An inequality for the analysis of variance

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Abstract

We prove a generalization to matrices and tensors of the Szőkefalvi-Nagy inequality and the Grüss-Popoviciu inequality. Our more general version is required in the analysis of variance (ANOVA).

1. Introduction and main result

The next theorem is our main result, it relates the sum of squares of a real array x with its range. The assumption is that x has zero mean in all directions. This is a standard assumption in the statistics applications that motivate our results, see Remark 1. Our result is a generalization of the Szőkefalvi-Nagy and Grüss-Popoviciu inequalities, see Section 3. Let $n_1, \dots, n_N \in \{2, 3, \dots\}$.

Theorem 1. *Let x be an $(n_1 \times \cdots \times n_N)$ array of real numbers such that x has zero mean in each of its N directions,*

$$\sum_{i_k=1}^{n_k} x_{i_1,\dots,i_k,\dots,i_N} = 0, \qquad \text{for any fixed } \{i_1, \dots, i_N\} \setminus \{i_k\}.$$

Let $x_{\min}$ and $x_{\max}$ denote the smallest and largest entries of x, respectively, and let δ denote the range of x,

$$\delta = x_{\max} - x_{\min}.$$

Let $j_1 \in \{1, 2, \dots, N\}$ such that n_{j_1} is (one of) the smallest n_j, and define

$$C_1 = \frac{1}{2} \cdot \prod_{j=1}^{N} n'_j, \qquad n'_j = \begin{cases} 1, & \text{if } j = j_1 \\ \dfrac{n_j}{n_j - 1}, & \text{otherwise.} \end{cases}$$

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If at least one n_j is odd, then let $j_2 \in \{1, 2, \ldots, N\}$ such that n_{j_2} is (one of) the smallest of the odd n_j. Define

$$C_2 = \frac{1}{4} \cdot \begin{cases} \prod_{j=1}^{N} n_j, & \text{if all } n_j \text{ are even,} \\ \prod_{j=1}^{N} n''_j, & \text{if at least one } n_j \text{ is odd.} \end{cases} \qquad n''_j = \begin{cases} n_j - \frac{1}{n_j}, & j = j_2, \\ n_j, & \text{otherwise.} \end{cases}$$

Then the following holds.

(i) *We have the following bounds for the total sum of squares:*

$$C_1 \cdot \delta^2 \le \sum_{\substack{i_1 \le n_1 \\ \vdots \\ i_n \le n_N}} x^2_{i_1,\ldots,i_n} \le C_2 \cdot \delta^2 \ .$$

(ii) *The lower bound is sharp. The extremal arrays are the tensor products v of (possibly permuted) vectors v_j of the following form,*

$$v = \frac{\delta}{2} \cdot v_1 \otimes \cdots \otimes v_N, \qquad v_j = \begin{cases} (1, -1, \underbrace{0, \ldots, 0}_{n_j - 2}), & j = j_1, \\ \Big(1, \underbrace{-\frac{1}{n_j - 1}, \ldots, -\frac{1}{n_j - 1}}_{n_j - 1}\Big), & j \in \{1, 2, \ldots, N\} \setminus \{j_1\} \ . \end{cases}$$

(iii) *The upper bound is sharp if all n_j are even (Case I, define $p = 2$), or if one n_{j_0} is odd and divides all the other n_j (Case II, define $p = n_{j_0}$). An example extremal is the Hankel tensor defined by first*

$$(x_{1,1,1,\ldots,1}, \ldots, x_{p,1,1,\ldots,1}) = \frac{\delta}{2} \cdot \begin{cases} (1, -1), & \text{Case I,} \\ (\underbrace{1, \ldots, 1}_{\lfloor p/2 \rfloor}, \underbrace{-1, \ldots, -1}_{\lceil p/2 \rceil}) + \frac{1}{p}, & \text{Case II,} \end{cases}$$

and secondly by the p-periodic Hankel property

$$x_{i_1,\ldots,i_n} = x_{i'_1,\ldots,i'_n} \qquad \text{for } i_1 + \cdots + i_n \equiv i'_1 + \cdots + i'_n \mod p \ .$$

