A method for generating realistic correlation matrices

Stephan Ramon Garcia        Johanna Hardin

June 30, 2011

Abstract

Simulating sample correlation matrices is important in many areas of statistics. Approaches such as generating normal data and finding their sample correlation matrix or generating random uniform $[-1,1]$ deviates as pairwise correlations both have drawbacks. We develop an algorithm for adding noise, in a highly controlled manner, to general correlation matrices. In many instances, our method yields results which are superior to those obtained by simply simulating normal data. Moreover, we demonstrate how our general algorithm can be tailored to a number of different correlation models. Finally, using our results with an existing clustering algorithm, we show that simulating correlation matrices can help assess statistical methodology.

1 Introduction

As computational resources continue to improve, researchers can take advantage of simulation studies to investigate properties and results associated with novel statistical methodology. In particular, simulating correlation matrices with or without a given structure can provide insight into the sensitivity of a model. There has been extensive work on simulating correlation matrices with random entries; that is, generating positive semidefinite matrices with all entries bounded by $[-1,1]$ and having ones on the diagonal. Seminal work by Marsaglia and Olkin [30] discusses distributional characteristics and eigenvalues of simulated random correlation matrices. Although there has been additional work expanding the ideas associated with generating random correlation matrices [8, 16, 21, 28, 35] and even randomly generating correlation matrices within particular settings [15, 33], to our knowledge there is no literature devoted to the problem of adding noise to given correlation structures.

We discuss the need to simulate realistic correlation matrices in a specific context. By realistic we mean not only that the correlation matrix has some prescribed structure (dependent upon the requirements of the particular application), but also that it is noisy. Simulating correlation matrices is important for a variety of situations. For example, methods that use simulated correlation matrices include probit analysis [29, 44], shrinkage estimation [2], meta-analysis [10], multiple comparisons [23], management science [32], and factor analysis [17], as well as clustering. Some clustering and classification methods simulate correlations (or covariances) using uniform
distributions \([20, 24, 25, 38]\). However, unconstrained randomly simulated correlation matrices are typically not positive semidefinite. Although we provide motivation and a detailed example using clustering, our method is applicable to any context where simulating realistic correlation matrices is important.

There is an enormous literature devoted to methods designed for unsupervised clustering. In particular, the clustering of microarray data has generated much recent interest. Clustering techniques can be quite powerful because they provide models or novel groupings in a setting where class labels are unknown. However, the lack of knowledge of underlying structure makes assessing clustering algorithms difficult in realistic settings. Indeed, there has been a call for work that seeks to determine the reproducibility of clustering methods instead of continued work on developing new clustering algorithms \([1,37]\).

Suppose that we are given a \(N \times N\) correlation matrix \(\Sigma = (\Sigma_{ij})_{i,j=1}^{N}\). Generating a noisy correlation matrix \(S = (S_{ij})_{i,j=1}^{N}\) based upon the template \(\Sigma\) can be difficult since noise must be added to \(\Sigma\) in such a way that \(S\) is positive semidefinite, and satisfies \(S_{ii} = 1\) and \(-1 \leq S_{ij} \leq 1\) for \(1 \leq i, j \leq N\). Moreover, for numerical purposes (e.g., generating data from \(S\)) one might also require an explicit upper bound on the condition number of \(S\) to ensure its numerical stability (e.g., for matrix inversion). Unfortunately, naively adding random noise to a correlation matrix can result in matrices which violate any or all of the above constraints.

### 1.1 Simulating Data for Evaluating Algorithms

Many clustering algorithms (e.g., hierarchical clustering, PAM \([22]\), HOPACH \([40]\), QT clustering \([14]\), WGCNA \([43]\)) use distances in lieu of raw data to partition or agglomerate observations into groups. Additionally, correlation distance has been used recently for high dimensional data reduction methods in order to apply functional data analysis \([5]\). A method for determining differential co-expression based only on correlation (and not raw data) is given by Choi and Kendziorski \([6]\). In fact, correlation has become a standard method for determining similarity between high throughput observations; distances are computed from one minus the correlation or one minus the absolute correlation. With most high throughput data, the relationships of interest are due to directional changes across experimental conditions (measured by correlation) as opposed to magnitude changes across experimental conditions (measured by Euclidean distance).

In order to assess the accuracy of a clustering algorithm, it is important to have a known group structure, many authors use a certain group structure and simulate normal data from that matrix. For example, in a recent paper, Tritchler et al. simulate normal data to assess a method for filtering genes prior to clustering and network analysis. Their clustering structure consists of within cluster correlations of 0.4 and between cluster correlations of 0 \([39]\). Using clustering to find differentially expressed genes, Hu et al. generate normal deviates in a two-cluster setting with one cluster of 100 observations correlated at 0.94, another cluster of 608 observations clustered at 0.9, and observations from different clusters correlated at 0.697 \([19]\).

We appreciate the difficulty in generating realistic data with known cluster stru-
ture. However, we believe that using normal deviates often adds an additional unnecessary layer of assumptions. In Section 4.1 we demonstrate that our method produces matrices that are more general than the class of matrices produced by finding the sample correlation of normally distributed data. Indeed, we do not believe that microarray data are normally distributed [13]. Instead of simulating normal data from a known correlation structure, we argue in favor of simulating correlation matrices directly based on a known correlation structure. The random correlation matrices can then be used to assess the algorithm at hand.

