On the maximal size of Large-Average and ANOVA-fit Submatrices in a Gaussian Random Matrix

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Abstract

We investigate the maximal size of distinguished submatrices of a Gaussian random matrix. Of interest are submatrices whose entries have average greater than or equal to a positive constant, and submatrices whose entries are well-fit by a two-way ANOVA model. We identify size thresholds and associated (asymptotic) probability bounds for both large-average and ANOVA-fit submatrices. Results are obtained when the matrix and submatrices of interest are square, and in rectangular cases when the matrix submatrices of interest have fixed aspect ratios. In addition, we obtain a strong, interval concentration result for the size of large average submatrices in the square case. A simulation study shows good agreement between the observed and predicted sizes of large average submatrices in matrices of moderate size.

Running title: Maximal submatrices of a Gaussian random matrix

Keywords: analysis of variance, data mining, Gaussian random matrix, large average submatrix, random matrix theory, second moment method

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1 Introduction

Gaussian random matrices (GRMs) have been a fixture in the application and theory of multivariate analysis for many years. Recent work in the field of random matrix theory has provided a wealth of information about the eigenvalues and eigenvectors of Gaussian, and more general, random matrices. Motivated by problems of data mining and the exploratory analysis of large data sets, this paper considers a different problem, namely the maximal size of distinguished submatrices in a GRM. Of interest are submatrices that are distinguished in one of two ways: (i) the average of their entries is greater than or equal to a positive constant or (ii) the optimal two-way ANOVA fit of their entries has average squared residual less than a positive constant.

Using arguments from combinatorial probability, we identify size thresholds and associated probability bounds for large average and ANOVA-fit submatrices. Results are obtained when the matrix and the submatrices of interest are square, and when the matrix and the submatrices of interest have fixed aspect ratios. In each case, the maximal size of a distinguished submatrix grows logarithmically with the dimension of the matrix, and depends in a polynomial-type fashion on the inverse of the constant that constitutes the threshold of distinguishability. In the rectangular case, the aspect ratio of the submatrix plays a more critical role than the aspect ratio of the matrix itself. In addition, we obtain upper and lower bounds for the size of large average submatrices in the square case. In particular, for $n \times n$ GRMs, the size of the largest square submatrix with average greater than $\tau > 0$ is eventually almost surely within in an interval of fixed width that contains the critical value $4\tau^{-2}(\ln n - \ln(4\tau^{-2}\ln n))$.

We assess our bounds for large average submatrices via a simulation study in which the size thresholds for large average submatrices are compared to the observed size of such submatrices in a Gaussian random matrix. For matrices with moderate size and aspect ratio, there is good agreement between the observed and predicted sizes.

Results of the sort established here fall outside the purview of random matrix theory and its techniques. Nevertheless, random matrix theory does provide some insight into the logarithmic scale of large average submatrices. This is discussed briefly in Section 1.3 below.

1.1 Exploratory Data Analysis

The results of this paper are motivated in part by the increasing application of exploratory tools such as biclustering to the analysis of large data sets. To be specific, consider an $m \times n$ data matrix X that is generated by measuring the values of m real-valued variables on each of n subjects or samples. The initial analysis of such data often involves an exploratory search for interactions among samples and variables. In genomic studies of cancer, sample-variable interactions can provide the basis for new insights and hypotheses concerning disease subtypes and genetic pathways, *c.f.* [8, 17, 6, 20, 21, 25].

Formally, sample-variable interactions correspond to distinguished submatrices of X. The task of identifying such submatrices is generally referred to as *biclustering*, two-way clustering or subspace clustering in the computer science and bioinformatics literature. There is presently a substantial body of work on biclustering methods, based on a variety of submatrix criteria; overviews can be found in [13, 10, 15] and the references therein. In particular, the biclustering methods by Tanay *et al.* [24] and by Shabalin *et al.* [18] search for submatrices whose entries have a large average value, while those of Cheng and Church [4] and Lazzeroni and Owen [12] search for submatrices whose entries are well fit by a two-way ANOVA model. The effectiveness of these procedures in the analysis of real data is considered in [18].

An exact or heuristic search among the (exponentially large) family of submatrices of a data matrix for those that are distinguished by their average or ANOVA fit leads naturally to a number of statistical questions related to multiple testing. For example, how large does a distinguished submatrix have to be in order for it to be considered statistically significant, and therefore potentially worthy of scientific interest? What is the statistical significance of a given distinguished submatrix? Quantitative answers require an appropriate null model for the observed data matrix, and in many cases, a GRM model is a natural starting point for analysis. When a GRM null is appropriate, the results of this paper provide partial answers to the questions above.

We note that answers to statistical questions like those above can have algorithmic implications. For example, knowing the minimal size of a significant submatrix can provide a useful filtering criterion for exhaustive or heuristic search procedures, or can drive the search procedure in a direct way. The biclustering method in [18] is based on a simple, Bonferroni corrected measure of statistical significance that arises in the initial analyses below.

1.2 Bipartite Graphs

Our results on large average submatrices can also be expressed in graph-theoretic terms, as every $m \times n$ matrix X is associated in a natural way with a bipartite graph $G = (V, E)$.

In particular, the vertex set V of G is the disjoint union of two sets V_1 and V_2, with $|V_1| = m$ and $|V_2| = n$, corresponding to the rows and columns of X, respectively. For each row $i \in V_1$ and column $j \in V_2$ there is an edge $(i, j) \in E$ with weight $x_{i,j}$. There are no edges between vertices in V_1 or between vertices in V_2. With this association, large average submatrices of X are in 1:1 correspondence with subgraphs of G having large average edge-weight. The complexity of finding the largest subgraph of G whose average edge weight is greater than a threshold appears to be unknown. However, it is shown in [5] that a slight variation of this problem, namely finding the maximum edge weight subgraph in a general bipartite matrix, is NP-complete. A randomized, polynomial time algorithm that finds a subgraph whose edge weight is within a constant factor of the optimum is described in [1], but this algorithm cannot readily be adapted to the problem considered here.

1.3 Connections with Random Matrix Theory

The theory of random matrices provides some insight into the relationship between large average submatrices and the singular value decomposition. In practice, the GRM assumption made here acts as a null hypothesis. If an observed matrix contains a large average submatrix whose size exceeds the thresholds given below, one may reject the GRM hypothesis, and subject the identified submatrix to further analysis. This suggest an alternative hypothesis, under which a fixed constant is added to every element of a select submatrix of the null matrix, effectively embedding a large average submatrix within a background of Gaussian noise. It is then natural to ask if the embedded submatrix affects the top singular value or singular vectors of the resulting matrix. We argue below that the answer is a qualified no.

Let W be an $m \times n$ Gaussian random matrix, representing the null distribution. Define a rank-one matrix $S = 2\tau ab^t$, where $\tau > 0$ is a fixed constant, and $a \in \{0,1\}^m$, $b \in \{0,1\}^n$ are indicator vectors having k and l non-zero components, respectively. The outer produce $a\, b^t$ defines a submatrix C whose rows and columns are indexed by the indicator vectors a and b, respectively. The matrix $Y = W + S$ is distributed according to an alternative hypothesis under which the fixed constant τ has been added to every entry of the submatrix C.

Suppose that the dimensions m, n, k and l grow (with n, say) in such a way that the matrix aspect ratio $m/n \to \alpha$ with $\alpha \in [1, \infty)$, and the submatrix aspect ratio k/l remains bounded away from zero and infinity. It is easy to see that the average of the $k \times l$ submatrix C in Y has distribution $\mathcal{N}(2\tau, (kl)^{-1})$, which is greater than τ with overwhelming probability when k and l are large. It follows from Proposition 1 that the probability of finding a $k \times l$ submatrix with average greater than τ in the matrix W is vanishingly small if k and l grow faster than $\log n$. Thus, we might expect to see evidence of C in the first singular value, or the associated singular vectors, of Y.