Remark 1. Our results are required in the analysis of variance (ANOVA) experimental design. They refine the computation of the worst case power—the power (i.e., the power function evaluated under the alternative) is the complement of the type II error probability—and thus they help decreasing the experimental size [19]. The "zero mean in all directions" condition is a standard assumption to ensure identifiability of parameters [5, pp. 157, 169, 178], [12, Sec. 3.3.1.1], [13, Sec. 5], [14, Sec. 5], [15, Sec. 4.1, p. 92], [16, p. 415, Sec. 7.2.i].

lower	2	3	4	5	6	7
	1	0.75	0.66	0.62	0.6	0.58

Table 1: Lower bounds for the sum of squares of $(n_1 \times n_2)$ matrices with range $\delta = x_{\max} - x_{\min} = 1$ that have zero mean rows and columns. The lower bound from Theorem 1 is tabled as a function of $\max(n_1, n_2)$. The lower bounds are sharp.

upper I	2	3	4	5	6	7
2	1	1.33	2	2.40	3	3.42
3		2	2.66	3.33	4	4.66
4			4	4.80	6	6.85
5				6	7.20	8.40
6					9	10.29
7						12

upper II	2	3	4	5	6	7
2	1	←	2	←	3	←
3		2	←↑	2.61	4	←
4			4	←	6	←
5				6	←↑	7.38
6					9	←
7						12

Table 2: Upper bounds for the sum of squares of $(n_1 \times n_2)$ matrices with range $\delta = x_{\max} - x_{\min} = 1$ that have zero mean rows and columns. In the first table (upper I) the upper bound from Theorem 1 is tabled as a function of n_1 and n_2. The upper bound is not sharp, in general, but the sharp bound cannot be less than the entry in the second table (upper II). In the second table the integer values are the sharp cases from Theorem 1. The non-integer values are obtained from examples found by local minimization, see Example 2(iv). The arrows point to neighboring values that can be re-used by padding the smaller matrix with zeros, see also Example 2(iv).

2. Examples

For $N = 1$, see Section 3. We summarize Theorem 1(i) for $N = 2, 3$.

Example 1. (i) Let x be a real $(n_1 \times n_2)$ matrix with zero mean rows and columns,

$$\sum_i x_{i,j_0} = \sum_j x_{i_0,j} = 0, \qquad \text{for any } i_0, j_0 \ .$$

Let $m_2 = \max(n_1, n_2)$. If at least one of n_1, n_2 is odd, then let p_1 denote the least odd number of n_1, n_2 and let p_2 denote the other number. Then for $\delta = x_{\max} - x_{\min}$, we have

$$\frac{\delta^2}{2} \cdot \frac{m_2}{m_2 - 1} \ \le \ \sum_{i,j} x_{i,j}^2 \ \le \ \frac{\delta^2}{4} \cdot \begin{cases} n_1 n_2, & n_1, n_2 \text{ even}, \\ \left(p_1 - \dfrac{1}{p_1}\right) \cdot p_2, & \text{otherwise.} \end{cases}$$

(ii) Let x be a real $(n_1 \times n_2 \times n_3)$ array with zero mean in all three directions,

$$\sum_i x_{i,j_0,k_0} = \sum_j x_{i_0,j,k_0} = \sum_k x_{i_0,j_0,k} = 0, \qquad \text{for any } i_0, j_0, k_0 \ .$$

Let $m_1 \le m_2 \le m_3$ denote n_1, n_2, n_3 sorted from least to greatest. If at least one of n_1, n_2, n_3 is odd, then let p_1 denote the least odd number of n_1, n_2, n_3 and let p_2, p_3 denote the other two numbers. Then for $\delta = x_{\max} - x_{\min}$, we have

$$\frac{\delta^2}{2} \cdot \frac{m_2 m_3}{(m_2 - 1)(m_3 - 1)} \ \le \ \sum_{i,j,k} x_{i,j,k}^2 \ \le \ \frac{\delta^2}{4} \cdot \begin{cases} n_1 n_2 n_3, & n_1, n_2, n_3 \text{ even}, \\ \left(p_1 - \dfrac{1}{p_1}\right) \cdot p_2 p_3, & \text{otherwise.} \end{cases}$$

We further illustrate Theorem 1 for $N = 2$.

