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BOOTSTRAPS REGULARIZE SINGULAR CORRELATION MATRICES

A PREPRINT

Christian Bongiorno

Université Paris-Saclay, CentraleSupélec,
Laboratoire de Mathématiques et Informatique pour les Systèmes Complexes,
91190, Gif-sur-Yvette, France

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ABSTRACT

I show analytically that the average of k bootstrapped correlation matrices rapidly becomes positive-definite as k increases, which provides a simple approach to regularize singular Pearson correlation matrices. If n is the number of objects and t the number of features, the averaged correlation matrix is almost surely positive-definite if $k > \frac{e}{e-1} \frac{n}{t} \simeq 1.58 \frac{n}{t}$ in the limit of large t and n . The probability of obtaining a positive-definite correlation matrix with k bootstraps is also derived for finite n and t . Finally, I demonstrate that the number of required bootstraps is always smaller than n . This method is particularly relevant in fields where n is orders of magnitude larger than the size of data points t , e.g., in finance, genetics, social science, or image processing.

Keywords Correlation · Regularization · High-Dimensionality

1 Introduction

Correlation and covariance matrices are fundamental dependence estimators in statistical inference. Their use includes risk minimization in finance [1], analysis of functional genomics [2], or image processing [3]. However, when the number of objects under study (n) exceeds the number of available data points (t), these matrices cannot be inverted. As a result, many standard inference methods cannot be applied directly. To overcome this issue, a large literature on eigenvalue regularization has been devoted to this issue over the last decades. The most relevant ones are the Ledoit-Wolf linear shrinkage [4] and the more recent non-linear shrinkage [5]. These methods, apart from regularizing singular correlation matrices, attempt to reduce the noise effect due to finite sample size. In addition, Ref. [6] proposes a recursive algorithm that aims to find the most similar positive-definite matrix to an initial problematic matrix that is not positive-definite. Similarly to the proposed method, this approach does not try to denoise the target matrix but corrects the eigenvalue distribution by removing the non-positive eigenvalues.

In this work, I propose a simple alternative approach based on bootstrap resampling to regularize correlation matrices with $z > 0$ zero degenerate eigenvalues. In particular, I prove that the probability to obtain a positive defined matrix from the average of k bootstrap resampling scenarios converges rapidly with respect to k to one provided that k is larger than $\frac{e}{e-1} \frac{n}{t}$.

2 The Bootstrap Average Correlation Matrix

Let $\mathbf{X} \in \mathbb{R}^{n \times t}$ be the data matrix and $\mathbf{C} \in \mathbb{R}^{n \times n}$ its Pearson correlation matrix. We assume that no column or row of \mathbf{X} is a linear combination of the others; this implies that \mathbf{C} has rank $r = \min\{n, t - 1\}$. Let $\mathbf{X}^{(b)} \in \mathbb{R}^{n \times t}$ be a bootstrap copy of \mathbf{X} obtained by sample replacement of the columns of \mathbf{X} , and $\mathbf{C}^{(b)}$ its correlation matrix. A generic element of $\mathbf{X}^{(b)}$ is $x_{ij}^{(b)} = x_{i\mathbf{h}_j^{(b)}}$, where $\mathbf{h}^{(b)}$ is a vector of dimension t obtained by random sampling with replacement of the elements of vector $(1, 2, \dots, t)$.

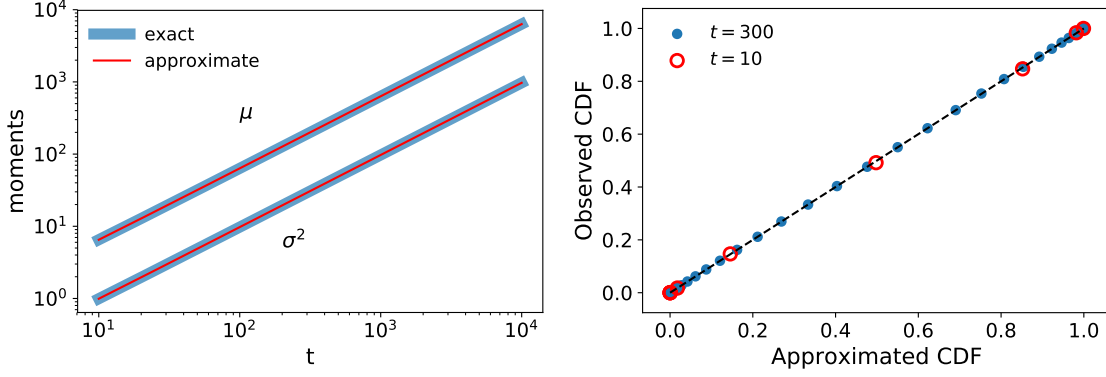


Figure 1: The left plot shows the exact (Eq. (3)) and approximate (eq. (4)) t -dependence of the first two moments of $\mathcal{P}(u_b)$ distribution of Eq. (2). The right plot shows the approximate Normal Cumulative Distribution Function (CDF) against the observed CDF obtained with 10^4 random sampling for every integer value of $u_b \in [0, t]$.