Given an $m \times n$ matrix U, let $s_1(U) \geq \cdots \geq s_m(U)$ denote its ordered singular values, and let $||U||_F = \sum_{i,j} u_{i,j}^2$ denote its Frobenius norm. The difference between the largest singular value of W and Y can be bounded as follows:

$$\begin{aligned}
(s_1(Y) - s_1(W))^2 &\leq \sum_{j=1}^{n} (s_j(Y) - s_j(W))^2 \\
&\leq \sum_{j=1}^{n} (s_j(Y - W))^2 \\
&= ||Y - W||_F^2 \;=\; ||Z||_F^2 \;=\; \tau^2\, k\, l.
\end{aligned} \tag{1}$$

The second line above follows an inequality of of Lidskii (*c.f.* Exercise 3.5.18 of [9]), and the third makes use of the fact that the Frobenius norm of a matrix is the sum of the squares of its singular values. By a basic result of Geman [7],

$$\frac{s_1(W)}{n^{1/2}} \to \left(1 + \alpha^{1/2}\right) \tag{2}$$

with probability one as n tends to infinity. If $k = o(m^{1/2})$ and $l = o(n^{1/2})$, inequality (1) implies that $n^{-1/2}|s_1(Y) - s_1(W)| \to 0$ with probability one, and therefore (2) holds with Y in place of W. In other words, the asymptotic behavior of $n^{-1/2}s_1(W)$ is unchanged under the alternative $Y = W + Z$ if the dimensions of the embedded submatrix C grow more slowly than $n^{1/2}$. (Recall that m is asymptotically proportional to n.)

For fixed τ and k, l such that $\log n << k, l << n^{1/2}$, the embedded submatrix C in Y is highly significant, but has no effect on the scaled limit of $s_1(Y)$. Under the same conditions, C is also not recoverable from the top singular vectors of Y. To be precise, let u_1 and v_1 be the left and right singular vectors of Y corresponding to the maximum singular value $s_1(Y)$. Using results of Paul [16] on the singular vectors of spiked population models, it can be shown that $a^t u_1$ and $b^t v_1$ tend to zero in probability as n tends to infinity. Thus the row and column index vectors of C are asymptotically orthogonal to the first left and right singular vectors of Y.

1.4 Overview

The next section contains probability bounds and a finite interval concentration result for the size of large average submatrices in the square case. Size thresholds and probability bounds for ANOVA submatrices in the square case are presented in Section 3. Thresholds and bounds in the rectangular case are given in Section 4. Section 5 contains a simulation study for large average submatrices. Sections 6 – 8 contain the proofs of the main results.

2 Thresholds and Bounds for Large Average Submatrices

Let $W = \{w_{i,j} : i, j \geq 1\}$ be an infinite array of independent $\mathcal{N}(0,1)$ random variables, and for $n \geq 1$, let $W_n = \{w_{i,j} : 1 \leq i, j \leq n\}$ be the $n \times n$ Gaussian random matrix equal to upper left hand corner of W. (The almost-sure asymptotics of Theorem 1 requires consideration of matrices W_n that are derived from a fixed, infinite array.) A submatrix of W_n is a collection $U = \{w_{i,j} : i \in A, j \in B\}$ where $A, B \subseteq \{1, \ldots, n\}$. The Cartesian product $C = A \times B$ will be called the index set of U, and we will write $U = W_n[C]$. The dimension of C is $|A| \times |B|$, where $|A|, |B|$ denote the cardinality of A and B, respectively. Note that the rows A need not be contiguous, and that the same is true of the columns B. When no ambiguity will arise, the index set C will also be referred to as a submatrix of W_n.

Definition: For any submatrix U of W_n with index set $C = A \times B$, let

$$F(U) \; = \; \frac{1}{|C|} \sum_{(i,j) \in C} w_{i,j} \; = \; \frac{1}{|A||B|} \sum_{i \in A, j \in B} w_{i,j}$$

be the average of the entries of U. Note that $F(U) \sim \mathcal{N}(0, |C|^{-1})$.

We are interested in the maximal size of square submatrices whose averages exceed a fixed threshold. This motivates the following definition.

Definition: Fix $\tau > 0$ and $n \geq 1$. Let $K_\tau(W_n)$ be the largest $k \geq 0$ such that W_n contains a $k \times k$ submatrix U with $F(U) \geq \tau$.

As the rows and columns of a submatrix need not be contiguous, the statistic $K_\tau(W_n)$ is invariant under row and column permutations of W_n. We may regard the Gaussian distribution of W_n as a null hypothesis for testing an observed $n \times n$ data matrix, and $K_\tau(\cdot)$ as a test statistic with which we can detect departures from the null. Our immediate goal is to obtain bounds on the probability that $K_\tau(W_n)$ exceeds a given threshold, and to identify a threshold for $K_\tau(W_n)$ that governs its asymptotic behavior. To this end, we begin the analysis of $K_\tau(W_n)$ using standard first moment type arguments, which are detailed below.

Let $\Gamma_k(n, \tau)$ be the number of $k \times k$ submatrices in W_n having average greater than or equal to τ. We begin by identifying the value of k for which $E\,\Gamma_k(n, \tau)$ is approximately equal to one. If $\mathcal{S}_k$ denotes the set of all $k \times k$ submatrices of W_n then

$$\Gamma_k(n, \tau) \;=\; \sum_{U \in \mathcal{S}_k} I\{F(W_n[U]) \geq \tau\}, \tag{3}$$

and consequently

$$E\,\Gamma_k(n, \tau) \;=\; |\mathcal{S}_k| \cdot P(F(W_n[U]) \geq \tau) \;=\; \binom{n}{k}^2 (1 - \Phi(\tau k)) \;\leq\; \binom{n}{k}^2 e^{-\frac{\tau^2 k^2}{2}}, \tag{4}$$

where in the last step we have used a standard bound on $1 - \Phi(\cdot)$. For $s \in (0, n)$ define

$$\phi_{n,\tau}(s) \;=\; (2\pi)^{-\frac{1}{2}}\, n^{n+\frac{1}{2}}\, s^{-s-\frac{1}{2}}\, (n-s)^{-(n-s)-\frac{1}{2}}\, e^{-\frac{\tau^2 s^2}{4}}. \tag{5}$$

Using the Stirling approximation of $\binom{n}{k}$, it is easy to see that $\phi_{n,\tau}(k)$ is an approximation of the square root of the final expression in (4). In particular, the rightmost expression in (4) is less than $2\phi_{n,\tau}(k)^2$. With this in mind, let $s(n, \tau)$ be any positive, real root of the equation

$$\phi_{n,\tau}(s) = 1. \tag{6}$$

The next result shows that $s(n, \tau)$ exists and is unique, and it provides an explicit expression for its value when τ is fixed and n is large.

Lemma 1. *Let $\tau > 0$ be fixed. When n is sufficiently large, equation (6) has a unique root $s(n, \tau)$, and*

$$s(n, \tau) \;=\; \frac{4}{\tau^2} \ln n \;-\; \frac{4}{\tau^2} \ln\left(\frac{4}{\tau^2} \ln n\right) \;+\; \frac{4}{\tau^2} \;+\; o(1) \tag{7}$$

where $o(1) \to 0$ as $n \to \infty$.

We show below that the asymptotic behavior of the random variables $K_\tau(W_n)$ is governed by the root $s(n, \tau)$ of equation (6). To begin, note that for values of k greater than $s(n, \tau)$, the expected number of $k \times k$ submatrices U of W_n with $F(U) \geq \tau$ is less than one. The next proposition shows that the probability of seeing such large submatrices is small.

Proposition 1. *Let $\tau > 0$ be fixed. For every $\epsilon > 0$, when n is sufficiently large,*

$$P\left(K_\tau(W_n) \geq s(n, \tau) + r\right) \;\leq\; \frac{4}{\tau^2}\, n^{-2\,r} \left(\frac{\ln n}{\tau^2}\right)^{2r+\epsilon} \tag{8}$$

for every $r = 1, \ldots, n$.

The proofs of Lemma 1 and Proposition 1 are given in Section 6. The arguments are similar to those in [23], with adaptations to the present setting. A result similar to

Proposition 1 can also be obtained from the comparison principle for Gaussian sequences (*cf.* [19]). To be specific, fix $k \geq 1$ and note that the family of random variables $\{F(U) : U \in \mathcal{S}_k\}$ is a Gaussian random field with $m = \binom{n}{k}^2$ elements that are pairwise positively correlated, and have a common $\mathcal{N}(0, k\tau)$ distribution. Then, by the comparison principle,

$$P\left(K_\tau(W_n) \geq k\right) \;=\; P\left(\max_{U \in \mathcal{S}_k} F(U) \geq \tau\right) \;\leq\; P\left(\max\{Z_1, ..., Z_m\} \geq \tau\right),$$

where $Z_1, \ldots, Z_m$ are independent $\mathcal{N}(0, k\tau)$ random variables. Using Poisson approximation based bounds such as those in Section 4.4 of [2], one may obtain a probability upper bound similar to that in (8).