Example 2. (i) For (3×6) matrices with zero mean rows and columns, we have

$$\frac{3}{5} \cdot \delta^2 \ \le \ \sum_{i,j} x_{i,j}^2 \ \le \ 4 \cdot \delta^2,$$

and lower/upper extremals (with $\delta = 1$) are

$$\frac{1}{10} \cdot \begin{pmatrix} 5 & -1 & -1 & -1 & -1 & -1 \\ -5 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \frac{1}{3} \cdot \begin{pmatrix} 2 & -1 & -1 & 2 & -1 & -1 \\ -1 & -1 & 2 & -1 & -1 & 2 \\ -1 & 2 & -1 & -1 & 2 & -1 \end{pmatrix} .$$

(ii) For (4×6) matrices with zero mean rows and columns, we have

$$\frac{3}{5} \cdot \delta^2 \ \le \ \sum_{i,j} x_{i,j}^2 \ \le \ 6 \cdot \delta^2,$$

and lower/upper extremals (with $\delta = 1$) are

$$\frac{1}{10} \cdot \begin{pmatrix} 5 & -1 & -1 & -1 & -1 & -1 \\ -5 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \frac{1}{2} \cdot \begin{pmatrix} 1 & -1 & 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 & -1 & 1 \end{pmatrix} .$$

(iii) For (5×5) matrices with zero mean rows and columns, we have

$$\frac{5}{8} \cdot \delta^2 \;\le\; \sum_{i,j} x_{i,j}^2 \;\le\; 6 \cdot \delta^2,$$

and lower/upper extremals (with $\delta = 1$) are

$$\frac{1}{8} \cdot \begin{pmatrix} 4 & -1 & -1 & -1 & -1 \\ -4 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \frac{1}{5} \cdot \begin{pmatrix} 3 & 3 & -2 & -2 & -2 \\ 3 & -2 & -2 & -2 & 3 \\ -2 & -2 & -2 & 3 & 3 \\ -2 & -2 & 3 & 3 & -2 \\ -2 & 3 & 3 & -2 & -2 \end{pmatrix}.$$

(iv) The upper bound in Theorem 1 is not sharp, in general. The sharp upper bound requires finding global extremals, which quickly become inaccessible as n_1, n_2 increase. But it is easy to close in on the sharp upper bound by finding local extremals, such as the following (3×5) and (5×7) matrices with sum of squares $C = 2.61 \cdot \delta^2$, and $C = 7.38 \cdot \delta^2$, respectively,

$$\frac{1}{7} \cdot \begin{pmatrix} 4 & -1 & -1 & -1 & -1 \\ -2 & 4 & -3 & 4 & -3 \\ -2 & -3 & 4 & -3 & 4 \end{pmatrix}, \qquad \frac{1}{9} \cdot \begin{pmatrix} 5 & 5 & -2 & -2 & -2 & -2 & -2 \\ 5 & -3 & 5 & 5 & -4 & -4 & -4 \\ -3 & 5 & -4 & 5 & 5 & -4 & -4 \\ -4 & -3 & 5 & -4 & -4 & 5 & 5 \\ -3 & -4 & -4 & -4 & 5 & 5 & 5 \end{pmatrix}.$$

Another option to close in on the sharp upper bound is padding an array with zeros that is extremal for a smaller size. For example, attaching a zero column to an extremal (3×6) matrix yields a (3×7) matrix with the same sum of squares, $C = 4 \cdot \delta^2$,

$$\frac{1}{3} \cdot \begin{pmatrix} 2 & -1 & -1 & 2 & -1 & -1 & 0 \\ -1 & -1 & 2 & -1 & -1 & 2 & 0 \\ -1 & 2 & -1 & -1 & 2 & -1 & 0 \end{pmatrix}.$$

3. Proof of Theorem 1

The case $N = 1$ of Theorem 1 reduces to the Szőkefalvi-Nagy and Grüss-Popoviciu inequalities, which we include by the next lemma. The equivalence is immediate, since the range of observations is invariant if we subtract the mean. In the lemma the lower bound is the Szőkefalvi-Nagy inequality [7, eq. (1)], [17, eq. (1.5)], see also Remark 2 below. The upper bound is the Grüss-Popoviciu inequality [1, Sec. 1.7], [9, p. 299, Sec. X.6], a discrete analogue of Grüss' inequality [6], referenced to [3, 11]. See also [2], [10, p. 46, Remark 1.7.9].