Typically, the $i,j$th entry $S_{ij}$ of a $N \times N$ correlation matrix $S = (S_{ij})_{i,j=1}^{N}$ is the Pearson correlation between the $i$th and $j$th objects. In particular, $S$ is symmetric, each entry lies between $-1$ and $1$, and the diagonal entries of $S$ are all equal to 1. Correlation matrices with such a structure can be constructed from any correlations computed on the pairs of entries associated with a particular row and column (e.g., Spearman correlation or biweight correlation [12]). In general, any positive semidefinite matrix is a covariance matrix [31, p. 3] and any such matrix corresponds to a correlation matrix. One approach for generating random correlation matrices draws independent observations from a uniform distribution on $[-1,1]$ as the entries of the correlation matrix [24,25]. Random entries of the correlation matrix will not necessarily create positive definite matrices, and any further processes based on inverting the correlation matrix will be impossible. The correlation matrix can provide a tremendous amount of information about the underlying data structure, but due to the required algebraic relations, generating a noisy correlation matrix which satisfies certain prescribed conditions is not trivial.

1.2 Three existing models

The goal of our work is to provide an algorithm for simulating correlation structures that:

- are realistic yet flexible in structure,
- contain sufficient noise for within group correlations,
- contain sufficient noise for between group correlations,
- can be used in lieu of simulating (Gaussian) data from the correlation matrix.

Again, to motivate the properties of the simulated correlation matrix, we point out (1) microarray data are typically not normally distributed, (2) many clustering and classification methods rely only on the distances (i.e., correlations) between observations and not their observed values, (3) it is important to build in possible structure or hierarchical relationships across different values.

It has been observed, though (to our knowledge) not investigated, that with high-throughput data, the dependencies between clusters are weak but existent. As Guo et al. declare, “[a]lthough it is true that weak connections between groups may exist, independence between groups is usually a reasonable assumption” [9].

Below we have outlined three methods for generating correlation matrices, each of which describes different dependence structures for simulating clusters of data. Our
paper offers a flexible way to generate correlation structures given any reasonable model of what we would expect across observational units.

### 1.2.1 Constant correlation model

A standard clustering structure is one with fixed correlations within a cluster and between clusters (often with correlation equal to zero between clusters). Hu et al.\cite{19} simulate observations correlated at the same level with off diagonal noise also specified. 

$$\Sigma = (\Sigma_{ij})_{i,j=1}^{N}$$

$$\Sigma_{ij} = \begin{cases} 
0.94 & 1 \leq i < j \leq 100, \\
0.697 & \text{for } 1 \leq i \leq 100 \leq j \leq 708, \\
0.90 & \text{for } 101 \leq i < j \leq 708,
\end{cases}$$

### 1.2.2 Toeplitz model

Another structure is one that models high correlation for observations which are close together in the correlation matrix and such that correlation values decrease for observations which are increasingly far away. In building a classification model, Guo et al.\cite{9} describe a Toeplitz structure (sometimes referred to as an auto-regressive structure) to the correlation matrix, where adjacent pairs of observations are highly correlated, and those further away are less correlated. Let

$$\Sigma_{k} = \begin{pmatrix}
1 & \rho_{k} & \rho_{k}^{2} & \rho_{k}^{3} & \cdots & \rho_{k}^{n_{k}-1} \\
\rho_{k} & 1 & \rho_{k} & \rho_{k}^{2} & \cdots & \rho_{k}^{n_{k}-2} \\
\rho_{k}^{2} & \rho_{k} & 1 & \rho_{k} & \cdots & \rho_{k}^{n_{k}-3} \\
\rho_{k}^{3} & \rho_{k}^{2} & \rho_{k} & 1 & \cdots & \rho_{k}^{n_{k}-4} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\rho_{k}^{n_{k}-1} & \rho_{k}^{n_{k}-2} & \rho_{k}^{n_{k}-3} & \rho_{k}^{n_{k}-4} & \cdots & 1
\end{pmatrix} \quad (1)$$

be the correlation matrix for $k$th cluster, given by the correlation value $\rho_{k}$. In this model, the between group correlations are set to zero. Additional classification models have used similar Toeplitz structure for simulating data from a correlation matrix\cite{7,20,34,11,45}. In fact, Huang et al. use a $U[0.5,1.5]$ distribution to simulate the variance components of the population in order add noise to the above prescribed structure.

### 1.2.3 Hub observation model

The last model is one that is hierarchical in nature based on a single hub-observation and the relationship of each observation to that original hub. Horvath et al.\cite{26,27,43} define a correlation structure with respect to a particular profile (or hub-observation). Each observation in the cluster is correlated with the hub-observation with decreasing strength (from a user supplied maximum correlation to a given minimum correlation).
Additionally, clusters are generated independently (that is, with correlation zero between clusters). For the $i$th observation ($i = 2, 3, \ldots, n$), the correlation between it and the hub-observation is given by, $\Sigma = (\Sigma_{ij})_{i,j=1}^{N}$:

$$\Sigma_{i,\text{hub}} = \rho_{\text{max}} - ((i-2)/(n-2)) \gamma (\rho_{\text{max}} - \rho_{\text{min}})$$

Note that the correlation between the $i$th observation and the hub will range from $\rho_{\text{max}}$ to $\rho_{\text{min}}$; the rate at which the correlations decay is controlled by the power, $\gamma$.

Motivated by the three existing models above, we provide an algorithm for adding noise to correlation matrices. Section 2 contains the theoretical details behind our procedure, while Section 3 concerns several specific applications in the contexts discussed above. In Section 4 we give an example of how simulated correlation matrices with realistic structure can be used to assess a statistical method.

2 The Basic Procedure

2.1 Preliminaries

Recall that if $A$ is a $N \times N$ symmetric matrix, then each of its eigenvalues is real and hence we may list them in descending order

$$\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_N(A),$$

where each eigenvalue is repeated according to its multiplicity. According to this convention, $A$ is positive semi-definite if and only if $\lambda_N(A) \geq 0$ and $A$ is positive definite if and only if $\lambda_N(A) > 0$.

