + d + g - 1 \leq N$.



Subcase 2-3. M is symmetric and
 $a + d + g > N$.

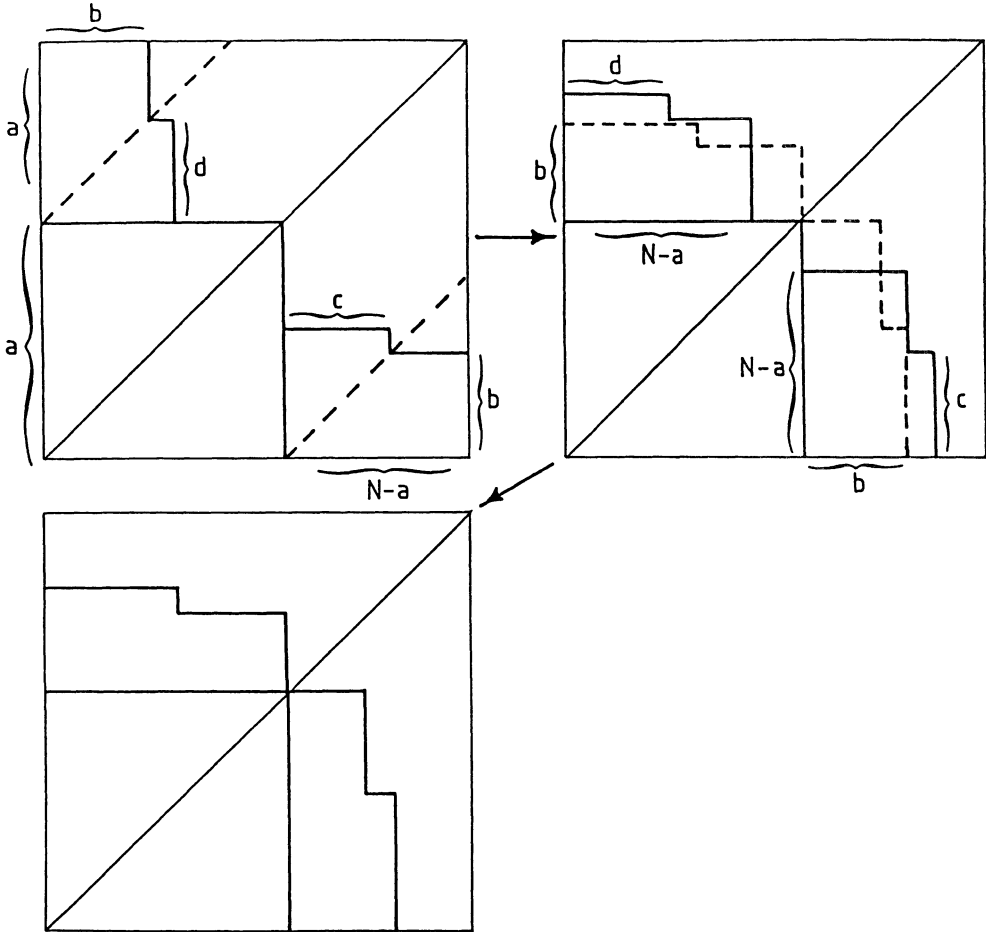


Subcase 2-4. M is nearly-symmetric and
 $a + d + g - 1 > N$.

The squares marked with \circ are moved to squares marked with \times .

From the principle of the contribution of a square follows that I_M increases under these transformations.

Case 3. $a > N/2$ and $N - a \geq b + 1$.