It follows from Proposition 1 and the Borel Cantelli Lemma that, with probability one, $K_\tau(W_n)$ is eventually less than or equal to $\lceil s(n,\tau) \rceil + 1 \leq s(n,\tau) + 2$. Our principal result, stated in Theorem 1 below, makes use of a second moment argument in order to obtain a corresponding lower bound. The proof is given in Section 8.

Theorem 1. *Let W_n, $n \geq 1$, be Gaussian random matrices derived from an infinite array W, and let $\tau > 0$ be fixed. With probability one, when n is sufficiently large,*

$$s(n,\tau) \;-\; \frac{4}{\tau^2} \;-\; \frac{12 \ln 2}{\tau^2} \;-\; 4 \;\leq\; K_\tau(\mathbf{W}_n) \;\leq\; s(n,\tau) + 2. \tag{9}$$

The difference between the upper and lower bounds in Theorem 1 is a constant that depends on τ, but is *independent* of the matrix dimension n. In particular the values of the random variable $K_\tau(W_n)$ are eventually concentrated on an interval that contains $s(n,\tau)$ and whose width is independent of n.

The lower bound in Theorem 1 can be further improved. An examination of the argument in Lemma 4 in the Appendix shows the inequality of the theorem still holds if the quantity $12 \ln 2$ is replaced with any constant greater than $8 \ln 2$.

Extending earlier work of Dawande *et al.* [5] and Koyuturk *et al.* [11], Sun and Nobel [22, 23] obtained a similar, two-point concentration result for the size of largest square submatrix of ones in an i.i.d. Bernoulli random matrix. Bollobás and Erdős [3], and Matula [14], established analogous results for the clique number of a regular random graph. (See [23] for additional references to work in the binary case.) The proof of Theorem 1 relies on a second moment argument, but differs from the proofs of these earlier results due to the continuous setting. In particular, the proof makes use of the fact that, under the Gaussian assumption made here, for any $k \times k$ submatrix U of W, there exist simple upper bound and lower bounds on $P(F(U) \geq \tau)$, and that the ratio of these bounds is of order τk.

3 Thresholds and Bounds for ANOVA Submatrices

In this section we derive bounds like those in Proposition 1 for the size of submatrices whose entries are well-fit by a two-way ANOVA model. Roughly speaking, the ANOVA criterion identifies submatrices whose rows (and columns) are shifts of one another.

Definition: For a submatrix U of W_n with index set $A \times B$, define

$$G(U) \ = \ \min \left\{ \frac{1}{(|A|-1)(|B|-1)} \sum_{i \in A, j \in B} (w_{ij} - a_i - b_j - c)^2 \right\},$$

where the minimum is taken over all real constants $\{a_i : i \in A\}$, $\{b_j : j \in B\}$ and c.

Under the ANOVA criterion, a submatrix U will warrant interest if $g(U)$ is less than a pre-defined threshold. Note that by standard arguments,

$$G(U) \ = \ \frac{1}{(|A|-1)(|B|-1)} \sum_{i \in A, j \in B} (w_{ij} - \overline{w}_{i.} - \overline{w}_{.j} + \overline{w}_{..})^2,$$

where $\overline{w}_{i.}$, $\overline{w}_{.j}$, and $\overline{w}_{..}$ denote the row, column, and the full submatrix averages, respectively.

Definition: Given $0 < \tau < 1$, let $L_\tau(W_n)$ be the largest value of k such that W_n contains a $k \times k$ submatrix U with $G(U) \leq \tau$.

Arguments similar to those in the proof of Proposition 1, in conjunction with a probability upper bound on the left tail of a χ^2 distribution, establish the following bound on $L_\tau(W_n)$. The proof is given in Section 7.

Proposition 2. *Let $\tau > 0$ be fixed. For every $\epsilon > 0$, when n is sufficiently large,*

$$P\left(L_\tau(W_n) \geq t(n,\tau) + r\right) \ \leq \ \frac{4}{h(\tau)} \left(\frac{\ln n}{h(\tau)}\right)^{2r+2+\epsilon} n^{-2r} \tag{10}$$

for every $r = 1, \ldots, n$, where

$$t(n,\tau) = \frac{4}{h(\tau)} \ln n - \frac{4}{h(\tau)} \ln\left(\frac{4}{h(\tau)} \ln n\right) + \frac{4}{h(\tau)} + 2$$

and

$$h(\tau) = 1 - \tau - \log(2 - \tau). \tag{11}$$

Proposition 2 and the Borel Cantelli Lemma imply that $L_\tau(W_n) \leq t(n,\tau) + 1$ eventually almost surely. The arguments used to lower bound $K_\tau(W_n)$ in Theorem 1 do not extend readily to $L_\tau(W_n)$, and we are not aware if a similar interval-concentration result holds in this case.

4 Thresholds and Bounds for Rectangular Submatrices

The probability bounds of Proposition 1 and 2 can be extended to non-square submatrices of non-square matrices by adapting the methods of proof detailed in Sections 6 and 7, respectively. We present the resulting bounds below, without proof. Similar results concerning submatrices of 1s in binary matrices can be found in [23].

Definition: Let $W(m,n)$ denote an $m \times n$ Gaussian random matrix, and let $\alpha > 0$ and $\beta \geq 1$ be fixed aspect ratios for the sample matrix and target submatrix respectively.

a. For $\tau > 0$ let $K_\tau(W : n, \alpha, \beta)$ be the largest integer k such that there exists a $\lceil \beta k \rceil \times k$ submatrix U in $W(\lceil \alpha n \rceil, n)$ with $F(U) \geq \tau$.

b. For $0 < \tau < 1$ let $L_\tau(W : n, \alpha, \beta)$ be the largest integer k such that there exists a $\lceil \beta k \rceil \times k$ submatrix U in $W(\lceil \alpha n \rceil, n)$ with $G(U) \leq \tau$.

Proposition 3. *Fix $\tau > 0$ and any $\epsilon > 0$. When n is sufficiently large,*

$$P\left(K_\tau(W : n, \alpha, \beta) \ \geq \ s(n, \tau, \alpha, \beta) + r\right) \ \leq \ n^{-(\beta+1)\,r} \left(\frac{\ln n}{\tau^2}\right)^{(\beta+1+\epsilon)r}$$

for each $1 \leq r \leq n$, where

$$s(n, \tau, \alpha, \beta) \ = \ \frac{2(1+\beta^{-1})}{\tau^2} \ln n - \frac{2(1+\beta^{-1})}{\tau^2} \ln\left[\frac{2(1+\beta^{-1})}{\tau^2} \ln n\right] + \frac{2}{\tau^2} \ln \alpha + C_1(\beta, \tau),$$

for some constant $C_1(\beta, \tau) > 0$.

Proposition 4. *Fix $0 < \tau < 1$ and any $\epsilon > 0$. When n is sufficiently large,*

$$P(L_\tau(W : n, \alpha, \beta) \ \geq \ t(n, \tau, \alpha, \beta) + r) \ \ \leq \ n^{-(\beta+1)\,r} \left(\frac{\ln n}{h(\tau)}\right)^{(\beta+1+\epsilon)r}$$

for each $1 \leq r \leq n$, where

$$t(n, \tau, \alpha, \beta) \ = \ \frac{2(1+\beta^{-1})}{h(\tau)} \ln n - \frac{2(1+\beta^{-1})}{h(\tau)} \ln\left[\frac{2(1+\beta^{-1})}{h(\tau)} \ln n\right] + h(\tau)^{-1} \ln \alpha + C_2(\beta, \tau),$$

for some constant $C_2(\beta, \tau) > 0$, where $h(\tau)$ is defined as in (11).

Remark: The bounds in Propositions 3 and 4 have a similar form. In each case, the bound is of the form $n^{-(\beta+1)\,r}$ times a polynomial in $\ln n$, and the leading term in $s(\cdot)$ and $t(\cdot)$ are of the form $(1 + \beta^{-1}) \ln n$ times a function of the threshold τ. We note the critical role played by the aspect ratio β of the target submatrix. By contrast, the aspect ratio α of the sample matrix plays a secondary role, its logarithm appearing only in the constant term of $s(\cdot)$ and $t(\cdot)$.