The norm of a $N \times N$ matrix $A$ is defined to be

$$\|A\| = \max_{\|v\|=1} \|Av\|,$$

which equals $\lambda_1(A)$ if $A$ is positive semi-definite. To be more specific, the expression (2) is often called the operator norm to distinguish it from other frequently used matrix norms (e.g., the Frobenius norm). The condition number [18, p. 336] of a symmetric matrix $A$ is defined to be

$$\kappa(A) = \begin{cases} \|A^{-1}\|\|A\| & \text{if } A \text{ is nonsingular}, \\ \infty & \text{if } A \text{ is singular}. \end{cases}$$

In particular, if $A$ is positive semi-definite, then we have

$$\kappa(A) = \begin{cases} \lambda_1(A) / \lambda_N(A) & \text{if } \lambda_N(A) > 0, \\ \infty & \text{if } \lambda_N(A) = 0. \end{cases}$$

In the following, we let $I_n$ denote the $n \times n$ identity matrix and $1_n$ denote the $n \times n$ matrix whose entries are all equal to 1.
2.2 An algorithm

Given a prototype correlation matrix \( \Sigma = (\Sigma_{ij})_{i,j=1}^{N} \), we might wish to add noise to \( \Sigma \) in a computationally efficient way such that the resulting matrix \( S \) is also a correlation matrix. Furthermore, we might also require effective bounds on the condition number \( \kappa(S) \) of \( S \) to ensure that \( S \) is a suitable candidate for certain numerical procedures (e.g., matrix inversion). For example, in the statistical software R, the default tolerance for detecting linear dependencies in the columns of a matrix is a condition number \( \leq 10^{15} \).

The following simple procedure, which we shall apply in more specialized settings (Section 3), accomplishes this task.

**Algorithm 1.** Let

1. \( \Sigma \) be a given \( N \times N \) correlation matrix,
2. \( 0 < \varepsilon < \lambda_N(\Sigma) \) (\( \varepsilon \) is the maximum noise level),
3. \( M \) be a positive integer (the dimension of the noise space).

Select \( N \) unit vectors \( u_1, u_2, \ldots, u_N \) from \( \mathbb{R}^M \) and form the \( M \times N \) matrix 

\[
U = (u_1 \mid u_2 \mid \cdots \mid u_N)
\]

whose columns are the \( u_i \). The \( N \times N \) matrix

\[
S = \Sigma + \varepsilon(U^T U - I)
\]

is a correlation matrix whose entries satisfy \( |S_{ij} - \Sigma_{ij}| \leq \varepsilon \) for \( 1 \leq i, j \leq N \) and whose condition number \( \kappa(S) \) satisfies

\[
\kappa(S) \leq \frac{\lambda_1(\Sigma)}{\lambda_N(\Sigma)} + \frac{(N - 1)\varepsilon}{\lambda_N(\Sigma) - \varepsilon}.
\]

Before justifying the procedure above, let us make a few remarks concerning the condition number of \( S \). It might be the case that a certain numerical procedure (e.g., matrix inversion in R) cannot handle a matrix which is poorly conditioned (i.e., with a large condition number). Therefore we might desire that \( \kappa(S) \leq \kappa_{\text{max}} \) for some fixed \( \kappa_{\text{max}} \), which depends upon the particular requirements of the software being employed. From (4), it is easy to see that any \( \varepsilon > 0 \) satisfying the additional constraint

\[
\varepsilon \leq \frac{\kappa_{\text{max}} \lambda_N(\Sigma) - \lambda_1(\Sigma)}{\kappa_{\text{max}} + (N - 1)}
\]

yields an \( S \) such that \( \kappa(S) \leq \kappa_{\text{max}} \).

**Justification of Algorithm 1.** Let \( E = U^T U \) so that

\[
E = \begin{pmatrix}
1 & u_1^T u_2 & \cdots & u_1^T u_N \\
u_2^T u_1 & 1 & \cdots & u_2^T u_N \\
\vdots & \vdots & \ddots & \vdots \\
u_N^T u_1 & u_N^T u_2 & \cdots & 1
\end{pmatrix}
\]

and note that \( E \) is symmetric and positive-semidefinite (i.e., \( \lambda_N(E) \geq 0 \)). Moreover, \( E \) is positive definite if and only if the \( u_i \) are linearly independent [18 Thm. 7.2.10].
Now recall that Geršgorin’s Disk Theorem \([18, \text{Thm. 6.1.1}]\) asserts that if \(A = (A_{ij})\) is a \(N \times N\) matrix, then for each eigenvalue \(\lambda\) of \(A\) there exists a corresponding index \(i\) such that
\[
|\lambda - A_{ii}| \leq \sum_{j=1, j \neq i}^{N} |A_{ij}|.
\]
By Geršgorin’s theorem and Cauchy-Schwarz, it follows that every eigenvalue \(\lambda\) of \(E\) satisfies
\[
|\lambda - 1| \leq \sum_{j=1}^{N} |u_j^T u_j| \leq (N - 1)
\]
whence \(0 \leq \lambda_i(E) \leq N\) for \(i = 1, 2, \ldots, N\).