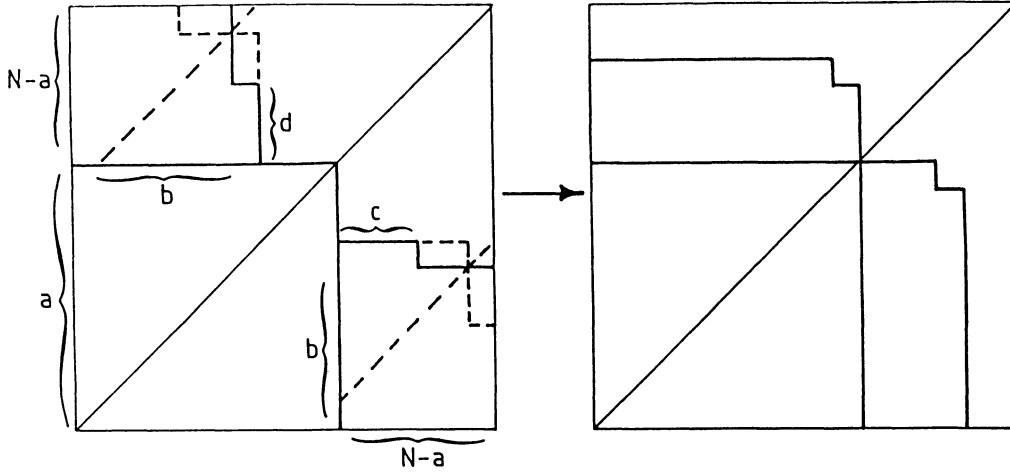
First we reflect the quasi-blocks with size $(N-a)b + d$, $(N-a)b + c$ resp. with respect to the lines $y = x + a$, $y = x - a$ resp. Then we spread out the quasi-blocks horizontally over $[0, a]$, vertically over $[0, a]$ resp.

Now we consider the complement of the obtained set A_M . This complement is of the type as in case 1 or 2. By the Complement Lemma I_{l-M} increases when I_M does. So, with the methods of cases 1 and 2 (applied to $l-M$) we can transform M to another matrix and in this way we prove that the maximum was not attained in M .

Case 4. $a > N/2$ and $N-a < b+1$.

First we reflect two quasi-blocks of size $(N-a)(N-a-1) + d$, $(N-a)(N-a-1) + c$ resp. with respect to the lines $y = x - (b+1) + N$, $y = x - N + b + 1$ resp., then we spread out the two quasi-blocks of size $(N-a-1)(b+1) + b+1 - (N-a-d)$, $(N-a-1)(b+1) + b+1 - (N-a-c)$ resp., horizontally over $[0, a]$, vertically over $[0, a]$ resp.

Now we consider its complement and by an argument as in case 3 we are finished.



Type B

The complement of type B is of type A.

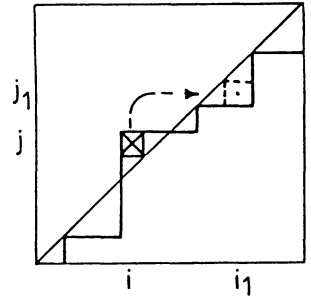
Again by the Complement Lemma we consider its complement and we deal with it as described above.

Now we have reached the matrices of the types I, II, III, IV and so we have proved Theorem 1. \square

Appendix 8. (4.3. Under the diagonal Lemma, Theorem 2)

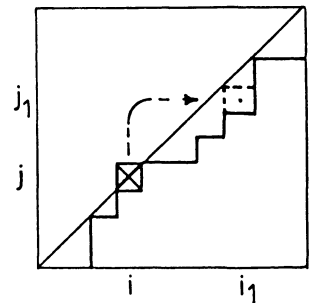
Case 1. $j > i$.

$$\begin{aligned}
 I_M - I_{M'} &= H_i V_i + H_j V_j + H_{i_1} V_{i_1} + H_{j_1} V_{j_1} \\
 &\quad - H_i(V_i - 1) - (H_j - 1)V_j - H_{i_1}(V_{i_1} + 1) \\
 &\quad - (H_{j_1} + 1)V_{j_1} \\
 &= H_i + V_j - H_{i_1} - V_{j_1} \geq (N - i + 1) + \\
 &\quad + j - (N - i_1) - (j_1 - 1) \\
 &= j - i + i_1 - j_1 + 2 \geq 3.
 \end{aligned}$$



Case 2. $j = i$.