We summarize the simple proof from [4, proof of Thm. 2] for the upper bound, adjusting it slightly such that it also yields the lower bound. The mean of $x_1, \ldots, x_n$ is denoted $\overline{x} = (x_1 + \cdots + x_n)/n$.

Lemma 1. *The variance of n real numbers $(x_1, \dots, x_n)$ is related with their range $\delta = x_{\max} - x_{\min}$ by*

$$\frac{1}{2} \cdot \delta^2 \;\le\; \sum_{i=1}^{n} (x_i - \overline{x})^2 \;\le\; \frac{n'}{4} \cdot \delta^2, \qquad n' = \begin{cases} n, & n \text{ even}, \\ n - \frac{1}{n}, & n \text{ odd}. \end{cases}$$

The extremals for the lower and upper bounds are the permutations of, repectively,

$$(x_{\min}, \underbrace{\mu, \dots, \mu}_{n-2}, x_{\max}), \qquad \mu = (x_{\max} - x_{\min})/2,$$

$$(\underbrace{x_{\min}, \dots, x_{\min}}_{k}, \underbrace{x_{\max}, \dots, x_{\max}}_{n-k}), \qquad k = \begin{cases} n/2, & n \text{ even}, \\ \lfloor n/2 \rfloor \text{ or } \lceil n/2 \rceil, & n \text{ odd}. \end{cases}$$

Proof. Fix $x_1 = x_{\min}$ and $x_n = x_{\max}$. Let $j \in \{2, \dots, n-1\}$ and differentiate the variance as a function of x_j,

$$\frac{\partial}{\partial x_j} \sum_{i=1}^{n} (x_i - \overline{x})^2 = \frac{\partial}{\partial x_j} \left[\sum_{i=1}^{n} x_i^2 - \frac{1}{n} \left(\sum_{i=1}^{n} x_i \right)^2 \right] = 2x_j - 2\overline{x} = 2(x_j - \overline{x}). \tag{1}$$

The first derivative contains the factor $x_j - \overline{x}$ and the second derivative $2(1 - 1/n)$ is a positive number. Thus the lower bound extremals must have $x_j = \overline{x}$ and the upper bound extremals must have $x_j = x_{\min}$ or $x_j = x_{\max}$. Selecting the largest variance among these upper bound extremal candidates completes the proof. □

Remark 2. The inequalities in Lemma 1 are often studied in a context where the real numbers x_i are roots of a polynomial, such as the eigenvalues of a symmetric matrix. For example, the original result for the lower bound [18, pp. 42–43, Thm. IX] is in fact an upper bound for the range $\delta = x_{\max} - x_{\min}$ of polynomial roots. The bound is an expression that is formed by two polynomial coefficients and that is equal to the variance, see [4], [8, p. 153, eq. (1.10)].

The simple proof of Lemma 1 does not apply to Theorem 1, since in general the range of x is not invariant, if we project x to mean zero in all directions. Only for $N = 1$ the range is invariant, since the projection reduces to subtracting the mean $x \mapsto x - \overline{x}$. For $N = 2, 3, \dots$, projecting x to mean zero in all directions:

- does not mean subtracting the overall mean or the tensor product of the directional means,
- is clearer, if we consider the discrete Fourier transform y of x, it means annihilating certain Fourier coefficients.

To see which coefficients should be set to zero, we formulate the next lemma.

Lemma 2. *Let x be an $(n_1 \times \cdots \times n_N)$ array of real or complex numbers and let y denote the discrete Fourier transform of x. Then the following equivalences hold:*

(i) *x has mean zero* $\Leftrightarrow$ $y_{1,\dots,1} = 0$,

(ii) *x has mean zero in all directions* $\Leftrightarrow$ $y_{i_1,\ldots,i_N} = 0$ *if any* $i_j = 1$.

Proof. The first equivalence follows from the definition of the first Fourier coefficient. The second equivalence specializes from the following fact, obtained from standard properties of the Fourier transform. If X denotes the smaller array obtained by summing x along the i_k direction and if Y denotes the restriction of y to $i_k = 1$, then Y is the discrete Fourier transform of X. □

Proof of Theorem 1.