We next define \(S\) by (3) and observe that \(S\) is of the form
\[
S = \begin{pmatrix}
1 & \sum_{12} + \varepsilon u_1^T u_2 & \cdots & \sum_{1N} + \varepsilon u_1^T u_N \\
\Sigma_{21} + \varepsilon u_2^T u_1 & 1 & \cdots & \sum_{2N} + \varepsilon u_2^T u_N \\
\vdots & \vdots & \ddots & \vdots \\
\sum_{N1} + \varepsilon u_N^T u_1 & \sum_{N2} + \varepsilon u_N^T u_2 & \cdots & 1
\end{pmatrix}.
\]
In particular, \(S\) is our original matrix \(\Sigma\) with “noise” terms \(\varepsilon u_i^T u_j\) of magnitude at most \(\varepsilon\) added to the off-diagonal entries. To analyze the impact of adding this noise, we require Weyl’s Inequalities \([18, \text{Thm. 4.3.1}]\), which assert that if \(A\) and \(B\) are \(N \times N\) symmetric matrices, then
\[
\lambda_j(A) + \lambda_N(B) \leq \lambda_j(A + B) \leq \lambda_j(A) + \lambda_1(B)
\]
for \(j = 1, 2, \ldots, N\). Applying the lower inequality in (7) with \(j = N, A = \Sigma - \varepsilon I_N, B = \varepsilon E\), we obtain
\[
0 < \lambda_N(\Sigma) - \varepsilon = \lambda_N(\Sigma - \varepsilon I_N) \leq \lambda_N(\Sigma - \varepsilon I_N) + \lambda_N(\varepsilon E) \leq \lambda_N(S)
\]
from which we conclude that \(S\) is positive definite. Next, we apply the upper inequality in (7) with \(j = 1\) which yields
\[
\lambda_1(S) \leq \lambda_1(\Sigma - \varepsilon I) + \lambda_1(\varepsilon E) \leq (\lambda_1(\Sigma) - \varepsilon) + N \varepsilon = \lambda_1(\Sigma) + (N - 1)\varepsilon.
\]
Putting this all together, we obtain the estimates
\[
0 < \lambda_N(\Sigma) - \varepsilon \leq \lambda_N(S) \leq \lambda_1(S) \leq \lambda_1(\Sigma) + (N - 1)\varepsilon.
\]
The inequality (4) follows since \(\kappa(S) = \lambda_1(S)/\lambda_N(S)\).

There are a few arguments that can be made in favor of adding noise in this manner. First of all, the procedure described above is easy to implement numerically, and it can be rapidly executed. Moreover, it offers a great deal of flexibility since the dimension \(M\) of the ambient space that the vectors \(u_1, u_2, \ldots, u_N\) are drawn from and the manner in which these vectors are selected is arbitrary and can be tailored to the particular
application at hand. Finally, our method is completely general in the sense that any
positive-definite \( N \times N \) matrix \( E \) having constant diagonal 1 can be factored as \( E = U^TU \) where \( U \) is some matrix whose columns are unit vectors (e.g., let \( U \) be the positive-
definite square root of \( E \)). In other words, regardless of the method one employs to
produce a positive-semidefinite matrix \( E = U^TU \) for use in (3), the same \( E \) can in
principle be generated using our approach.

Let us now say a few words about the manner in which the vectors \( u_i \) are selected.
If \( M \) is very small (e.g., \( 2 \leq M \leq 5 \)), then many of the dot products \( u_i^T u_j \) will be
relatively large in magnitude. For many purposes, this yields a very noisy coefficient
matrix \( S \) based upon the original template \( \Sigma \). Moreover, even if \( M \) is relatively large,
then the matrix \( E = U^TU \) can be computed extremely rapidly since generating the
unit vectors \( u_i \) and computing the dot products \( u_i^T u_j \) involve relatively straightforward
computations (e.g., no eigenvalue calculations).

There are of course many other ways which one could select the \( u_i \). If one wishes
the \( u_i^T u_j \) to be consistently large in magnitude while also ensuring that \( E \) has full
rank, one lets \( M \geq N \) and then selects numbers \( \alpha_1, \alpha_2, \ldots, \alpha_N \) at random from \([-1,1] \)
using a continuous probability density function \( f(x) \) on \([-1,1] \) which favors extreme
values (e.g., \( f(x) = |x| \), \( f(x) = \frac{2 - 2\sqrt{1-x^2}}{4\pi} \), or a Beta distribution transformed to exist
on the range \([-1,1] \)). One then replaces the numbers \( u_i^T u_j \) in (6) by
\[
\alpha_i \alpha_j + \sqrt{(1 - |\alpha_i|^2)(1 - |\alpha_j|^2)} u_i^T u_j.
\] (8)
In effect, one is replacing the \( u_i \in \mathbb{R}^M \) with the unit vectors \( (\alpha_i, \sqrt{1 - |\alpha_i|^2} u_i) \in \mathbb{R}^{M+1} \).
These vectors tend to be highly correlated (but linearly independent) since the numbers
\( \alpha_i \) favor extreme values in the interval \([-1,1] \).

3 Recipes

Using the basic procedure (Algorithm 1) described above for adding noise to a given
correlation matrix, we can modify our approach to take advantage of certain known
structures. For the constant correlation structure (Subsection 3.1) and Toeplitz struc-
ture (Subsection 3.2) we first calculate sharp bounds on the smallest eigenvalues of the
template correlation matrix \( \Sigma \) and then apply Algorithm 1 to obtain the noisy corre-
lation matrix \( S \). A similar computational approach to the hub correlation structure is
discussed in Subsection 3.3. Each model is expanded to describe a population based on
multiple clusters with the same underlying structure (and different sizes and parameter
values).