$$\begin{aligned}
 I_M - I_{M'} &= H_i V_i + H_{i_1} V_{i_1} + H_{j_1} V_{j_1} \\
 &\quad - (H_i - 1)(V_i - 1) - H_{i_1}(V_{i_1} + 1) \\
 &\quad - (H_{j_1} + 1)V_{j_1} \\
 &= H_i + V_j - 1 - H_{i_1} - V_{j_1} \geq \\
 &\quad \geq (N - i + 1) + i - 1 - (N - i_1) - (j_1 - 1) \\
 &= i_1 - j_1 + 1 \geq 2.
 \end{aligned}$$



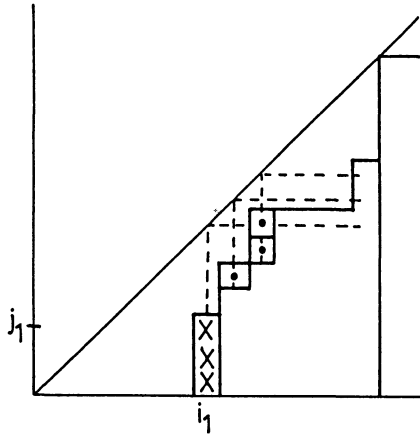
The conclusion follows directly.

Appendix 9. (4.7. Moving to the diagonal Lemma, Theorem 2).

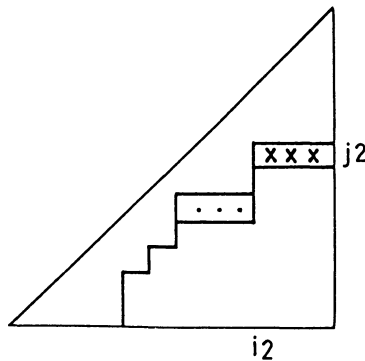
Assume that M is not of this kind. Take the first corner strictly under the diagonal (i_1, j_1) and the last one (i_2, j_2) (so i_1 minimal and i_2 maximal).

We first prove that we may assume that if (i_1, j_1) is a corner strictly under the diagonal then $(i_1 + 1, i_1 - 1)$ or $(i_1 + 1, i_1)$ is a corner.

If this is not the case, then we can move ones from the i_1 th column to the $j_1 + 1$ th row (or, when $M_{i_1+1, j_1+1} = 1$ to a row at higher level) and so on, until the second corner (i, j) strictly under the diagonal (with $i > i_1$ minimal) has the desired form. When the i_1 th column is exhausted, we continue with moving ones from the $i_1 + 1$ th column etc. We make the crucial observation that after the moving of ones to columns to the right these ones changes I_M by horizontal sections on a higher level; thus with smaller sections. So I_M does not increase.



Analogously we can assume that if (i_2, j_2) is the last corner strictly under the diagonal (with i_2 maximal) then $(j_2 + 1, j_2 - 1)$ or $(j_2, j_2 - 1)$ is a corner point.



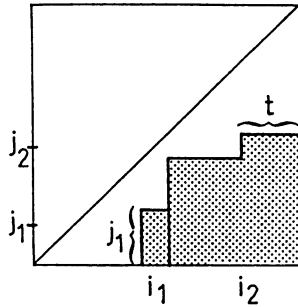
We now consider two cases:

Case 1. $i_1 = j_2$.

We use the Windowing Lemma. There are j_1 ones in the i_1 th column. Assume there are t ones in the j_2 th row (windowed).

Moving a one from (i_1, j_1) to $(i_2 - 1, j_2)$ yields

$$I_M - I_{M'} = j_1 t - (j_1 - 1)(t + 1) = t - j + 1$$



and moving a one from (i_2, j_2) to $(i_1, j_1 + 1)$ yields

$$I_M - I_{M'} = j_1 t - (j_1 + 1)(t - 1) = j - t + 1.$$

At least one of these transformations decreases I_M , so the minimum was not attained.

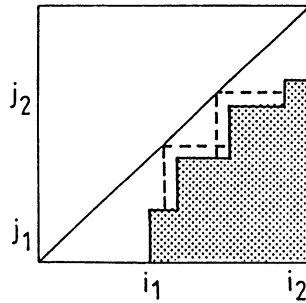
Case 2. $i_1 < j_2$.

