On the Limitation of Spectral Methods: From the Gaussian Hidden Clique Problem to Rank-One Perturbations of Gaussian Tensors

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Abstract

We consider the following detection problem: given a realization of asymmetric matrix \$X\$ of dimension \$n\$, distinguish between the hypothesisthat all upper triangular variables are i.i.d. Gaussians variables with mean 0 and variance \$1\$ and the hypothesis that there is aplanted principal submatrix \$B\$ of dimension \$L\$ for which all upper triangular variables are i.i.d. Gaussians with mean \$1\$ and variance \$1\$, whereasall other upper triangular elements of \$X\$ not in \$B\$ are i.i.d.Gaussians variables with mean 0 and variance \$1\$. We refer to this asthe 'Gaussian hidden clique problem'. When $L=(1+epsilon) \ sqrt\{n\}\$ (\$epsilon ; 0\$), it is possible to solve this detection problem with probability $1 - o_1(1)$ by computing the spectrum of \$X\$ and considering the largest eigenvalue of \$X\$. We prove that when \$L ; (1-epsilon) sqrt {n}\$ no algorithm that examines only theeigenvalues of \$X\$can detect the existence of a hiddenGaussian clique, with error probability vanishing as \$n to infty\$. The result above is an immediate consequence of a more general result on rankoneperturbations of \$k\$-dimensional Gaussian tensors. In this context we establish a lower bound on the critical signal-to-noise ratio below which a rank-one signal cannot be detected.

1 Paper Body

Consider the following detection problem. One is given a symmetric matrix X = X(n) of dimension n, such that the n2 + n entries (Xi,j) i?j are mutually independent random variables. Given (a realization of) X one would like to distinguish between the hypothesis that all random variables Xi,j have the same distribution F0 to the hypothesis where there is a set U? [n], with L := -U—, so that all random variables in the submatrix XU := (Xs,t:s,t?U) have a distribution F1 that is different from the distribution of all other elements in

X which are still distributed as F0 . We refer to XU as the hidden submatrix. 1

The same problem was recently studied in [1, 8] and, for the asymmetric case (where no symmetry assumption is imposed on the independent entries of X), in [6, 18, 20]. Detection problems with similar flavor (such as the hidden clique problem) have been studied over the years in several fields including computer science, physics and statistics. We refer to Section 5 for further discussion of the related literature. An intriguing outcome of these works is that, while the two hypothesis are statistically distinguishable as soon as L? C log n (for C a sufficiently large constant) [7], practical algorithms require significantly larger L. In this paper we study the class of spectral (or eigenvaluebased) tests detecting the hidden submatrix. Our proof technique naturally allow to consider two further generalizations of this problem that are of independent interests. We briefly summarize our results below. The Gaussian hidden clique problem. This is a special case of the above hypothesis testing setting, whereby F0 = N(0, 1)and F1 = N(1, 1) (entries on the diagonal are defined slightly differently in order to simplify calculations). Here and below N(m, ? 2) denote the Gaussian distribution of mean m and variance? 2. Equivalently, let Z be a random matrix from the Gaussian Orthogonal Ensemble (GOE) i.e. Zij? N(0, 1/n) independently for i ; j, and Zii? N(0, 2/n). Then, under hypothesis H1,L we have X = n?1/2 1U 1T U + Z (1U being the indicator vector of U), andunder hypothesis H0, X = Z (the factor n in the normalization is for technical convenience). The Gaussian hidden clique problem can be thought of as the following clustering problem: there are n elements and the entry (i, j) measures the similarity between elements i and j. The hidden submatrix corresponds to a cluster of similar elements, and our goal is to determine given the matrix whether there is a large cluster of similar elements or alternatively, whether all similarities are essentially random (Gaussian) noise. Our focus in this work is on the following restricted hypothesis testing question. Let ?1? ?2?????? ?n be the ordered eigenvalues of X. Is there a test that depends only on ?1, . . . , ?n and that distinguishes H0 from H1,L ?reliably,? i.e. with error probability converging to 0 as n? ?? Notice that the eigenvalues distribution does not depend on U as long as this is independent from the noise Z. We can therefore think of U as fixed for this? question. Historically, the first polynomial time algorithm for detecting a planted clique of size O(n) in a random graph [2] relied on spectral methods (see Section 5 for more details). This is one reason for our interest in spectral tests for the Gaussian hidden clique problem. ? If L ? (1 + ?) n then [11] implies that a simple test checking whether ?1 ? 2 + ? for some ? = ?(?); 0 is reliable for the Gaussian hidden clique problem. We prove that this result is tight,? in the sense that no spectral test is reliable for L? (1??) n. Rank-one matrices in Gaussian noise. Our proof technique builds on a simple observation. Since the noise Z is invariant under orthogonal transformations 1. the above question is equivalent to the following testing problem. For ? ? R?0. and v? Rn, kvk2 = 1 a uniformly random unit vector, test H0:?X = Z versus H1, X = ?vvT + Z. (The correspondence between the two problems yields? = L/ n.) Again, this problem (and a closely related asymmetric version [22])