5 Simulation Study for Large Average Submatrices

The size thresholds and probability bounds presented in Sections 2 - 4 are asymptotic, and it is reasonable to ask if they apply to matrices of moderate size. To this end, we carried out a simulation study in which we compared the size of large average submatrices in simulated Gaussian data matrices with the bounds predicted by the theory. An exhaustive search for large average submatrices is not computationally feasible. Our study was based on a simple search algorithm for large average submatrices that is used in the biclustering procedure of Shabalin *et al.* [18]. Analogous application of existing ANOVA based biclustering procedures does not appear to be straightforward, so the simulation study was restricted to the large average criteria.

The search algorithm from [18] operates as follows. Given an $m \times n$ data matrix W and integers $1 \leq k \leq m$ and $1 \leq l \leq n$, a random subset of l columns of W is selected. The sum of each row over the selected set of l columns is computed, and the rows corresponding to the k largest sums are selected. Then the sum of each column over the selected set of k rows is computed, and the columns corresponding to the l largest sums are selected. This alternating update of row and column sets is repeated until a fixed point is reached, and the average of the resulting $k \times l$ matrix is recorded. The basic search procedure is repeated N times, and the output of the search algorithm is the largest of the N observed submatrix averages. The search algorithm is not guaranteed to find the $k \times l$ submatrix of W with maximum average. However, the algorithm provides a lower bound on the maximum average value of $k \times l$ submatrices We conducted two experiments, one for square matrices and one for rectangular matrices.

Square matrices. We considered matrices of size $n = 200$ and $n = 500$. Results from the case $n = 200$ are summarized in Figure 1. For a fixed $k \geq 1$, we generated a 200×200 Gaussian random matrix W, and then used the search algorithm described above to find a lower bound, τ_k, on the maximum average of the $k \times k$ submatrices of W using $N = 10000$ iterations of the search procedure. Different random matrices W were generated for different values of k. The upper and lower bounds of Theorem 1 begin to diverge when $\tau \leq 1/2$, so we restricted attention to values of k for which $\tau_k > 1/2$. In this case k ranged from 1 to 55. A linear interpolation of the pairs (τ_k, k) appears as the red curve in Figure 1. We have also plotted the threshold function $s(n, \tau)$ derived in Lemma 1, omitting the $o(1)$ term, as well as the upper and lower bounds from Theorem 1. As can be seen from the figure, there is good agreement between the observed and predicted sizes of large average submatrices. In

Figure 1: Results of 200 x 200 simulations

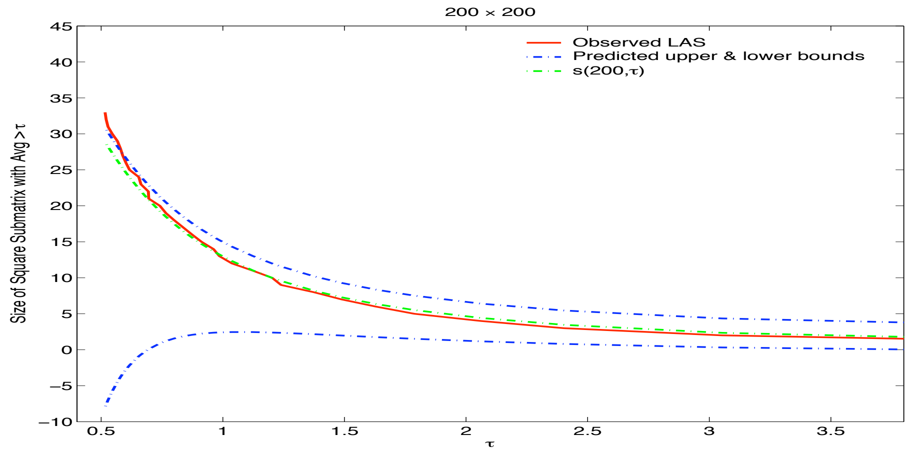
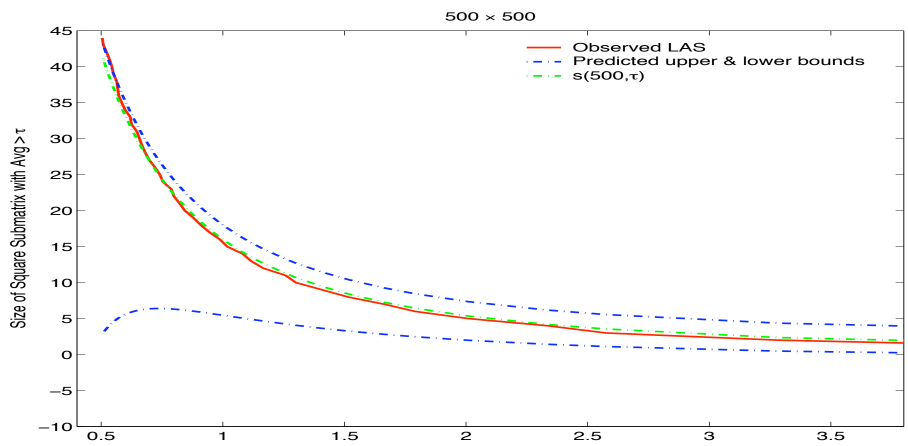


Figure 2: Results of 500 x 500 simulations

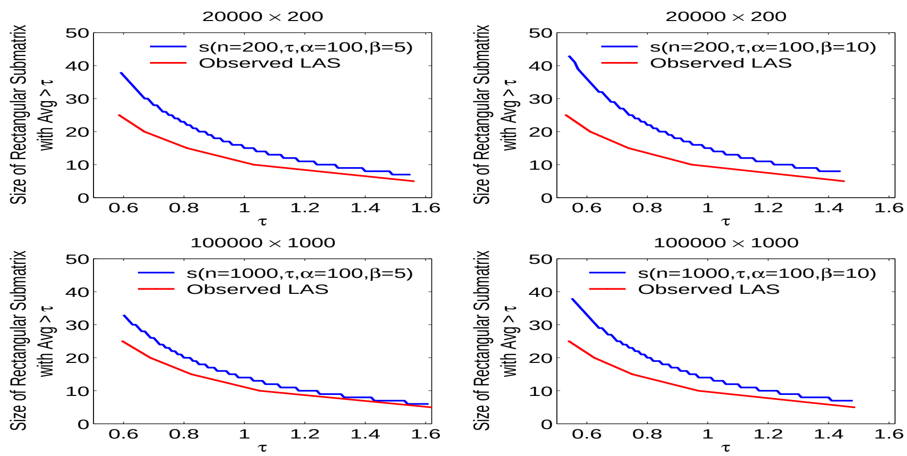


particular, for the range $\tau \geq 1/2$ the observed sizes of large average submatrices fall within the upper and lower bounds of the theorem.

Simulations for matrix size $n = 500$ were carried out in a similar fashion. The results, based on $N = 10000$ iterations of the search procedure for each value of k, are summarized in Figure 2. Restricting attention to $\tau_k > 1/2$ leads to matrix sizes k between 1 and 55 As in the case $n = 200$ there is good agreement between the observed and predicted sizes of large average submatrices, and the observed sizes of large average submatrices fall within the upper and lower bounds of Theorem 1.

Non-Square matrices. We also carried out two simulation studies for rectangular

Figure 3: Results for rectangular simulations



matrices of sizes $20,000 \times 200$ and $100,000 \times 1000$ (matrix aspect ratio $\alpha = 100$). These sizes reflect those commonly seen in high-throughput genomic data. In each case, we looked for submatrices with aspect ratio $\beta = 5$ and $\beta = 10$. For each fixed $k \in \{5, 10, 15, 20, 25\}$, we generated a Gaussian random matrix of the appropriate size and then used the search algorithm with $N = 10000$ iterations to identify $\beta k \times k$ submatrices with large average. The results are summarized in the (interpolated) red curves of Figure 5. The theoretical upper bounds from Proposition 3 are plotted in blue for comparison. In each case the observed maxima lie below the theoretical upper bound; the gap decreases with decreasing β and increasing τ.