Assume there are t ones in the j_2 th row. Moving a one from (i_1, j_1) to $(i_2 - 1, j_2)$ now yields

$$I_M - I_{M'} = H_{i_1}^w - V_{j_2}^w,$$

and moving a one from (i_2, j_2) to $(i_1, j_1 + 1)$ yields

$$I_M - I_{M'} = V_{j_2}^w - H_{i_1}^w.$$



If $H_{i_1}^w \neq V_{j_2}^w$, then clearly the minimum was not attained.

If $H_{i_1}^w = V_{j_2}^w$, then we can move ones from the i_1 th column to the j_2 th row (while I_M is invariant) until the column is exhausted or the row is full (i.e. the diagonal is reached); in both cases we have one corner less lying strictly under the diagonal.

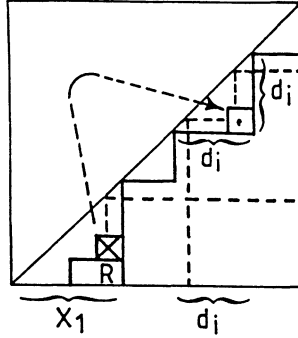
We conclude that we may assume that M has at most 2 corners lying strictly under the diagonal, and that in this case the first corner changes I_M by horizontal sections at a higher level than the second corner.

Appendix 10. (4.8. Less inequality between differences, Theorem 2).

8a. $x_1 \geq d_i \quad \forall i.$

First we prove that we may assume that $x_1 \geq d_i$ for all i .

Assume that $x_1 < d_i$ for some i , then we can move a one from R to $(x_{i+1}, x_i + 1)$ while I_M decreases (consider the changing of I_M by $(N - x_1) - (N - d_i) = d_i - x_1 > 0$, so the minimum was not attained).



8b. $x_1 \leq 2d_i \quad \forall i.$

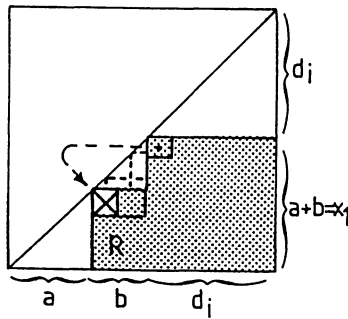
We now give an upper bound for x_1 .

Assume that the R ones lie in a $a \times b$ rectangle

$$\{(i, j): a + 1 \leq i \leq a + b, 1 \leq j \leq a\}.$$

Because of local reflection it is no restriction to assume that $a \geq b$.

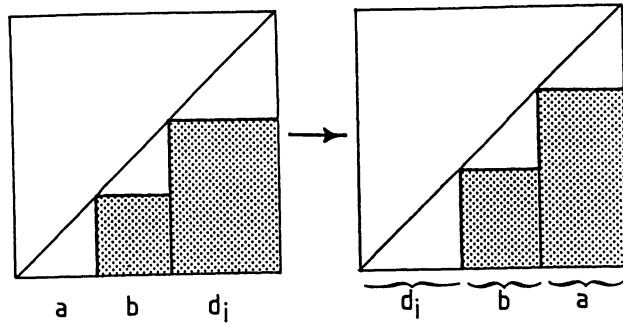
After a rearrangement we have the situation as in the picture.



First assume $R < a \cdot b$ and $b \geq 2$ (the case $b = 1$ is left as an exercise to the reader, use 8c). Then it is possible to move a one from $(x_1 + 1, x_1)$ to $(a + 1, a)$. This gives a decreasing of I_M by $a - d_i$ (consider the changing of I_M).

So we can assume that $d_i \geq a \geq b$, which implies $x_1 = a + b \leq 2d_i$.