This paper derives an approximate expression of the probability that the smallest eigenvalue λ_0 of the correlation matrix $\langle \mathbf{C} \rangle := k^{-1} \sum_{i=0}^k \mathbf{C}^{(i)}$ is larger than zero as a function of the number of bootstrap copies. The minimum number of bootstrap copies k^+ , that guarantees $\langle \mathbf{C} \rangle$ to be positive-definite within a chosen confidence level, shows a real transition in the large-system limit, defined here as $n, t \rightarrow \infty$ at fixed q .

3 The Distribution of the Number of Null Eigenvalues

The first step is to obtain a probability distribution of the number of zero eigenvalues z_b of a given bootstrap correlation matrix $\mathbf{C}^{(b)}$. One has

$$z_b = \max\{n + 1 - u_b, 0\}, \quad (1)$$

where u_b is the number of unique column indices sampled from \mathbf{X} in the b -bootstrap copy. The exact probability distribution of u_b is known to be [7]

$$\mathcal{P}(u_b) = \frac{\mathcal{S}_2(t, u_b) t!}{t^t (t - u_b)!} \quad (2)$$

where $\mathcal{S}_2(t, u_b)$ is the Sterling number of the second kind. Such a distribution has mean and variance

$$\begin{aligned} \mu(t) &= t \left[1 - \left(1 - \frac{1}{t}\right)^t \right] \\ \sigma^2(t) &= t \left(1 - \frac{1}{t}\right)^t + t^2 \left(1 - \frac{1}{t}\right) \left(1 - \frac{2}{t}\right)^t - t^2 \left(1 - \frac{1}{t}\right)^{2t}. \end{aligned} \quad (3)$$

In the limit of large t , eqs (3) become

$$\begin{aligned} \mu(t) &\approx \left(1 - \frac{1}{e}\right) t + \frac{1}{2e} \\ \sigma^2(t) &\approx \left(\frac{e-2}{e^2}\right) t + \frac{3-e}{2e^2}. \end{aligned} \quad (4)$$

Furthermore, it is worth noticing that the deviation of the empirical $\mathcal{P}(u_b)$ from a normal $\mathcal{N}(\mu(t), \sigma(t))$ is negligible for even for moderately large t [7], as reported in the right-hand side plot of Fig. 1.

If we consider a condition characterized by an abundance of expected zero eigenvalues, i.e., $n \gg t$, then the probability distribution of z_b according to Eq. (1) can be approximate by a Normal distribution

$$\mathcal{P}(z_b) \approx \mathcal{N}(n + 1 - \mu(t), \sigma(t)). \quad (5)$$

Now that the distribution of the zero eigenvalues for the single bootstrap copy is known, we can answer the original question, and consider k bootstrap copies of \mathbf{X} such that $\langle \mathbf{C} \rangle := k^{-1} \sum_{i=1}^k \mathbf{C}^{(i)}$.

To make further progress, it is necessary to recall the geometrical properties of the space associated to degenerate eigenvalues. Let us suppose that $\mathbf{C}^{(i)}$ has z_i zero eigenvalues. Then the set of eigenvectors associated with these zero eigenvalues defines a hyper-plane V_i of dimension z_i embedded in an n dimensional space. Each vector \mathbf{w} that lies in V_i verifies $\mathbf{w} \mathbf{C}^{(i)} \mathbf{w}' = 0$; however, if there is at least another $j \neq i$ whose z_j zero eigenvalues of $\mathbf{C}^{(j)}$ define hyper-plane V_j such that $\dim(V_i \cap V_j) \not\geq 1$, then $\mathbf{w} \mathbf{C}^{(j)} \mathbf{w}' > 0$; and thus $\mathbf{w} \langle \mathbf{C} \rangle \mathbf{w}' > 0$ for every vector \mathbf{w} that lies in V_i or V_j .