Proof. **Step I** (lower bound). Without loss of generality we assume

$$n_1 \leq \cdots \leq n_N \ . \tag{2}$$

By permuting the array without affecting the zero mean conditions, we can assume that the maximum of x is at the $(1,\ldots,1)$ position,

$$x_{\max} = x_{1,\ldots,1}. \tag{3}$$

We also assume that x is not constant, thus the minimum has at least one coordinate k different from the maximum,

$$x_{\min} = x_{i_1,\ldots,i_N}, \qquad i_k \neq 1 \ . \tag{4}$$

Let X be the restriction of x to $i_k = 1$. Thus X is a layer of x that contains $x_{\max}$ but avoids $x_{\min}$. Let Y denote the discrete Fourier transform of X. We use the Fourier transform normalized such that it is unitary,

$$\sum |X_-|^2 = \sum |Y_-|^2, \tag{5}$$

where the notation means summation over all entries of the array. The Fourier transform definition thus involves a normalization constant $\sqrt{P}$, where P is the number of entries of X, which is

$$P = \prod_{\substack{1\leq j\leq N \\ j\neq k}} n_j \ . \tag{6}$$

The normalization constant also occurs in the inverse Fourier transform and related formulas, such as

$$X_{1,\ldots,1} = \frac{1}{\sqrt{P}} \cdot \sum Y_-. \tag{7}$$

Next, the triangle inequality implies

$$\left(\sum Y_-\right)^2 \leq K \cdot \sum |Y_-|^2, \tag{8}$$

where K is the number of non-zero entries of Y. By Lemma 2 the zero mean conditions on X imply that the Fourier transform Y vanishes at $y_{i_1,\ldots,i_N}$, if $i_j = 1$, for any $j \in \{1,\ldots,N\}\backslash\{k\}$. Hence,

$$K \leq \prod_{\substack{1\leq j\leq N \\ j\neq k}} (n_j - 1) \ . \tag{9}$$

Combining the above and noting that X is real, we obtain

$$\begin{aligned} x_{\max}^2 = x_{1,\dots,1}^2 = X_{1,\dots,1}^2 &= \frac{1}{P} \cdot \left(\sum Y_-\right)^2 \\ &\le \frac{K}{P} \cdot \sum |Y_-|^2 = \frac{K}{P} \cdot \sum |X_-|^2 = \frac{K}{P} \cdot \sum X_-^2 \ . \end{aligned} \tag{10}$$

The arguments above for the layer X that contains $x_{\max}$ also work for the parallel layer $\widetilde{X}$ that contains $x_{\min}$ and hence,

$$\begin{aligned} x_{\max}^2 + x_{\min}^2 &\le \frac{K}{P} \cdot \sum X_-^2 + \frac{K}{P} \cdot \sum \widetilde{X}_-^2 \\ &= \frac{K}{P} \cdot \left(\sum X_-^2 + \sum \widetilde{X}_-^2\right) \le \frac{K}{P} \cdot \sum x_-^2 \ . \end{aligned} \tag{11}$$

Since

$$(x_{\max} - x_{\min})^2 \le (x_{\max} + x_{\min})^2 + (x_{\max} - x_{\min})^2 = 2(x_{\max}^2 + x_{\min}^2), \tag{12}$$

we thus conclude that

$$\frac{(x_{\max} - x_{\min})^2}{2} \cdot \prod_{\substack{1 \le j \le N \\ j \ne k}} \frac{n_j}{n_j - 1} \le (x_{\max}^2 + x_{\min}^2) \cdot \frac{P}{K} \le \sum x_-^2 \ . \tag{13}$$

Step II (upper bound, if all n_j are even). Let $n = n_1 \cdots n_N$. Reshape the $(n_1 \times \cdots \times n_N)$ array x into one long vector v of length n. Note v has mean zero. Apply to v the Grüss-Popoviciu inequality, which is the upper bound in Lemma 1.

Step III (upper bound, if at least one n_j is odd). Let $n = n_1 \cdots n_N$ and let p denote the least odd number of $n_1, \dots, n_N$. We can split the $(n_1 \times \cdots \times n_N)$ array x into n/p many vectors v_k of length p, such that each v_k has mean zero. Apply to each v_k the Grüss-Popoviciu inequality. □

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