has been studied in the literature, and it follows from [11] that a reliable test exists for ??1+?. We provide a simple proof (based on the second moment method) that no test is reliable for ? ; 1 ? ?. Rank-one tensors in Gaussian noise. It turns that the same proof applies to an even more general problem: detecting a rank-one signal in a noisy tensor. We carry out our analysis in this more general setting for two reasons. First, we think that this clarifies the what aspects of the model are important for our proof technique to apply. Second, the problem estimating tensors from noisy data has attracted significant interest recently within the machine learning community [15, 21]. Nk n More precisely, we consider a noisy tensor X? R, of the form X = ? v?k + Z, where Z is Gaussian noise, and v is a random unit vector. We consider the problem of testing this hypothesis against H0: X = Z. We establish a threshold ?k2nd such that no test can be reliable for ?; ?k2nd (in particular ?22nd = 1). Two differences are worth remarking for k? 3 with respect to the more familiar matrix case k = 2. First, we do not expect the second moment bound ?k2nd to be tight, i.e. a reliable test to exist for all? ; ?k2nd. On the other hand, we can show that it is tight up to 1

By this we mean that, for any orthogonal matrix R ? O(n), independent of Z, RZRT is distributed as Z.

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a universal (k and n independent) constant. Second, below ?k2nd the problem is more difficult than the matrix version below ?22nd = 1: not only no reliable test exists but, asymptotically, any test behaves asymptotically as random guessing. For more details on our results regarding noisy tensors, see Theorem 3.

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Main result for spectral detection

Let Z be a GOE matrix as defined in the previous section. Equivalently if G is an (asymmetric) matrix with i.i.d. entries Gi, j? N(0, 1),

1 Z= ? G + GT . (1) 2n For a deterministic sequence of vectors $v(n),\,kv(n)k2$ = 1, we consider the two hypotheses

 $\rm H0: X=Z, (2)~H1,?: X=?vvT+Z$.? A special? example is provided by the Gaussian hidden clique problem in which case ? = L/n and v = 1U / L for some set U ? [n], —U — = L, (H0: X = Z, (3) H1,L: X = ?1n 1U 1T U + Z. Observe that the distribution of eigenvalues of X, under either alternative, is invariant to the choice of the vector v (or subset U), as long as the norm of v is kept fixed. Therefore, any successful algorithm that examines only the eigenvalues, will distinguish between H0 and H1,? but not give any information on the vector v (or subset U , in the case of H1,L). We let Q0 = Q0 (n) (respectively, Q1 = Q1 (n)) denote the distribution of the eigenvalues of X under H0 (respectively H1 = H1,? or H1,L). A spectral statistical test for distinguishing between H0 and H1 (or simply a spectral test) is a measurable map Tn: (?1, . . . , ?n) 7? {0, 1}. To formulate precisely what we mean by the word distinguish, we introduce the following notion. Definition 1. For each n? N, let P0,n, P1,n be two probability measures on the same measure space (?n, Fn). We say that the sequence (P1,n) is contiguous with respect

to (P0,n) if, for any sequence of events An? Fn, $\lim P0,n$ (An) = 0? $\lim P0,n$ P1,n (An) = 0 . (4) n??n??