When $R = a \cdot b$ we can reach the situation $x_1 \leq 2d_i$ by local reflecting

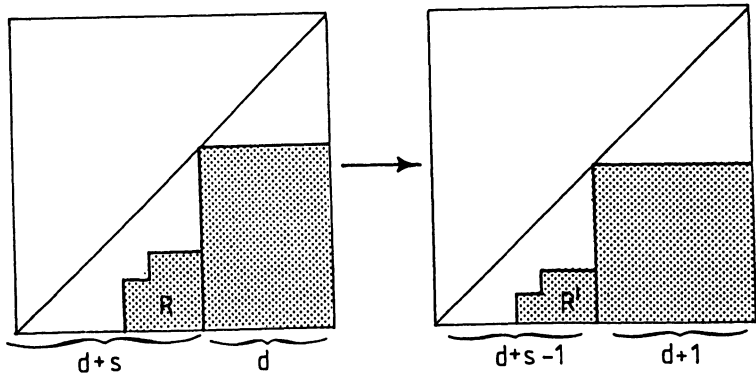


$$8c. R \geq (s-1)(d+1).$$

In this substep we give a lower bound for R . Because

$$s-1 + \frac{(d+s-1)^2}{4} - \frac{(d-s+1)^2}{4} = (s-1)(d+1)$$

we may assume that $R - s + 1 < (d+s-1)^2/4$ (otherwise the statement is trivially true).



After local reflections we obtain the situation as in the first above picture and by the Windowing Lemma we restrict our attention to the $R + (d+s)d$ ones in that picture. Because

$$R + (d+s)d = (R-s+1) + (d+s-1)(d+1)$$

we can transform the matrix and obtain the second picture with $R' = R - s + 1$. This is possible because $R - s + 1 < (d+s-1)^2/4$.

Note that $R_1 > 0$, else $I_{M'}$ is trivially smaller than I_M . We have

$$\begin{aligned} I_{M'} - I_M &= (R-s+1)(d+1) - Rd \\ &= R - (s-1)(d+1) \end{aligned}$$

and the statement follows.

$$8d. d \leq d_i \leq d+1 \quad \forall i.$$

We will prove that the d_i 's cannot differ more than 1 from each other. Assume that $d_i = d + v$ for some i and some $v \geq 2$.

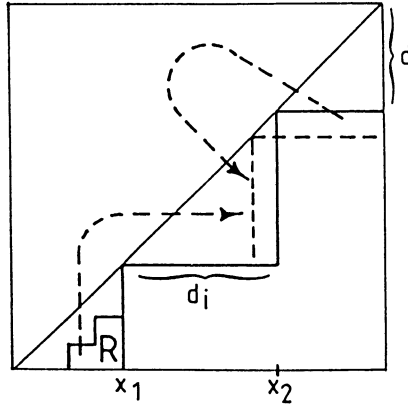
This implies $s = x_1 - d \geq d_i - d = v$ and $R \geq (s - 1)(d + 1) \geq v - 1$.

After the usual local reflections and rearrangements and windowing we obtain the next situation (see figure below).

We decrease d_i by one, and we add that to d , in practice this means the following. We move d ones from the x_2 th row and $v - 1$ ones from R to the x_2 th column and we obtain a matrix with $R' = R - v + 1$. We have

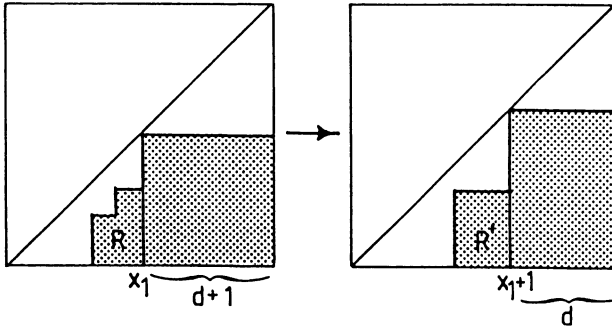
$$\begin{aligned} I_M - I_{M'} &= R(d + d_i) + x_1 d_i d - (R - v + 1)(d + d_i) - x_1(d_i - 1)(d + 1) \\ &= (v - 1)(d + d_i - x_1) > 0. \end{aligned}$$

So the minimum was not attained, and the statement is proved.



8e. $R \leq sd$ if $d_i = d + 1$ for some i .