6 Proof of Lemma 1 and Proposition 1

Proof of Lemma 1: Let $\tau > 0$ be fixed, and note that

$$\ln \phi_{n,\tau}(s) \;=\; (n + \frac{1}{2}) \ln n - (s + \frac{1}{2}) \ln s - (n - s + \frac{1}{2}) \ln(n - s) - \frac{\tau^2 s^2}{4} - \frac{1}{2} \ln 2\pi. \qquad (12)$$

Differentiating $\ln \phi_{n,\tau}(s)$ with respect to s yields

$$\frac{\partial \ln \phi_{n,\tau}(s)}{\partial s} \;=\; \frac{1}{2(n-s)} + \ln(n - s) - \frac{1}{2s} - \ln s - \frac{s\tau^2}{2}.$$

The last expresssion is negative when $2\tau^{-2} \ln n < s < 4\tau^{-2} \ln n$; we now consider the value of $\ln \phi_{n,\tau}(s)$ for s outside this interval. A straightforward calculation shows that for $0 < s \leq 2\tau^{-2} \ln n$,

$$\ln \phi_{n,\tau}(s) \;\geq\; s \left(\ln(n - 2\tau^{-2} \ln n) - \frac{s\tau^2}{4} - \ln \ln n - \ln 2\tau^{-2} \right) - \frac{1}{2} \ln s - \frac{1}{2} \ln 2\pi,$$

which is positive when n is sufficiently large. In order to address the other extreme, note that from (12) we have

$$\ln \phi_{n,\tau}(s) \;\leq\; s\left(\ln(n-s) - \frac{s\tau^2}{4} - \ln s\right) - \frac{1}{2}\ln s + (n+1/2)\ln\left(\frac{n}{n-s}\right). \qquad (13)$$

It is easy to check that the right hand side of the above inequality is negative when $s > n-2$. Considering separately the cases $s+2 < n < (2\ln 2)^{-1} s\ln s$ and $n \geq (2\ln 2)^{-1} s\ln s$, one may upper bound the final term above by $(s\ln s)/2 + (\ln 2)/2$ and $2s + (\ln 2)/2$, respectively. Thus, for $s < n-2$, we have

$$\ln \phi_{n,\tau}(s) \;\leq\; s\left(\ln(n-s) - \frac{s\tau^2}{4} - \ln s\right) - \frac{1}{2}\ln s + 2s + \frac{s\ln s}{2} + \frac{\ln 2}{2},$$

and in particular, for $4\tau^{-2}\ln n \leq s < n-2$,

$$\ln \phi_{n,\tau}(s) \;\leq\; s\left(2 - \frac{\ln s}{2}\right) - \frac{1}{2}\ln s + \frac{\ln 2}{2} \;<\; 0$$

when n (and therefore s) is sufficiently large. Thus for large n there exists a unique solution $s(n,\tau)$ of the equation $\phi_{n,\tau}(s) = 1$ with $s(n,\tau) \in (2\tau^{-2}\ln n, 4\tau^{-2}\ln n)$.

Taking logarithms of both sides of the equation $\phi_{n,\tau}(s) = 1$ and rearranging terms yields the expression

$$\frac{1}{2}\ln\frac{n}{n-s} + n\ln\frac{n}{n-s} - (s+\frac{1}{2})\ln s + s\ln(n-s) - \frac{\tau^2 s^2}{4} \;=\; \frac{\ln 2\pi}{2}. \qquad (14)$$

The argument above shows that the (unique) solution of this equation belongs to the interval $(2\tau^{-2}\ln n, 4\tau^{-2}\ln n)$, so we consider the case in which s and n/s tend to infinity with n. Dividing both sides of (14) by s yields

$$\ln(n-s) - \frac{s\tau^2}{4} - \ln s \;=\; -1 + O(\frac{\ln s}{s}),$$

which, after adding and subtracting terms, can be rewritten in the equivalent form

$$\ln n - \frac{s\tau^2}{4} - \ln\ln n \;=\; \ln\left(\frac{s}{\ln n}\right) - \ln\left(\frac{n-s}{n}\right) - 1 + O(\frac{\ln s}{s}). \qquad (15)$$

For each $n \geq 1$, define $R(n)$ via the equation

$$s(n,\tau) \;=\; 4\tau^{-2}\ln n - 4\tau^{-2}\ln\ln n + R(n).$$

Plugging the last expression into (15), we find that $R(n) = \frac{4}{\tau^2}(1 - \ln\frac{4}{\tau^2}) + o(1)$, and the result follows from the uniqueness of $s(n,\tau)$.

Proof of Proposition 1: Fix $\tau > 0$. If $\lceil s(n,\tau)\rceil + r > n$ the bound (1) holds trivially; in the case of equality, it follows from a standard Gaussian tail bound when n is sufficiently large. Fix $n \geq 1$ for the moment and suppose that $l = \lceil s(n,\tau) \rceil + r \leq n-1$. By Markov's inequality and the definition of $\phi_{n,\tau}(\cdot)$,

$$\begin{aligned} P(M_\tau(W_n) \geq s(n,\tau)+r) &= P(M_\tau(W_n) \geq l) \\ &= P(U_l(n,\tau) \geq 1) \\ &\leq EU_l(n,\tau) \\ &\leq 2\phi_{n,\tau}^2(l) \;\leq\; 2\phi_{n,\tau}^2(s(n,\tau)+r). \end{aligned} \tag{16}$$

Let $\gamma = e^{-\tau^2/4}$ and, to reduce notation, denote $s(n,\tau)$ by s_n. Under the constraint on r, a straightforward calculation shows that one can decompose the final term above as follows:

$$2\phi_{n,\tau}^2(s_n+r) \;=\; 2\,\phi_{n,\tau}^2(s_n)\,\gamma^{2rs_n}\,[\,A_n(r)\,B_n(r)\,C_n(r)\,D_n(r)\,]^2 \tag{17}$$

where

$$A_n(r) \;=\; \left(\frac{n-r-s_n}{n-s_n}\right)^{-n+r+s_n-\frac{1}{2}} \qquad B_n(r) \;=\; \left(\frac{r+s_n}{s_n}\right)^{-s_n-\frac{1}{2}}$$

$$C_n(r) \;=\; \left(\frac{n-s_n}{r+s_n}\,\gamma^{s_n}\right)^r \qquad D_n(r) \;=\; \gamma^{r^2}$$

It is enough to bound the right hand side of (17) as n increases and $r = r(n)$ is such that $\lceil s(n,\tau) \rceil + r \leq n-1$. By definition, $\phi_{n,\tau}(s_n) = 1$, and for each fixed $\epsilon > 0$,

$$\max_{r\geq 1} \frac{2\gamma^{2rs_n}}{n^{-2r}\left(\frac{2\ln n}{\tau^2}\right)^{2r+\epsilon}} \to 0 \;\;\text{as}\;\; n \to \infty.$$

Thus it suffices to show that the product $A_n(r)\,B_n(r)\,C_n(r)\,D_n(r)$ is uniformly bounded in r. To begin, note that for any fixed $0 < \delta < 4$,

$$C_n(r)^{\frac{1}{r}} \;=\; \frac{n-s_n}{r+s_n}\,\gamma^{s_n} \;\leq\; \frac{n}{s_n}\,\gamma^{s_n} \;\leq\; \frac{4}{4-\delta}\,e^{-1}\cdot o(1).$$

The last term will be less than one when δ is sufficiently small. The term $B_n(r) \leq 1$ for each $r \geq 1$, so it only remains to show that $\max_{r\geq 1} A_n(r)\cdot D_n(r)$ is bounded as a function of n. A straightforward calculation shows that $\ln A_n(r) \leq r$, and consequently, $\ln A_n(r)\cdot D_n(r) \leq r - \frac{\tau^2 r^2}{4}$, a quadratic function of r that is bounded from above.

7 Proof of Proposition 2

For any $k \times k$ submatrix U of the Gaussian random matrix W_n, it follows from standard arguments that $(k-1)^2 G(U)$ has a χ^2 distribution with $(k-1)^2$ degrees of freedom. In order to bound the quantity $P(G(U) \leq \tau)$, which arises in the analysis of $L_\tau(W_n)$, we require an initial result relating the right and left tails of the χ^2 distribution.