3.1 Constant correlation structure

The first correlation structure is based on constant correlations within each cluster
and between each cluster (values of the correlation differ for each relationship). In
particular, observe that the approach below yields a noisy correlation matrix which
has a significant amount of noise on the off-diagonal blocks. We argue that this is
more realistic than simply assuming that all of these entries are zero.
Algorithm 2. Let

- $K$ denote a positive integer (the number of clusters) and $k = 1, 2, \ldots, K$,
- $n_k$ be a positive integer (the size of the $k$th cluster),
- $N = \sum_{k=1}^{K} n_k$ (size of the desired matrix),
- $\rho_k$ such that $0 \leq \rho_k < 1$ (baseline correlation in the $k$th cluster),
- $\rho_{\min} = \min\{\rho_1, \rho_2, \ldots, \rho_K\}$ (minimum correlation in any cluster),
- $\rho_{\max} = \max\{\rho_1, \rho_2, \ldots, \rho_K\}$ (maximum correlation in any cluster),
- $\delta$ such that $0 \leq \delta < \rho_{\min}$ (baseline noise between clusters),
- $\Sigma_k$ be the $n_k \times n_k$ matrix

$$\Sigma_k = \begin{pmatrix}
1 & \rho_k & \cdots & \rho_k \\
\rho_k & 1 & \cdots & \rho_k \\
\vdots & \vdots & \ddots & \vdots \\
\rho_k & \rho_k & \cdots & 1
\end{pmatrix}, \quad (9)$$

(correlation matrix for $k$th cluster),
- $\Sigma = (\Sigma_{ij})_{i,j=1}^{N}$ be the $N \times N$ matrix having the blocks $\Sigma_k$ along the diagonal and $0$s elsewhere,
- $\varepsilon$ such that $0 \leq \varepsilon < 1 - \rho_{\max}$ (maximum entry-wise random noise),
- $M$ be a positive integer (the dimension of the noise space).

Select $N$ unit vectors $u_1, u_2, \ldots, u_N$ from $\mathbb{R}^M$. The $N \times N$ matrix $S = (S_{ij})_{i,j=1}^{N}$ defined by

$$S_{ij} = \begin{cases} 
1 & \text{if } i = j, \\
\rho_k + \varepsilon u_i^T u_j & \text{if } i, j \text{ are in the } k\text{th cluster and } i \neq j, \\
\delta + \varepsilon u_i^T u_j & \text{if } i, j \text{ are in different clusters},
\end{cases} \quad (10)$$

is a correlation matrix whose condition number satisfies

$$\kappa(S) \leq \frac{N(1 + \varepsilon) + 1}{1 - \rho_{\max} - \varepsilon}. \quad (11)$$

Justification of Algorithm 2. In order to introduce a significant amount of noise to the off-diagonal blocks, we work instead with the modified correlation matrix

$$\Sigma' = \begin{pmatrix}
\Sigma_1 - \delta \mathbb{1}_{n_1} \\
\Sigma_2 - \delta \mathbb{1}_{n_2} \\
\vdots \\
\Sigma_K - \delta \mathbb{1}_{n_K}
\end{pmatrix} + \delta \mathbb{1}_{N}, \quad (12)$$
where \(1_n\) denotes the \(n \times n\) matrix whose entries are all 1. Since
\[
\Sigma_k - \delta 1_n = (1 - \rho_k)I_n + (\rho_k - \delta)1_n,
\]
it follows that
\[
\lambda_j(\Sigma_k - \delta 1_n) = \begin{cases} 
  n_k(\rho_k - \delta) + (1 - \rho_k) & \text{if } j = 1, \\
  1 - \rho_k & \text{if } j = 2, 3, \ldots, n_k,
\end{cases}
\]
and that the eigenspace corresponding to the largest eigenvalue of \(\Sigma_k - \delta 1_n\) is spanned by the vector \(1_n = (1, 1, \ldots, 1) \in \mathbb{R}^{n_k}\). In particular, the eigenspace corresponding to the eigenvalue \(1 - \rho_k\) is \((n_k - 1)\)-dimensional and any eigenvector \(v = (v_1, v_2, \ldots, v_{n_k})\) belonging to this eigenspace is orthogonal to \(1_n\) (i.e., satisfies \(\sum_{i=1}^{n_k} v_i = 0\)).

If we augment \(v\) by placing \(N - n_k\) zeros appropriately, we obtain a vector
\[
v' = (0, 0, \ldots, 0, v_1, v_2, \ldots, v_{n_k}, 0, 0, \ldots, 0) \in \mathbb{R}^{N}
\]
which is an eigenvector of \(\Sigma'\) corresponding to the eigenvalue \(1 - \rho_k\) since \(A \cdot v' = (1 - \rho_k) \cdot v'\) and \(1_N \cdot v' = 0\). It follows that the lowest \(N - K\) eigenvalues of \(\Sigma\) are the numbers \(1 - \rho_k\), each repeated \(n_k - 1\) times. In particular,
\[
\lambda_N(\Sigma') = 1 - \rho_{\text{max}}.
\]
An upper bound on the eigenvalues of \(\Sigma\) follows from (7) and (13):
\[
\lambda_1(\Sigma') \leq \lambda_1(A) + \lambda_1(\delta 1_N)
\leq \max_{1 \leq k \leq K} \{n_k(\rho_k - \delta) + (1 - \rho_k)\} + N\delta
\leq N(1 - \delta) + 1 + N\delta
= N + 1.
\]

Plugging the matrix \(\Sigma'\) into Algorithm 1 and using the preceding estimates for \(\lambda_1(\Sigma')\) and \(\lambda_N(\Sigma')\) into (4) we obtain the desired estimate (11) for \(\kappa(S)\).

3.2 Toeplitz correlation structure

The Toeplitz structure assumes that as observations are farther away, they are less correlated. The Toeplitz structure has been used extensively in classification and discriminant analysis as a model for group correlations [7,9,34,41,45]. In particular, the model assumes that each pair of adjacent observations is highly correlated and that the correlations between the \(i\)th and \(j\)th observations decay exponentially with respect to \(|i - j|\).