It is important to point out that eigenvectors associated to z_i zero eigenvalues can be assumed to be ‘‘randomly’’ chosen with the constraint to be orthogonal with V_i^\perp , the space defined by the eigenvectors associated with the $n - z_i$ non-zero eigenvalues; this because they do not carry any information about the correlation matrix $\mathbf{C}^{(i)}$ since they explain zero variance. Therefore every rotation of the basis of V_i constrained to be orthogonal with V_i^\perp will produce exactly the same matrix $\mathbf{C}^{(i)}$. In the $k = 2$ case, the probability that $\dim(V_1 \cap V_2) \not\geq 1$ will be approximately 1 if $z_1 + z_2 \leq n$ and 0 otherwise. It is possible to visualize this relationship easily in a three-dimensional space, i.e., $n = 3$. In case of two random straight lines, that have dimensions $z_1 = 1$ and $z_2 = 1$, the probability that they intersect in a straight line is almost zero since they must be coincident; differently, if we consider two random planes $z_1 = 2$ and $z_2 = 2$ they will intersect in a straight line almost surely apart from only configurations in which they are parallels. The above-discussed approximation, in the case of the spectral decomposition, is valid if the probability that the orthogonal spaces V_1^\perp and V_2^\perp defined from the $n - z_1$ and $n - z_2$ non-zero eigenvalues perfectly overlap is negligible. In a bootstrap resampling, when t is sufficiently large, this probability is approximately zero, as this requires to sample the same column indices of \mathbf{X} for both bootstrap realizations, in other words, $\mathbf{C}^{(1)} = \mathbf{C}^{(2)}$.

More generally, for k bootstrap copies, every hyper-plane V_i will verify $\dim(V_i \cap V_j) \not\geq 1$ for at least one $j \neq i$ with probability 1 if

$$\zeta := \sum_{i=1}^k z_i \leq (k - 1)n. \quad (6)$$

If the above inequality holds, then $\langle \mathbf{C} \rangle$ has no zero eigenvalue. From Eq. (6), one can derive an upper bound for the number of bootstrap copies required. In fact, even if all bootstrap correlations have $n - 1$ null eigenvalues, no more than $k = n$ bootstrap copies are necessary to obtain a positive definite matrix $\langle \mathbf{C} \rangle$.

According to Eq. (5), the distribution of ζ can be approximated by a sum of k identical normal distributions that converges to

$$\mathcal{P}(\zeta) \approx \mathcal{N}\left(k(n + 1 - \mu(t)), \sqrt{k}\sigma(t)\right). \quad (7)$$

Therefore, the probability that the smallest eigenvalue λ_0 of $\langle \mathbf{C} \rangle$ is larger than zero can be obtained from the cumulative distribution function of $\mathcal{P}(\zeta)$ estimated at $(k - 1)n$, that is

$$\mathcal{P}(\lambda_0 > 0) \approx \mathcal{P}(\zeta \leq (k - 1)n) = \int_{-\infty}^{(k-1)n} \mathcal{P}(\zeta) d\zeta \approx \frac{1}{2} \left[1 + \operatorname{erf}\left(\frac{[\mu(t) - 1]k - n}{\sigma(t)\sqrt{2k}}\right) \right] \quad (8)$$

The above equation suggests to set a threshold α such that $\mathcal{P}(\lambda_0 > 0) > 1 - \alpha$, i.e. $1 - \operatorname{erf}(a) = \alpha$ (for example, $a \approx 1.82$ for $\alpha = 0.01$). One can then define the number of bootstraps required to achieve $\mathcal{P}(\lambda_0 > 0) > 1 - \alpha$ by setting the argument of the erf function to a , which gives

$$k^+(a) \simeq \frac{a^2\sigma^2(t) + [\mu(t) - 1]n + \sqrt{a^4\sigma^4(t) + 2a^2\sigma^2(t)[\mu(t) - 1]n}}{[\mu(t) - 1]^2} \quad (9)$$

A bi-dimensional mapping of the values of $k^+(a)$ with $a = 1.82$ as function of n and t , shown in Fig. 2 left, shows that the number of bootstrap copies k^+ required to have a positive defined $\langle \mathbf{C} \rangle$ is quite small, at least for not too extreme values of $q = n/t$.