Lemma 2. *Suppose that $X \sim \chi^2_\ell$ for some $\ell \geq 3$. Then for $0 < t < \ell - 2$ we have*

$$P(X \leq t) \;\leq\; P(X \geq 2\ell - 4 - t).$$

Proof of Lemma 2: Let f denote the density function of X and let $0 < t < \ell - 2$. Since

$$P(X \leq t) \;=\; \int_0^t f(s)\, ds \quad \text{and} \quad P(X \geq 2\ell - 4 - t) \;\geq\; \int_{2\ell-4-t}^{2\ell-4} f(s)\, ds,$$

it suffices to show that

$$\frac{f(s)}{f(2\ell - 4 - s)} \;\leq\; 1 \quad \text{for all } 0 < s < \ell - 2. \tag{18}$$

To this end, note that the ratio in (18) can be rewritten as follows:

$$\begin{aligned}
\frac{f(s)}{f(2\ell - 4 - s)} \quad &= \quad \frac{s^{(\ell-2)/2}\, e^{-s/2}}{(2\ell - 4 - s)^{(\ell-2)/2}\, e^{-(2\ell-4-s)/2}} \\
&= \quad \left[\left(1 - \frac{2\ell - 4 - 2s}{2\ell - 4 - s}\right) e^{2(\ell-2-s)/(\ell-2)} \right]^{(\ell-2)/2}. \\
&= \quad \left[\left(1 - \frac{1}{u}\right) e^{\frac{2}{2u-1}} \right]^{(\ell-2)/2} \quad \text{with} \;\; u = \frac{2\ell - 4 - s}{2\ell - 4 - 2s}.
\end{aligned} \tag{19}$$

As s tends to $\ell - 2$, u tends to infinity, and therefore

$$\lim_{s \to (\ell-2)} \frac{f(s)}{f(2\ell - 4 - s)} \;=\; \lim_{u \to \infty} \left(1 - \frac{1}{u}\right) e^{\frac{2}{2u-1}} \;=\; 1.$$

Thus, it suffices to show that for $u \in (1, \infty)$, the final term in (19) is an increasing function of u. Differentiating with respect to u we find that

$$\frac{d}{du} \left(1 - \frac{1}{u}\right) e^{\frac{2}{2u-1}} \;=\; \frac{(2u-1)^2 - 4(u-1)u}{u^2(2u-1)^2}\, e^{\frac{2}{2u-1}} \;>\; 0$$

where the inequality follows from the fact that $u > 1$. Inequality (18) follows immediately.

Proof of Proposition 2: To begin, note that if X has a χ^2 distribution with ℓ degrees of freedom, then by a standard Chernoff bound,

$$P(X \geq r) \;\leq\; \min_{0<s<\frac{1}{2}} (1 - 2s)^{-\frac{\ell}{2}}\, e^{-sr} \;=\; \left[\left(\frac{\ell}{r}\right) e^{\left(\frac{r}{\ell} - 1\right)} \right]^{-\ell/2} \tag{20}$$

Let $\tau > 0$ be fixed. Fix $n \geq 1$ for the moment and let $r \geq 1$ be such that $k = \lceil t(n, \tau) \rceil + r \leq n$, where $t(n, \tau)$ is defined as in the statement of Proposition 2. Let U be any $k \times k$ submatrix of W_n, and let $\ell = (k-1)^2$. As noted above, the random variable

$\ell\, G(U)$ has a χ^2 distribution with ℓ degrees of freedom, so by Lemma 2 and inequality (20),

$$\begin{aligned} P(G(U) \le \tau) &= P(\ell\, G(U) \le \ell\,\tau) \le P\left(\ell\, G(U) \ge (2-\tau)\ell - 4\right) \\ &\le \exp\left\{ -\frac{\ell}{2}\left[\frac{(2-\tau)\ell-4}{\ell} - 1 + \ln\frac{\ell}{(2-\tau)\ell-4}\right]\right\} \\ &= \exp\left\{-\frac{\ell}{2}\left[(1-\tau)-\ln(2-\tau)\right]\right\} \exp\left\{\left[2+\frac{\ell}{2}\ln\left(1-\frac{4}{\ell(2-\tau)}\right)\right]\right\}. \end{aligned}$$

One may readily show that the second term above is $O(1)$. It then follows from a first moment argument that

$$P(L_\tau(W_n)\ge k) \le \binom{n}{k}^2 P(G(U)\le\tau) \le C\binom{n}{k}^2 q^{(k-1)^2} \le C\binom{n}{k-1}^2 q^{(k-1)^2}\cdot n^2 \quad (21)$$

where C is a finite constant and

$$q = \exp\left\{\frac{1}{2}[-(1-\tau)+\ln(2-\tau)]\right\}.$$

Fix $\epsilon > 0$. By following the proofs of Lemma 1 and Proposition 1, replacing τ^2 with $h(\tau) = 1-\tau-\ln(2-\tau)$, one can show that for every $r \ge 1$ such that

$$k = \left\lceil \frac{4}{h(\tau)}\ln n - \frac{4}{h(\tau)}\ln\left(\frac{4}{h(\tau)}\ln n\right) + \frac{4}{h(\tau)}\right\rceil + 2 + r$$

is at most n, we have

$$\binom{n}{k-1}^2 q^{(k-1)^2} \le \frac{4}{h(\tau)}\left(\frac{\ln n}{h(\tau)}\right)^{2r+2+\epsilon} n^{-2r-2},$$

and the result then follows from (21).

8 Proof of Theorem 1

In what follows we make use of standard bounds on the tails of the Gaussian distribution, namely that $(3s)^{-1}e^{-s^2/2} \le 1-\Phi(s) \le s^{-1}e^{-s^2/2}$ for $s \ge 3$. The proof of Theorem 1 is based on several preliminary results. The first result bounds the ratio of the variance of $\Gamma_k(\tau, n)$ and the square of its expected value, a quantity that later arises from an application of Chebyshev's inequality.

Lemma 3. *Fix $\tau > 0$. There exist integers $n_0, k_0 \ge 1$ and a positive constant C depending on τ but independent of k and n, such that for any $n \ge n_0$ and any $k \ge k_0$,*

$$\frac{\mathrm{Var}\ \Gamma_k(\tau,n)}{(E\,\Gamma_k(\tau,n))^2} \le C\,k^4 \sum_{l=1}^{k}\sum_{r=1}^{k} \frac{\binom{k}{l}\binom{n-k}{k-l}}{\binom{n}{k}} \frac{\binom{k}{r}\binom{n-k}{k-r}}{\binom{n}{k}} \exp\left\{\frac{rl\tau^2}{2}\left(1+\frac{k^2-rl}{k^2+rl}\right)\right\}. \quad (22)$$

Proof: Let $\mathcal{S}_k$ denote the collection of all $k \times k$ submatrices of W_n. It is clear that

$$E\,\Gamma_k(n,\tau) = \sum_{U \in \mathcal{S}_k} P(F(U) > \tau) = \binom{n}{k}^2 (1 - \Phi(k\tau))\,. \tag{23}$$

In a similar fashion, we have

$$E\,\Gamma_k^2(n,\tau) \;=\; \sum_{U_i, U_j \in \mathcal{S}_k} P(F(U_i) > \tau \text{ and } F(U_j) > \tau)$$

Note that the joint probability in the last display depends only on the overlap between the submatrices U_i and U_j. For $1 \le r, l \le k$ define

$$G(r,l) \;=\; P(F(U) > \tau \text{ and } F(V) > \tau)$$

where U and V are two fixed $k \times k$ submatrices of W having r rows and l columns in common. Then $E\,\Gamma_k(n,\tau) = \binom{n}{k}^2 G(0,0)^{1/2}$, and a straightforward counting argument shows that

$$E\,\Gamma_k^2(n,\tau) \;=\; \sum_{r=0}^{k}\sum_{l=0}^{k} \binom{n}{k}^2 \binom{k}{r}\binom{n-k}{k-r}\binom{k}{l}\binom{n-k}{k-l}\, G(r,l).$$