Let \(0 \leq \rho < 1\) and consider the \(n \times n\) Toeplitz matrix
\[
T_n = \begin{pmatrix}
1 & \rho & \rho^2 & \rho^3 & \cdots & \rho^{n-1} \\
\rho & 1 & \rho & \rho^2 & \cdots & \rho^{n-2} \\
\rho^2 & \rho & 1 & \rho & \cdots & \rho^{n-3} \\
\rho^3 & \rho^2 & \rho & 1 & \cdots & \rho^{n-4} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \ddots \\
\rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \rho^{n-4} & \cdots & 1
\end{pmatrix}
\]
(14)
whose \(ij\)th entry is \(\rho^{|i-j|}\). Using the spectral theory of self-adjoint Toeplitz operators, it is possible to show that \(T_n\) is positive-definite and that its eigenvalues satisfy

\[
\frac{1 - \rho}{1 + \rho} \leq \lambda_j(T_n) \leq \frac{1 + \rho}{1 - \rho} \tag{15}
\]

for \(j = 1, 2, \ldots, n\) (see Appendix A for details). We also remark that the preceding bounds are quite sharp in the sense that

\[
\lim_{n \to \infty} \lambda_1(T_n) = \frac{1 + \rho}{1 - \rho}, \quad \lim_{n \to \infty} \lambda_n(T_n) = \frac{1 - \rho}{1 + \rho}, \tag{16}
\]

as the size \(n\) of the matrix tends to infinity. In light of the explicit bounds (15), a straightforward application of Algorithm 1 yields the following procedure.

**Algorithm 3.** Let

- \(K\) denote a positive integer (the number of clusters) and \(k = 1, 2, \ldots, K\),
- \(n_k\) be a positive integer (the size of the \(i\)th cluster),
- \(N = \sum_{k=1}^{K} n_k\) (size of the desired matrix),
- \(\rho_k\) be such that \(0 \leq \rho_k < 1\) (correlation factor in the \(k\)th cluster),
- \(\rho_{\text{max}} = \max\{\rho_1, \rho_2, \ldots, \rho_K\}\) (maximum correlation factor),
- \(\Sigma_k\) be the \(n_k \times n_k\) Toeplitz correlation matrix

\[
\Sigma_k = \begin{pmatrix}
1 & \rho_k & \rho_k^2 & \rho_k^3 & \cdots & \rho_k^{n_k-1} \\
\rho_k & 1 & \rho_k & \rho_k^2 & \cdots & \rho_k^{n_k-2} \\
\rho_k^2 & \rho_k & 1 & \rho_k & \cdots & \rho_k^{n_k-3} \\
\rho_k^3 & \rho_k^2 & \rho_k & 1 & \cdots & \rho_k^{n_k-4} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\rho_k^{n_k-1} & \rho_k^{n_k-2} & \rho_k^{n_k-3} & \rho_k^{n_k-4} & \cdots & 1
\end{pmatrix} \tag{17}
\]

(correlation matrix for \(k\)th cluster),
- \(\Sigma = (\Sigma_{ij})_{i,j=1}^{N}\) be the \(N \times N\) matrix having blocks \(\Sigma_k\) along the diagonal,
- \(0 < \varepsilon < \frac{1 - \rho_{\text{max}}}{1 + \rho_{\text{max}}}\) (maximum entry-wise random noise),
- \(M\) be a positive integer (the dimension of the noise space).

Select \(N\) unit vectors \(u_1, u_2, \ldots, u_N\) from \(\mathbb{R}^M\) and form the \(M \times N\) matrix \(U = (u_1 u_2 \cdots | u_n)\) whose columns are the \(u_i\). The \(N \times N\) matrix

\[
S = \Sigma + \varepsilon(U^T U - I) \tag{18}
\]

is a correlation matrix whose entries satisfy \(|S_{ij} - \Sigma_{ij}| \leq \varepsilon\) and whose condition number satisfies

\[
\kappa(S) \leq \frac{1 + \rho_{\text{max}} + (N - 1)\varepsilon}{1 - \rho_{\text{max}} - \varepsilon}. \tag{19}
\]
Among other things, let us remark that for typical values of $\rho$ (e.g., Guo, Hastie, and Tibshirani let $\rho = 0.9$ in [9]) the noise level $\varepsilon$ can be made quite large compared to most of the entries in each $\Sigma_k$. This occurs because the eigenvalue estimates [15] are strong and because the off-diagonal entries of each $\Sigma_k$ are small (due to exponential decay) if one is far away from the main diagonal. Thus the approach outlined above yields a flexible method for introducing noise into the Toeplitz model. In fact, one can introduce so much noise (while still obtaining a correlation matrix with controlled condition number) that the original block-Toeplitz structure becomes difficult to discern.

3.3 Hub correlation structure

The hub correlation structure assumes a known correlation between a hub observation (typically the first observation) and each of the other observations. Moreover, one typically assumes that the correlation between the 1st and the $i$th observation decays as $i$ increases.

Let us describe a typical example that has been considered frequently in the literature. Suppose that the first row (and hence column) of a $n \times n$ correlation matrix $A$ is to consist of the prescribed values

$$A_{11} = 1, \quad A_{1i} = \rho_{\text{max}} - (\rho_{\text{max}} - \rho_{\text{min}}) \left( \frac{i - 2}{n - 2} \right)^\gamma,$$

which decreases (linearly if $\gamma = 1$) from $A_{12} = \rho_{\text{max}}$ to $A_{1n} = \rho_{\text{min}}$ for $2 \leq i \leq n$. For instance, this model is considered in Horvath et al. [26, 27, 43]. For the sake of simplicity, we consider the linear case $\gamma = 1$ and adopt a more convenient notation. Rather than specifying $\rho_{\text{max}}$ and $\rho_{\text{min}}$, we specify only $\rho_{\text{max}}$ and work instead with the step size $\tau = (\rho_{\text{max}} - \rho_{\text{min}})/(n - 2)$.