To have a rough estimate of the transition point k^+ for $\mathcal{P}(\lambda_0 > 0) \approx 1$ in the limit of large n , we can substitute $t = n/q$, and compute the k^* of the inflection point of the error function, obtained for the argument of erf equals to zero

$$k^* = \frac{2enq}{2(e - 1)n + (1 - 2e)q}. \quad (10)$$

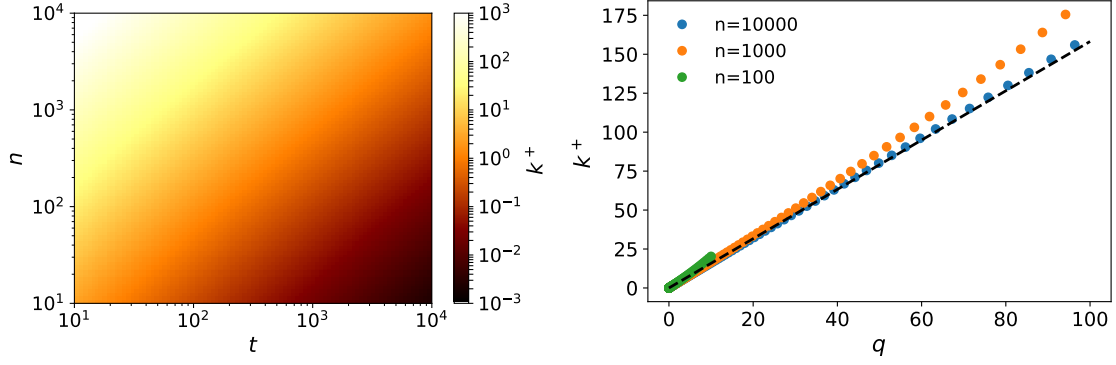


Figure 2: The left plot shows a color map of the analytical value of $k^+(a)$, with $a = 1.82$, for different n and t . The right plot shows the analytical (dots) and large-system limit (dotted line) values of k^+ obtained for t that span a geometric progression range in $[10, 10^4]$ such that $q \in [1, 100]$. The large-system limit is obtained from Eq.(12).

The large-system limit of the first derivative slope at the inflection point if the error function diverges to infinity

$$\lim_{n \rightarrow \infty} \frac{d}{dk} \left. \frac{k [2(e-1)n - 2eq + q] - 2enq}{2q \sqrt{k \left[\frac{2(e-2)n}{q} - e + 3 \right]}} \right|_{k=k^*} = \infty. \quad (11)$$

This means that $\mathcal{P}(\lambda_0 > 0)$ has a real transition in the large-system limit. The value of the inflection point of Eq. (10), in the large-system limit, converges to

$$\lim_{n \rightarrow \infty} k^* = \lim_{n \rightarrow \infty} k^+(a) = \frac{e}{(1-e)} q \approx 1.58 \frac{n}{t} \quad (12)$$

The right-hand side of Fig. 2 shows that this approximation can provide a quite accurate estimation of the magnitude of k^+ even for n small when q is not extremely large.

In summary, both the approximate distribution of $\mathcal{P}(\lambda_0 > 0)$ of Eq. (8) and the bound limits k^+ of Eqs. (9) show a very good agreement with the observations, reported in Fig. 3.

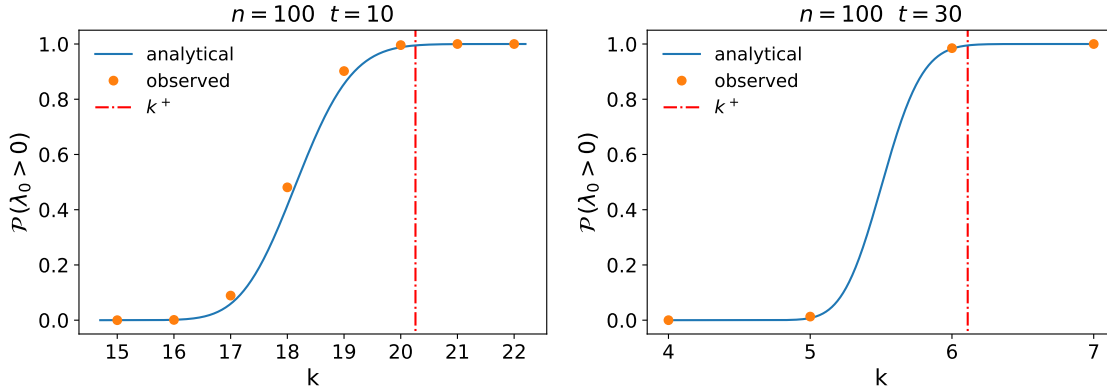


Figure 3: Observed and predicted probability that $\langle \mathbf{C} \rangle$ has no zero eigenvalues with k bootstrap copies, for various n and t . The figure shows the predicted $k^+(a)$ limit, with $a = 1.82$. The simulations are obtained by sampling \mathbf{X} from a standardized multivariate normal distribution.

4 Discussion

I have shown that the average correlation matrix of k bootstrap copies converges to a positive-defined matrix for k much smaller than the order of the matrix. Such a matrix can be used in many applications which require to invert C , such as risk optimization. An extensive comparative analysis of the performance of these approaches will be addressed in future works.

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