In particular,

$$\begin{aligned}
\frac{\operatorname{Var}\Gamma_k(n,\tau)}{(E\,\Gamma_k(n,\tau))^2} \;&=\; \sum_{r=0}^{k}\sum_{l=0}^{k} \frac{\binom{k}{l}\binom{n-k}{k-l}}{\binom{n}{k}}\,\frac{\binom{k}{r}\binom{n-k}{k-r}}{\binom{n}{k}} \left(\frac{G(r,l)}{G(0,0)}\right) - 1. \\
&=\; \sum_{r=1}^{k}\sum_{l=1}^{k} \frac{\binom{k}{l}\binom{n-k}{k-l}}{\binom{n}{k}}\,\frac{\binom{k}{r}\binom{n-k}{k-r}}{\binom{n}{k}} \left(\frac{G(r,l)}{G(0,0)} - 1\right).
\end{aligned}$$

where we have used the fact that $\binom{k}{l}\binom{n-k}{k-l}/\binom{n}{k}$ is a probability mass function, and that $G(0,l) = G(r,0) = G(0,0)$. When $k\tau \ge 3$ we have $G(0,0) = (1-\phi(k\tau))^2 \ge (3k\tau)^{-2} e^{-k^2\tau^2}$, and it therefore suffices to show that for $1 \le r, l \le k$,

$$G(r,l) \;\le\; C\,k^2 \exp\left\{-k^2\tau^2 + \frac{rl\tau^2}{2}\left(1 + \frac{k^2 - rl}{k^2 + rl}\right)\right\} \tag{24}$$

where $C > 0$ depends on τ but is independent of k and n. Inequality (24) is readily established when $r = l = k$, so we turn our attention to bounding $G(r,l)$ when $1 \le rl < k^2$. In this case

$$G(r,l) \;=\; \frac{\sqrt{rl}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{rlt^2}{2}}\, P\left(F(U \cap V^c) \ge \frac{k^2\tau - rlt}{\sqrt{k^2 - rl}}\right)^2 dt$$

where U, V are submatrices of W_n having r rows and l columns in common. Let $\overline{\Phi}(x) = 1 - \Phi(x)$. Note that $G(r,l) = D_0 + D_1$ where

$$D_0 \;=\; \frac{\sqrt{rl}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{rlt^2}{2}}\, \overline{\Phi}^2\left(\frac{k^2\tau - rlt}{\sqrt{k^2 - rl}}\right) I\{k^2\tau - rlt < 1\}\, dt \tag{25}$$

and

$$D_1 \;=\; \frac{\sqrt{rl}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{rlt^2}{2}}\, \overline{\Phi}^2\left(\frac{k^2\tau - rlt}{\sqrt{k^2 - rl}}\right) I\{k^2\tau - rlt \geq 1\}\, dt. \tag{26}$$

Consider first the term D_1 defined in (26). As $rl \neq k^2$ and $k^2\tau - rlt \geq 1$, the normal tail bound yields

$$\begin{aligned}
\overline{\Phi}\left(\frac{k^2\tau - rlt}{\sqrt{k^2 - rl}}\right) \;&\leq\; \frac{\sqrt{k^2 - rl}}{\sqrt{2\pi}(k^2\tau - rlt)}\; \exp\left\{-\frac{(k^2\tau - rlt)^2}{2(k^2 - rl)}\right\} \\
&=\; O(\sqrt{k^2 - rl})\; \exp\left\{-\frac{(k^2\tau - rlt)^2}{2(k^2 - rl)}\right\}.
\end{aligned}$$

Plugging the last expression into (26), the exponential part of the resulting integrand is

$$-\frac{(k^2\tau - rlt)^2}{(k^2 - rl)} - \frac{rlt^2}{2},$$

which (after lengthy but straightforward algebra) can be expressed as

$$-k^2\tau + \frac{rl\tau^2}{2}\left(1 + \frac{k^2 - rl}{k^2 + rl}\right) - \frac{rl(k^2 + rl)}{2(k^2 - rl)}\left((\tau - t) + \tau\left(\frac{k^2 - rl}{k^2 + rl}\right)\right)^2.$$

It then follows that

$$\begin{aligned}
D_1 \;&\leq\; O(k^2 - rl)\; \exp\left\{-k^2\tau^2 + \frac{rl\tau^2}{2}\left(1 + \frac{k^2 - rl}{k^2 + rl}\right)\right\} \\
&\times\sqrt{\frac{k^2 - rl}{k^2 + rl}} \times \int_{\infty}^{\infty} \sqrt{\frac{rl(k^2 + rl)}{k^2 - rl}}\, \exp\left\{-\frac{rl(k^2 + rl)}{2(k^2 - rl)}\left(\tau - t + \frac{\tau(k^2 - rl)}{k^2 + rl}\right)^2\right\} dt
\end{aligned}$$

The term preceding the integral is less than one, and the integral is equal to one. Thus D_1 is less than the right side of (24).

We next consider the term D_0 defined in (25). Note that $k^2\tau - rlt < 1$ is equivalent to $t > (k^2\tau - 1)/rl$, and therefore

$$D_0 \;\leq\; \int_{(k^2\tau - 1)/rl}^{\infty} \frac{\sqrt{rl}}{\sqrt{2\pi}}\, e^{-\frac{rlt^2}{2}}\, dt \;=\; \overline{\Phi}\left(\frac{k^2\tau - 1}{\sqrt{rl}}\right) \;\leq\; \frac{k\sqrt{rl}}{\sqrt{2\pi}(k^2\tau - 1)} e^{-\frac{(k^2\tau - 1)^2}{2rl} - \ln k}.$$

Comparing the last term above with (24), it suffices to show that when k is sufficiently large,

$$\frac{(k^2\tau - 1)^2}{2rl} + \ln k \;\geq\; \left(k^2 - \frac{rl}{2}\right)\tau^2$$

or equivalently

$$(k^2 - rl)^2\,\tau^2 \;-\; 2k^2\tau \;+\; 1 \;+\; 2rl\ln k \;\geq\; 0. \tag{27}$$

Suppose first that $rl \geq k^2 - k/\sqrt{\ln k}$. In this case, the left side of the expression above is at least

$$-2k^2\tau \;+\; 1 \;+\; 2rl\ln k \;\geq\; -2k^2\tau \;+\; 1 \;+\; 2(k^2 - k/\sqrt{\ln k})\,\ln k \;>\; 0$$

when k is sufficiently large. Suppose now that $k^2 - rl > k/\sqrt{\ln k}$. As a quadratic function of τ, the left side of (27) takes its minimum at $\tau = k^2/(k^2 - rl)^2$, and the corresponding value is $rl\,[-2k^2 + rl + 2(k^2 - rl)^2 \ln k]/(k^2 - rl)^2$. In this case, the assumption $k^2 - rl > k/\sqrt{\ln k}$ implies

$$-2k^2 \;+\; rl \;+\; 2(k^2 - rl)^2 \,\ln k \;>\; rl \;>\; 0.$$

This establishes (27) and complete the proof.

Lemma 4. *Let $\tau > 0$ be fixed. When k is sufficiently large, for every integer n satisfying the condition*

$$k \;\le\; \frac{4}{\tau^2}\,\ln n \;-\; \frac{4}{\tau^2}\ln\left(\frac{4}{\tau^2}\ln n\right) \;-\; \frac{12\ln 2}{\tau^2} \tag{28}$$

we have the bound

$$\frac{\mathrm{Var}\;\Gamma_k(\tau, n)}{(E\,\Gamma_k(\tau, n))^2} \;\le\; k^{-2}.$$

Remark: For the proof of Theorem 1, it is enough to show that the sum over k of the ratio above is finite, and for this purpose the upper bound k^{-2} is sufficient.