Note that contiguity is not in general a symmetric relation. In the context of the spectral statistical tests described above, the sequences An in Definition 1 (with Pn = Q0 (n) and Qn = Q1 (n)) can be put in correspondence with spectral statistical tests Tn by taking An = $\{(?1, \ldots, ?n) : Tn (?1, \ldots, ?n) : Tn (?1, \ldots, ?n) : Tn (?1, \ldots, ?n) \}$? ?n) = 0}. We will thus say that H1 is spectrally contiguous with respect to H0 if Qn is contiguous with respect to Pn. Our main result on the Gaussian hidden clique problem is the following. ? Theorem 1. For any sequence L = L(n) satisfying lim supn?? L(n)/ n; 1, the hypotheses H1,L are spectrally contiguous with respect to H0.

2.1

Contiguity and integrability

Contiguity is related to a notion of uniform absolute continuity of measures. Recall that a probability measure? on a measure space is absolutely continuous with respect to another probability measure? if for every measurable set A, ?(A) = 0 implies that ?(A) = 0, in which case there exists a ?-integrable, nonnegative function f? d? d? (the Radon-Nikodym derivative of? with respect to ?), R so that ?(A) = A f d? for every measurable set A. We then have the following known useful fact: 3

Lemma 2. Within the setting of Definition 1, assume that P1,n is absolutely continuous with respect dP1,n its Radon-Nikodym derivative. to P0,n, and denote by ?n? dP0,n (a) If \limsup ?? E0,n (?2n); ?, then (P1,n) is contiguous with respect to (P0,n). (b) If $\lim_{n \to \infty} P(2n) = 1$, then $\lim_{n \to \infty} P(2n) = 1$, then $\lim_{n \to \infty} P(2n) = 1$. kP0,n? P1,n kTV = 0, where k? kTV denotes the total variation distance, i.e. kP0,n ? P1,n kTV ? \sup —P0,n (A) ? P1,n (A)k. A 2.2

Method and structure of the paper

Consider problem (2). We use the fact that the law of the eigenvalues under both H0 and H1,? are invariant under conjugations by a orthogonal matrix. Once we conjugate matrices sampled under the hypothesis H1,? by an independent orthogonal matrix sampled according to the Haar distribution, we get a matrix distributed as X = ?vvT + Z, (5) where u is uniform on the n-dimensional sphere, and Z is a GOE matrix (with off-diagonal entries of variance 1/n). Letting P1,n denote the law of ?uuT + Z and P0,n denote the law of Z, we show that P1,n is contiguous with respect to P0,n, which implies that the law of eigenvalues Q1 (n) is contiguous with respect to Q0 (n). To show the contiguity, we consider a more general setup, of independent interest, of Gaussian dP1.n tensors of order k, and in that setup show that the Radon-Nikodym derivative?n,L = dP0,n is uniformly square integrable under P0,n; an application of Lemma 2 then quickly yields Theorem 1. The structure of the paper is as follows. In the next section, we define formally the detection problem for a symmetric tensor of order k? 2. We show the existence of a threshold under which detection is not possible (Theorem 3), and show how Theorem 1 follows from this. Section 4 is devoted to the proof of Theorem 3, and concludes with some additional remarks and consequences of Theorem 3. Finally, Section 5 is devoted to a description of the relation between the Gaussian hidden clique problem and hidden clique problem in computer science, and related literature.

3

A symmetric tensor model and a reduction

Exploiting rotational invariance, we will reduce the spectral detection problem to a detection problem involving a standard detection problem between random matrices. Since the latter generalizes to a tensor setup, we first introduce a general Gaussian hypothesis testing for k-tensors, which is of independent interest. We then explain how the spectral detection problem reduces to the special case of $\mathbf{k}=2$.

3.1

Preliminaries and notation

We use lower-case boldface for vectors (e.g. u, v) and upper-case boldface for matrices and tensors (e.g. Pn X, Z). The ordinary scalar product and 'p norm over vectors are denoted by hu, vi=i=1 ui vi, and kvkp. We write Sn?1 for the unit sphere in n dimensions

 $Sn?1\ ?\ x\ ?\ Rn: kxk2=1$. (6) Nk n Given X ? R a real k-th order tensor, we let {Xi1 ,...,ik }i1 ,...,ik denote its coordinates. The Nk n outer product of two tensors is X ? Y, and, for v ? Rn , we define v?k = v ? ? ? ? ? v ? R Nk n R as as the k-th outer power of v. We define the inner product of two tensors X, Y ? X hX, Yi = Xi1 ,??? ,ik Yi1 ,??? ,ik . (7) i1 ,??? ,ik ?[n]