This time we transform as follows:



From

$$R + x_1(d + 1) = R' + (x_1 + 1)d$$

follows

$$R' = R + s.$$

The second configuration is possible because

$$\frac{(x_1 + 1)^2}{4} = \frac{x_1^2}{4} + \frac{x_1}{2} + \frac{1}{4} > R + s = R'.$$

We have

$$I_M - I_{M'} = R(d + 1) - (R + s)d = R - sd$$

and the minimality of I_M implies

$$R \leq sd.$$

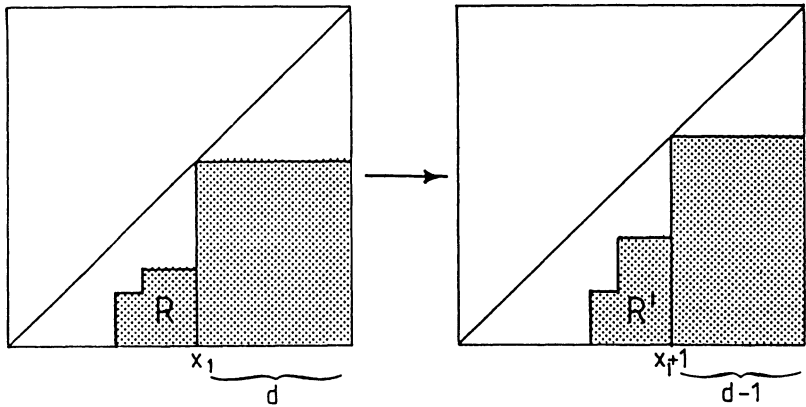
8f. $R \leq (s + 1)(d - 1)$ or $R = d^2$.

To prove this we consider some cases:

Case 1. $s = d$. Because $R \leq \frac{1}{4}x_1^2 = d^2$ and $(s + 1)(d - 1) = d^2 - 1$ in this case, the statement is clearly true.

Case 2. $s = d - 1$. Because $R \leq (x_1 + 1)/2 \cdot (x_1 - 1)/2 = (s + 1)(d - 1)$ in this case it is trivially true.

Case 3. $s \leq d - 2$.



This last time we transform the first configuration with $R + x_1 d$ ones to the second with $R' + (x_1 + 1)(d - 1)$ ones ($R' = R + s + 1$). This last configuration is possible because

$$\frac{(x_1 + 1)^2}{4} = \frac{x_1^2}{4} + \frac{x_1}{2} + \frac{1}{4} \geq R + \frac{2s + 2}{2} + \frac{1}{4} > R + s + 1.$$

We have

$$I_{M'} - I_M = (R + s + 1)(d - 1) - Rd = (s + 1)(d - 1) - R$$

and the statement follows from the minimality of M .

Appendix 11. (4.9, 4.10, 4.11, Theorem 2)

4.9. Representation by a triple

We represent a $N \times N$ matrix M of types VI, VII and VIII by a triple

$$(d, p, R).$$

If M is of type VI or VII we define $p := \ell$. We extend the parameter s to type VI, where we define $s := d$ and we extend the parameter q to types VI and VII, where we define $q := 0$.

We prove that (for fixed N) there corresponds at most one matrix M of the types VI, VII, VIII to a triple (d, p, R) .

LEMMA. *Let N, d, p, R be integers. Then there exists at most one $N \times N$ matrix M of types VI, VII, VIII with the triple (d, p, R) .*

Proof. We have

$$s + q(d + 1) = N - (p + 1)d$$

with $0 \leq s \leq d$. This implies

$$q = \text{int} \left(\frac{N - (p + 1)d}{d + 1} \right)$$

and

$$s = N - (p + 1)d - q(d + 1).$$

Further, K follows now from

$$N^2 - 2K = pd^2 + q(d + 1)^2 + (d + s)^2 - 2R. \quad \square$$

REMARK. The solution of the problem of the despot is represented by the triple $(4, 4, 11)$. The other parameters are $N = 38$, $K = 639$, $q = 3$, $s = 3$.

Let $\mathcal{M}_{N,K}^* \subset \mathcal{M}_{N,K}$ be the subclass of matrices M with $M_{i,i} = 0$ for all i . It is more realistic to consider this problem over $\mathcal{M}_{N,K}^*$ instead of $\mathcal{M}_{N,K}$.