Proof: Let n satisfy the condition (28). By Lemma 3, it suffices to show that

$$k^4 \sum_{l=1}^{k}\sum_{r=1}^{k} \frac{\binom{k}{l}\binom{n-k}{k-l}}{\binom{n}{k}}\,\frac{\binom{k}{r}\binom{n-k}{k-r}}{\binom{n}{k}}\;\exp\left\{\frac{rl\tau^2}{2}\left(1 + \frac{k^2 - rl}{k^2 + rl}\right)\right\} \;\le\; k^{-2}. \tag{29}$$

In order to establish (29), we will show that each term in the sum is less than k^{-8}. To begin, note that

$$\frac{\binom{k}{l}\binom{n-k}{k-l}}{\binom{n}{k}} \;\le\; \frac{\binom{k}{l}\,k^l\,(n-k)^{k-l}}{(n-k)^k} \;=\; \binom{k}{l}\,k^l(n-k)^{-l},$$

and that $(n-k)^{-l} = O(n^{-l})$ when $l \le k = O(n^{1/2})$. Thus for some constant $C > 0$,

$$\frac{\binom{k}{l}\binom{n-k}{k-l}}{\binom{n}{k}}\,\frac{\binom{k}{r}\binom{n-k}{k-r}}{\binom{n}{k}} \;\le\; C\binom{k}{r}\binom{k}{l}\,k^{r+l}\,n^{-(r+l)}.$$

Rewriting (28) as $\ln n \ge \frac{\tau^2 k}{4} + \ln(\frac{4}{\tau^2}\ln n) + 3\ln 2$ yields the bound

$$\begin{aligned} &n^{-(r+l)}\,\exp\left\{\frac{rl\tau^2}{2}\left(1 + \frac{k^2 - rl}{k^2 + rl}\right)\right\} \\ &\quad\le\; e^{-3\,(r+l)\,\ln 2}\left(\frac{4}{\tau^2}\ln n\right)^{-(r+l)}\;\exp\left\{\frac{\tau^2}{2}\left(rl\frac{2k^2}{k^2 + rl} \;-\; \frac{k}{2}(r+l)\right)\right\}. \end{aligned}$$

Combining the last three displays, and using the fact that $k \le \frac{4}{\tau^2}\ln n$ by assumption, it suffices to show that

$$\binom{k}{r}\binom{k}{l}\,e^{-3(r+l)\ln 2}\,\exp\left\{\frac{\tau^2}{2}\left(rl\frac{2k^2}{k^2 + rl} - \frac{k}{2}(r+l)\right)\right\} \;\le\; k^{-8}. \tag{30}$$

In order to establish (30), we consider two cases for $r+l$. Suppose first that $r+l \leq \frac{3k}{4}$. By elementary arguments

$$\binom{k}{r}\binom{k}{l} \leq \binom{2k}{r+l} \leq (2k)^{r+l} \quad \text{and} \quad rl\,\frac{2k^2}{k^2+rl} \;\leq\; \frac{(r+l)^2}{4}\,\frac{2k^2}{k^2+rl} \;\leq\; \frac{(r+l)^2}{2}.$$

It follows from these inequalities that

$$\begin{aligned}
&\binom{k}{r}\binom{k}{l}\,\exp\left\{\frac{\tau^2}{2}\left[rl\frac{2k^2}{k^2+rl} \;-\; \frac{k}{2}(r+l)\right]\right\} \\
&\leq\;\; \exp\left\{\frac{\tau^2}{2}\left[\frac{(r+l)^2}{2} \;-\; \frac{k}{2}(r+l)\right] \;+\; (r+l)\,\ln 2k\right\} \\
&=\;\; \exp\left\{\frac{\tau^2(r+l)}{2}\left[\frac{(r+l)}{2} \;-\; \frac{k}{2} \;+\; \frac{2\ln 2k}{\tau^2}\right]\right\} \\
&\leq\;\; \exp\left\{\frac{\tau^2(r+l)}{2}\left[\frac{3k}{8} \;-\; \frac{k}{2} \;+\; \frac{2\ln 2k}{\tau^2}\right]\right\}.
\end{aligned}$$

As the exponent above is negative when k is sufficiently large, (30) follows. Suppose now that $r+l \geq \frac{3k}{4}$. From the simple bounds $r+l \geq 2\sqrt{rl}$ and $k^2+rl \geq 2\sqrt{k^2rl}$ we find that

$$rl\,\frac{2k^2}{k^2+rl} \;-\; \frac{k}{2}(r+l) \;\leq\; \frac{2rlk^2}{2\sqrt{k^2rl}} \;-\; k\sqrt{rl} \;=\; 0,$$

and it suffices to bound the initial terms in (30). But clearly,

$$\binom{k}{r}\binom{k}{l}e^{-3(r+l)\ln 2} \;\leq\; 2^{2k}\cdot 2^{-\frac{9k}{4}},$$

which is less than k^{-8} when k is sufficiently large.

Proof of Theorem 1: Proposition 1 and the Borel-Cantelli lemma imply that eventually almost surely $K_\tau(W_n) \leq \lceil s(n,\tau)\rceil + 1$. Thus, we only need to establish an almost sure lower bound on $K_\tau(W_n)$. To this end, define functions

$$f(n) \;=\; \frac{4}{\tau^2}\ln n - \frac{4}{\tau^2}\ln\left(\frac{4}{\tau^2}\ln n\right) - \frac{12\ln 2}{\tau^2} \quad \text{and} \quad g(k) \;=\; \min\{n \geq 1, \lfloor f(n)\rfloor = k\}$$

for integers $n \geq 1$ and $k \geq 1$, respectively. It is easy to see that $f(n)$ is strictly increasing for large values of n, and clearly $f(n)$ tends to infinity as n tends to infinity. A straightforward argument shows that $g(k)$ has the same properties Thus for every sufficiently large integer n, there exists a unique integer $k = k(n)$ such that $g(k) \leq n < g(k+1)$.

Fix $m \geq 1$ and consider the event A_m that for some $n \geq m$ the random variable $K_\tau(W_n)$ is less than the lower bound specified in the statement of the theorem. More precisely, define

$$A_m \;=\; \bigcup_{n\geq m}\left\{K_\tau(W_n) \;\leq\; s(n,\tau) - \frac{12\ln 2}{\tau^2} - \frac{4}{\tau^2} - 3\right\}.$$

To establish the lower bound, it suffices to show that $P(A_m) \to 0$ as $m \to \infty$. To begin, note that when m is large

$$A_m \subseteq \bigcup_{k \geq \lfloor f(m) \rfloor} \bigcup_{g(k) \leq n < g(k+1)} \left\{ K_\tau(W_n) \leq s(n,\tau) - \frac{12 \ln 2}{\tau^2} - \frac{4}{\tau^2} - 4 \right\}.$$

Fix $n \geq m$ sufficiently large, and let $k = k(n)$ be the unique integer such that $g(k) \leq n < g(k+1)$. The definition of $g(k)$ and the monotonicity of $f(\cdot)$ ensures that $k = \lfloor f(g(k)) \rfloor \leq f(n) < k+1$. In conjunction with the definition of $f(n)$ and Lemma 1, this inequality implies that

$$\begin{aligned} 1 &= k+1-k > f(n) - \lfloor f(g(k)) \rfloor \geq f(n) - f(g(k)) \\ &= s(n,\tau) - s(g(k),\tau) + o(1), \end{aligned}$$

and therefore $s(n,\tau) < s(g(k),\tau) + 1 + o(1)$. Define

$$r(k) = \left\lfloor s(g(k),\tau) - \frac{12 \ln 2}{\tau^2} - \frac{4}{\tau^2} \right\rfloor.$$

From the bound on $s(n,\tau)$ above and the fact that $K_\tau(W_{g(k)}) \leq K_\tau(W_n)$, we have

$$\begin{aligned} \left\{ K_\tau(W_n) \leq s(n,\tau) - \frac{12 \ln 2}{\tau^2} - \frac{4}{\tau^2} - 3 \right\} &\subseteq \left\{ K_\tau(W_{g(k)}) \leq r(k) - 1 + o(1) \right\} \\ &\subseteq \left\{ K_\tau(W_{g(k)}) \leq r(k) - 1 \right\}, \end{aligned}$$

where the last relation makes use of the fact that K_τ and $r(k)$ are integers. Thus we find that

$$A_m \subseteq \bigcup_{k \geq \lfloor f(m) \rfloor} \left\{ K_\tau(W_{g(k)}) \leq r(k) - 1 \right\}.$$

Consider the events above. For fixed k,

$$P(K_\tau(W_{g(k)}) \leq r(k) - 1) = P(\Gamma_{r(k)}(\tau, g(k)) = 0) \leq \frac{\operatorname{Var} \Gamma_{r(k)}(\tau, g(k))}{(E\, \Gamma_{r(k)}(\tau, g(k)))^2} \tag{31}$$

where we have used the fact that for a non-negative integer-valued random variable X

$$P(X = 0) \leq P(|X - EX| \geq EX) \leq \frac{\operatorname{Var} X}{(EX)^2}$$

by Chebyshev's inequality. As $r(k) \leq f(g(k))$, Lemma 4 ensures that the final term in (31) is less than k^{-2}, and the Borel-Cantelli lemma then implies that $P(A_m) \to 0$ as $m \to \infty$. This completes the proof of Theorem 1.

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