4

We define the Frobenius (Euclidean) norm of a tensor X by kXkF = norm by

p hX, Xi, and its operator kXkop? max{hX, u1????? uk i:?i? [k], kui k2? 1}. (8)

It is easy to check that this is indeed a norm. For the special case k=2, it reduces to the ordinary '2 matrix operator norm (equivalently, to the largest singular value of X). For a permutation ? ? Sk , we will denote by X? the tensor with permuted indices X?i1 ,??? ,ik = X?(i1),??? ,?(ik) . We call the tensor X symmetric if, for any permutation ? ? Sk , X? = X. It is proved [23] that, for symmetric tensors, we have the equivalent representation kXkop ? $\max\{-hX, u?k i - : max\}$

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kuk2 ? 1}. (9)
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We define R? R?? with the usual conventions of arithmetic operations.

The symmetric tensor model and main result

Nk n We denote by G? R a tensor with independent and identically distributed entries Gi1,???, ik? N(0, 1) (note that this tensor is not symmetric). Nk n We define the symmetric standard normal noise tensor Z? R by 1 Z= k!

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r
2 X ? G . n
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(10) ??Sk

Note that the subset of entries with unequal indices form an i.i.d. collection $\{Zi1\ ,i2\ ,...,ik\ \}i1\ j????jik\ ?\ N(0,\ 2/(n(k!)))$. Nk n With this normalization, we have, for any symmetric tensor A? R o n

1~kAk2F . (11) E ehA,Zi = exp n We will also use the fact that Z is invariant in distribution under conjugation by orthogonal transformations, that is, that for any orthogonal matrix U ? O(n), {Zi1 ,...,ik } has the same distribution as Q P k { j1 ,...,jk U '=1 i' ,j' ? Zj1 ,...,jk }. Given a parameter ? ? R?0 , we consider the following model for a random symmetric tensor X: X ? ? v?k + Z , (12)

with Z a standard normal tensor, and v uniformly distributed over the unit sphere Sn?1. In the case k=2 this is the standard rank-one deformation of a GOE matrix. (k)

We let P? = P? denote the law of X under model (12). Theorem 3. For k? 2, let ?k2nd

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r 1 ? k log(1 ? q 2 ) . ? inf q q?(0,1) Assume ? ; ?k2nd . Then, for any k ? 3, we have lim P? ? P0 TV = 0 . n??
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Further, for k=2 and ? ; ?k2nd=1, P? is contiguous with respect to P0 . A few remarks are in order, following Theorem 3. First, it is not difficult to derive the asymptotic ?k2nd=5

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\begin{array}{l}
p \\
\log(k/2) + ok (1) \text{ for large } k. \\
(13) \\
(14)
\end{array}
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Second, for k=2 we get using $\log(1\ ?\ q\ 2)$? ?q 2 , that ?k2nd = 1. Recall that for k=2 and ? ¿ 1, it is known that the largest eigenvalue of X, ?1 (X) converges almost surely to (? + 1/?) [11]. As a consequence kP0 ? P? kTV ? 1 for all ? ¿ 1: the second moment bound is tight. For k ? 3, it follows by the triangle inequality that kXkop ? ? kZkop , and further lim supn?? kZkop ? ?k almost surely as n ? ? [19, 5] for some bounded ?k . It follows that kP0 ? P? kTV ? 1 for all ? ? ¿ 2?k [21]. Hence, the second moment bound is off by a k-dependent factor. For large k, 2?k = 2 log k + Ok (1) and hence the factor is indeed bounded in k. Behavior below the threshold. Let us stress an important qualitative difference between k = 2 and k ? 3, for ? ¡ ?k2nd . For k ? 3, the two models are indistinguishable and any test is essentially as good as random guessing. Formally, for any measurable function T : ?k Rn ? {0, 1}, we have

 $\lim P0 (T(X) = 1) + P? (T(X) = 0) = 1 . (15) n??$

For k = 2, our result implies that, for ? ; 1, kP0 ? P? kTV is bounded away from 1. On the other hand, it is easy to see that it is bounded away from 0 as well, i.e. 0 ; lim inf kP0 ? P? kTV ? lim sup kP0 ? P? kTV ; 1 . n??

(16) n??