There are a variety of ways to generate the remainder of such a correlation matrix. Using any hub structure correlation matrix, we can find the smallest eigenvalue which gives a bound on the noise needed in Algorithm 1. For example, we can use a Toeplitz structure to fill out the remainder of the hub correlation matrix and, using the well-developed theory of truncated Toeplitz matrices [3,4], obtain strong eigenvalue bounds which can be fed directly into Algorithm 1 directly.

**Algorithm 4.** Let

- $K$ denote a positive integer (the number of clusters) and $k = 1, 2 \ldots, K$,
- $n_k$ be a positive integer (the size of the $i$th cluster),
- $N = \sum_{k=1}^{K} n_k$ (size of the desired matrix),
- $\rho_k$ (maximum correlation in the first row of $k$th cluster),
- $\delta_k$ (step size in first row/column of $k$th cluster),
- $\alpha_{k,1} = 1$ and $\alpha_{k,i} = \rho_k - \tau_k(i - 2)$ (correlations between hub and observations),
• $\Sigma_k$ be the $n_k \times n_k$ hub-Toeplitz correlation matrix

$$\Sigma_k = \begin{pmatrix}
1 & \alpha_{k,2} & \alpha_{k,3} & \alpha_{k,4} & \cdots & \alpha_{k,n_k} \\
\alpha_{k,2} & 1 & \alpha_{k,2} & \alpha_{k,3} & \cdots & \alpha_{k,n_k-1} \\
\alpha_{k,3} & \alpha_{k,2} & 1 & \alpha_{k,2} & \cdots & \alpha_{k,n_k-2} \\
\alpha_{k,4} & \alpha_{k,3} & \alpha_{k,2} & 1 & \cdots & \alpha_{k,n_k-3} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\alpha_{k,n_k} & \alpha_{k,n_k-1} & \alpha_{k,n_k-2} & \alpha_{k,n_k-3} & \cdots & 1
\end{pmatrix} \quad (20)$$

(correlation matrix for $k$th cluster),

• $\Sigma = (\Sigma_{ij})_{i,j=1}^N$ be the $N \times N$ matrix having blocks $\Sigma_k$ along the diagonal,

• $0 < \varepsilon < \min \left\{ 1 - \rho_k - \frac{3}{4} \tau_k : 1 \leq k \leq K \right\}$ ($\varepsilon$ is the maximum noise level),

• $M$ be a positive integer (the dimension of the noise space).

Select $N$ unit vectors $u_1, u_2, \ldots, u_N$ from $\mathbb{R}^M$ and form the $M \times N$ matrix $U = (u_1 | u_2 | \cdots | u_N)$ whose columns are the $u_i$. The $N \times N$ matrix

$$S = \Sigma + \varepsilon (U^T U - I) \quad (21)$$

is a correlation matrix whose entries satisfy $|S_{ij} - \Sigma_{ij}| \leq \varepsilon$ and whose condition number satisfies the bound (4) where

$$\lambda_1(\Sigma) \leq \max \left\{ 1 + (n_k - 1) \rho_k - \tau_k \frac{(n_k - 2)(n_k - 1)}{2} : 1 \leq k \leq K \right\}, \quad (22)$$

$$\lambda_N(\Sigma) \geq \min \left\{ 1 - \rho_k - \frac{3}{4} \tau_k : 1 \leq k \leq K \right\}. \quad (23)$$

Justification of Algorithm 4. By Gershgorin’s Disk Theorem [18, Thm. 6.1.1], the largest eigenvalue $\lambda_1(\Sigma_k)$ of $\Sigma_k$ satisfies

$$\lambda_1(\Sigma_k) \leq 1 + \rho_k + (\rho_k - \tau_k) + \cdots + (\rho_k - (n_k - 2)\tau_k)$$

$$= 1 + (n_k - 1) \rho_k - \tau_k \frac{(n_k - 2)(n_k - 1)}{2}.$$

This immediately yields (22). On the other hand, it is possible to show that the smallest eigenvalue of $\Sigma_k$ satisfies

$$\lambda_{n_k}(\Sigma_k) \geq 1 - \rho_k - \frac{3}{4} \tau_k. \quad (24)$$

To be brief, one regards the original $n_k \times n_k$ Toeplitz matrix $\Sigma_k$ as the upper-left principal submatrix of a $(2n_k-1) \times (2n_k-1)$ symmetric circulant matrix, the eigenvalues of which can be exactly computed using well-known techniques [3, p. 32]. A series of algebraic manipulations and a standard eigenvalue interlacing result [3, Thm. 9.19] yields the desired inequality (24), from which (23) follows. We thank A. Böttcher, the author of [3,4], for pointing this out to us.
3.4 Extensions

Before proceeding, let us remark that Algorithm 1 is applicable to any given positive definite correlation matrix. The amount of noise which can be added to the original matrix is determined by its smallest eigenvalue. As we have seen, for several specific classes of correlation matrices, one can obtain simple, but powerful, lower bounds on this lowest eigenvalue. For such correlation matrices, we have provided explicit, specialized algorithms which provide a significant amount of noise while also maintaining quantitative control over the condition number of the resulting matrix.

4 Results

4.1 Simulated Data

One method for generating a noisy correlation matrix is to simulate normal data from an original template and find the sample correlation matrix from the data. Varying the sample size of the generated data can create correlation matrices which are more or less variable (in magnitude). However, the nature of the variability (distribution) is similar across different sample sizes. In particular, the majority of the entries in a given sample correlation matrix generated from normal data are quite close to the template matrix. Only a handful of observations deviate from the template substantially. Additionally, the sample size needed in order to get a large amount of variability could be smaller than the dimension of the correlation matrix (thus producing sample correlation matrices that are not positive definite).