Theorem 2 shows that this makes no difference for these values of the parameters.

4.10. Ordering on the triples

Let M_1, M_2 be $N \times N$ matrices of types VI, VII or VIII with triples (d_1, p_1, R_1) and (d_2, p_2, R_2) . We write

$$M_1 \ll M_2$$

if $(d_1 = d_2 \text{ and } p_1 = p_2 \text{ and } R_1 < R_2)$ or if $(d_1 = d_2 \text{ and } p_1 < p_2)$ or if $d_1 > d_2$.

We call M_2 the *successor* of M_1 if

$$M_1 \ll M_2$$

and if there exists no matrix M_3 such that

$$M_1 \ll M_3 \ll M_2.$$

4.11. The successor

LEMMA. Let M be a $N \times N$ matrix of types VI, VII or VIII with K ones and with triple (d, p, R) . The successor M_2 of M is (distinguishing 16 cases) listed below. Let K_2 be the number of ones of the successor.

No.	Type M	Description case	Triple successor	Type successor	K_2
1	VI	$R < d^2$	$(d, p, R + 1)$	VI	$K + 1$
2	VII	$R < (s + 1)(d - 1)$	$(d, p, R + 1)$	VII	$K + 1$
3	VIII	$R < s \cdot d$	$(d, p, R + 1)$	VIII	$K + 1$
4	VI	$R = d^2$	$(d, p + 1, 1)$	VII	$K + 1$
5	VII	$R = (s + 1)(d - 1), p = 1, s = d - 3$	$(d - 1, 1, d^2 - 2d)$	VI	K
6	VII	$R = (s + 1)(d - 1), p = 1, s = d - 2$	$(d - 1, 2, 1)$	VII	$K + 1$
7	VII	$R = (s + 1)(d - 1), p = 1, s = d - 1$	$(d - 1, 1, 1)$	VIII	$K + 1$
8	VII	$R = (s + 1)(d - 1), p \geq 2, s = d - 2$	$(d - 1, 2, 1)$	VIII	$K + 1$
9	VII	$R = (s + 1)(d - 1), p \geq 2, s = d - 1$	$(d - 1, 1, 1)$	VIII	$K + 1$
10	VII	$R = (s + 1)(d - 1), p = 1, s \leq d - 4$	$(d - 1, 1, (s + 1)d)$	VII	K
11	VII	$R = (s + 1)(d - 1), p \geq 2, s \leq d - 3$	$(d - 1, 1, (s + 1)d)$	VIII	K
12	VIII	$R = sd, q = 1, s = d - 1$	$(d, p + 1, d^2 - 1)$	VI	K
13	VIII	$R = sd, q = 1, s = d$	$(d, p + 2, 1)$	VII	$K + 1$
14	VIII	$R = sd, q \geq 2, s = d$	$(d, p + 2, 1)$	VIII	$K + 1$
15	VIII	$R = sd, q = 1, s \leq d - 2$	$(d, p + 1, s(d + 1))$	VII	K
16	VIII	$R = sd, q \geq 2, s \leq d - 1$	$(d, p + 1, s(d + 1))$	VIII	K

We leave the proof as an exercise to the reader.

In the cases 5, 10, 11, 12, 15 and 16 we have $K_2 = K$. Some easy calculations show that in these cases we also have $I_{M_2} = I_M$. It is also easy to verify that if $M_1 \ll M_2 \ll M_3$ then $K_1 < K_3$.

These facts prove our next lemma.

LEMMA. Let M_1, M_2, M_3 be $N \times N$ matrices of types VI, VII or VIII, with K_1, K_2, K_3 resp. ones.

If $M_1 \ll M_2$ then $K_2 = K_1 + 1$ or $K_2 = K_1$ and $I_{M_2} = I_{M_1}$.

If $M_1 \ll M_2 \ll M_3$ then $K_3 > K_1$.

Now the theorem follows in the case $\frac{1}{4}N^2 < K < \frac{1}{2}N(N - 1)$.

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