Indeed, consider for instance the statistics $S={\rm Tr}(X).$ Under P0 , S ? N(0, 2), while under P? , S ? N(?, 2). Hence

? ? lim inf kP0 ? P? kTV ? kN(0, 1) ? N(?/ 2, 1)kTV = 1 ? 2? ? ? ; 0 (17) n?? 2 2 ? Rx 2 (Here ?(x) = ?? e?z /2 dz/ 2? is the Gaussian distribution function.) The same phenomenon for rectangular matrices (k = 2) is discussed in detail in [22].

3.3

Reduction of spectral detection to the symmetric tensor model, k = 2

Recall that in the setup of Theorem 1, Q0,n is the law of the eigenvalues of X under H0 and Q1,n is the law of the eigenvalues of X under H1,L . Then Q1,n is invariant by conjugation of orthogonal matrices. Therefore, the detection problem is not changed if we replace $X=n?1/2\ 1U\ 1T\ U+Z$ by b? RXRT = ?1 R1U (R1U)T+RZRT, X n

(18)

where R ? O(n) is an orthogonal matrix sampled according to the Haar measure. A direct calculation yields $b=?vvT+Z,\,e~X$

(19)?

e is a GOE matrix (with offwhere v is uniform on the n dimensional sphere, ?=L/n, and Z e are independent of one another. diagonal entries of variance 1/n). Furthermore, v and Z b Note that P1,n=P(k=2) with ?=L/?n. We can relate the detection Let P1,n be the law of X. ? problem of H0 vs. H1,L to the detection problem of P0,n vs. P1,n as follows. Lemma 4. (a) If P1,n is contiguous with respect to P0,n then P1,L is spectrally contiguous with respect to P1,n kTV? kP0,n? P1,n kTV. In view of Lemma 4, Theorem 1 is an immediate consequence of Theorem 3.

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Proof of Theorem 3

The proof uses the following large deviations lemma, which follows, for instance, from [9, Proposition 2.3]. 6

Lemma 5. Let v a uniformly random vector on the unit sphere Sn?1 and let hv, e1 i be its first coordinate. Then, for any interval [a, b] with ?1 ? a ; b ? 1 n1 o 1 lim log P(hv, e1 i ? [a, b]) = max log(1 ? q 2) : q ? [a, b] . (20) n?? n 2 Proof of Theorem 3. We denote by ? the Radon-Nikodym derivative of P? with respect to P0 . By definition E0 ? = 1. It is easy to derive the following formula Z n n? 2 o n? ? = exp ? + hX, v?k i ?n (dv) . (21) 4 2 where ?n is the uniform measure on Sn?1 . Squaring and using (11), we get Z n n? o 2 E0 ?2 = e?n? /2 E0 exp hX, v1 ?k + v2 ?k i ?n (dv1)?n (dv2) 2 Z n n? 2

o 2

v1 ?k + v2 ?k 2 ?n (dv1)?n (dv2) = e?n? /2 exp F 4 Z o n n? 2 hv1 , v2 ik ?n (dv1)?n (dv2) = exp 2 Z n n? 2 o hv, e1 ik ?n (dv) , = exp 2 (22)

where in the first step we used (11) and in the last step, we used rotational invariance. Let F?: [?1, 1]? R be defined by F? (q)?

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1 ? 2 qk + log(1 ? q 2) . 2 2
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(23)

Using Lemma 5 and Varadhan?s lemma, for any ?1 ? a ; b ? 1, Z n n? 2 o n o hv, e1 ik I(hv, e1 i ? [a, b]) ?n (dv) = exp n max F? (q) + o(n) . exp 2 q?[a,b] It follows from the definition of ?k2nd that max—q—?? F? (q) ; 0 for

for some c(?) \not 0 and all n large enough. Next notice that, under ?n , hv, e1 i = G/(G2 + Zn?1)1/2 where G ? N(0, 1) and Zn?1 is a ?2 with n ? 1 degrees of freedom independent of G. Then, letting Zn ? G2 + Zn?1 (a ?2 with n degrees of freedom) o n n? 2 —G—k I(—G/Zn1/2 — ? ?) + e?c(?)n E0 ?2 ? E exp k/2 2 Zn n n? 2 —G—k o 1/2 ? E exp I(—G/Z — ? ?) I(Z ? n(1 ? ?)) n?1 n 2 Znk/2

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2 k + en? ? /2 P Zn?1 ? n(1 ? ?) + e?c(?)n n n1?(k/2) ? 2
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2 k k 2 ? E exp —G— I(—G— ? 2?n) + en? ? /2 P Zn?1 ? n(1 ? ?) + e?c(?)n k/2 2(1 ? ?) Z 2?n

1?k/2k 2 k 2 x ?x2 /2 =? eC(?,?)n dx + en? ? /2 P Zn?1 ? n(1 ? ?) + e?c(?)n , (26) 2? 0 where C(?, ?) = ? 2 /(2(1 ? ?)k/2). Now, for any ? ; 0, we can (and will) choose ? small enough

2 k so that both en? ? /2 P Zn?1 ? n(1~?~?) ? 0 exponentially fast (by tail bounds on ?2 random variables) and, if k ? 3, the argument of the exponent in the integral in the right hand side of (26) 7

is bounded above by ?x2 /4, which is possible since the argument vanishes at x? = 2C(?, ?)n1/2 . Hence, for any ? ι 0, and all n large enough, we have Z 2?n 1?k/2 k 2 x ?x2 /2 eC(?,?)n E0 ?2 ? ? dx + e?c(?)n , (27) 2? 0 for some c(?) ι 0. Now, for k ? 3 the integrand in (27) is dominated by e?x to 1. Therefore, since E0 ?2 ? (E0 ?)2 = 1, k?3:

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2 /4 and converges pointwise (as n ? ?) lim E0 ?2 = 1 . n?? (28)
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For k = 2, the argument is independent of n and can be integrated immediately, yielding (after taking the limit?? 0) k=2:

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1 lim sup E0 ?2 ? p . n?? 1 ? ?2 (29)
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(Indeed, the above calculation implies that the limit exists and is given by the right-hand side.) The proof is completed by invoking Lemma 2.

Related work

5

known when k = o(n). In the decision version of the planted clique problem. one seeks an efficient algorithm that distinguishes between a random graph distributed as G(n, 1/2) or a random graph containing a planted clique of size k? (2+?) log n (for? ¿ 0; the natural threshold for the problem is the size of the largest clique in a random sample of G(n, 1/2), which is asymptotic to 2 log n [14]). No polynomial time? algorithm is known for this decision problem if k = o(n). As another example, consider the following setting introduced by [4] (see also [1]): one is given a realization of a n-dimensional Gaussian vector x :=(x1, ..., xn) with i.i.d. entries. The goal is to distinguish between the following two hypotheses. Under the first hypothesis, all entries in x are i.i.d. standard normals. Under the second hypothesis, one is given a family of subsets C := {S1, ..., Sm} such that for every 1? k? m, Sk? {1, ..., n} and there exists an i ? $\{1,\,\ldots\,,\,m\}$ such that, for any ? ? Si , x? is a Gaussian random variable with mean ? \downarrow 0 and unit variance whereas for every ? ? / Si , x? is standard normal. (The second hypothesis does not specify the index i, only its existence). The main question is how large? must be such that one can reliably distinguish between these two hypotheses. In [4], ? are vertices in certain undirected graphs and the family C is a set of pre-specified paths in these graphs. The Gaussian hidden clique problem is related to various applications in statistics and computational biology [6, 18]. That detection is statistically possible when L log n was established? in [1]. In terms of polynomial time detection, [8] show that detection is possible when L = ?(n) for the symmetric cases. As noted, no polynomial time algorithm is known for the Gaussian hidden clique? problem when k = o(n). In? [1, 20] it was hypothesized that the Gaussian hidden clique problem should be difficult when L n. The closest results to ours are the ones of [22]. In the language of the present paper, these authors consider a rectangular matrix of the form X = ? v1 v2T + Z ? Rn1 ?n2 whereby Z has i.i.d. entries Zij? N(0, 1/n1), v1 is deterministic of unit norm, and v2 has entries which are i.i.d. N(0, 1/n1), independent of Z. They consider the problem of testing this distribution against ? = 0. Setting $c = \lim ?? nn12$, it is proved in [22] that the distribution of the singular values of X under the?? null and the alternative are mutually contiguous if?; c and not mutually contiguous if?; c. While [22] derive some more refined results, their proofs rely on advanced tools from random matrix theory [13], while our proof is simpler, and generalizable to other settings (e.g. tensors). 8

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