To demonstrate the restriction associated with simulating normal data as a way to find sample correlation matrices, we generate multiple correlation matrices using both normal samples and our method. The three normal structures (sample sizes 25, 250, 1000) show the same tendencies with more spread for smaller sample sizes. The three simulations using our method are based on uniform random vectors in $\mathbb{R}^2$ (GH1) and $\mathbb{R}^{25}$ (GH3) as well as uniform random vectors in $\mathbb{R}^2$ with an additional $\alpha$ component from a Beta(1,2) distribution as in equation (8) (GH2). For each simulation we used a constant correlation structure with three groups comprised of sample sizes of $(n_1 = 100, n_2 = 50, n_3 = 80)$, within cluster correlations of $(\rho_1 = 0.7, \rho_2 = 0.7, \rho_3 = 0.4)$, and between cluster correlations of $\delta = 0.25$.

Figure 1 shows the spread of entry-wise differences between the sample correlation matrices and the template for the six simulation scenarios. We see that the Garcia-Hardin (GH) scenarios are able to add larger noise terms than the normal simulation. Figure 2 shows the distribution of differences. Depending on the application, one might prefer large noise components, uniform noise component, or bell-shaped noise components. Each of those structures is easily generated by the algorithms outlined in the paper.

To demonstrate the effectiveness of our method, we simulate data from three models to show that noise added to a known structure can help to evaluate a clustering algorithm. For illustrative purposes, we use the PAM algorithm [22] to cluster and the adjusted Rand statistic [36,42] to measure the degree of concordance between the clus-
|       | \( p_1 \) | \( p_2 \) | \( p_3 \) | \( \delta \) | \( \|\varepsilon_i\| = 0 \) |
|-------|-------|-------|-------|--------|-------------------|
| GH1   | 0.7   | 0.7   | 0.4   | 0.25   | \( \varepsilon_i \in \mathbb{R}^2, \|\varepsilon_i\| = 0.29 \) |
| GH2   | 0.7   | 0.7   | 0.4   | 0.25   | \( \varepsilon_i \in \mathbb{R}^2, \|\varepsilon_i\| = 0.29, \alpha \sim \text{Beta}(1, 2) \) |
| GH3   | 0.7   | 0.7   | 0.4   | 0.25   | \( \varepsilon_i \in \mathbb{R}^{25}, \|\varepsilon_i\| = 0.29 \) |
| Norm25| 0.7   | 0.7   | 0.4   | 0.25   | 25 vectors       |
| Norm250| 0.7  | 0.7   | 0.4   | 0.25   | 250 vectors      |
| Norm1000| 0.7 | 0.7   | 0.4   | 0.25   | 1000 vectors     |

Table 1: Six different correlation matrix generating scenarios. GH1, GH2, and GH3 use the algorithms given in the paper for constant correlation. The normal simulations use the template matrix with the given sample size of random vectors. Each correlation matrix is based on a setting of 3 clusters with sizes (100, 50, 80).

Clustering output and the truth. Using silhouette width, the unsupervised PAM algorithm will give the optimal number of clusters. The adjusted Rand statistics models the degree of concordance between the PAM results and the truth. An adjusted Rand of 1 indicates perfect concordance; an adjusted Rand of zero indicates a random partition.

For each of the models we tested, we created the correlation matrix (including noise) using the appropriate algorithm. For constant correlation, we used Algorithm 2 to obtain a matrix of the form \( \text{CC1} \). Algorithm 3 was used to obtain a matrix with a Toeplitz structure as in equation (18). We used Algorithm 1 for adding noise to a general structure, and the adjustment of the algorithm to simulate the hub-Toeplitz structure as in equation (21).

### 4.2 Constant Correlation

To assess simulating the constant correlation using the parameter settings below we use Algorithm 2. All simulations were done in the 3 cluster setting with sample sizes of \( (n_1 = 100, n_2 = 50, n_3 = 80) \).

|       | \( p_1 \) | \( p_2 \) | \( p_3 \) | \( \delta \) | \( \|\varepsilon_i\| = 0.25 \) |
|-------|-------|-------|-------|--------|-------------------|
| CC1   | 0.7   | 0.7   | 0.4   | 0.25   | \( \varepsilon_i \in \mathbb{R}^{25}, \|\varepsilon_i\| = 0.29 \) |
| CC2   | 0.7   | 0.7   | 0.4   | 0.25   | \( \varepsilon_i \in \mathbb{R}^2, \|\varepsilon_i\| = 0.29 \) |
| CC3   | 0.8   | 0.75  | 0.7   | 0.65   | \( \varepsilon_i \in \mathbb{R}^2, \|\varepsilon_i\| = 0.15 \) |
| CC4   | 0.8   | 0.75  | 0.7   | 0.50   | \( \varepsilon_i \in \mathbb{R}^2, \|\varepsilon_i\| = 0.10 \) |

Clustering Results

For each of the scenarios, we simulated 1000 correlation matrices. We then clustered the data using PAM; the clustering results were assessed by determining the number of clusters the algorithm produced (truth was 3 clusters) as well as the concordance between the clustering results and the truth (1 gives perfect concordance).
Figure 1: Each boxplot represents the distribution of the entry-wise differences between the generated correlation matrix and the template structure.

| Scenario | CC1 | CC2 | CC3 | CC4 |
|----------|-----|-----|-----|-----|
| min # clusters | 3   | 7   | 2   | 3   |
| median # clusters | 3   | 12  | 11  | 3   |
| max # clusters | 3   | 17  | 15  | 3   |
| median adj Rand | 0.950 | 0.303 | 0.300 | 1   |

Table 2: Results from optimal number of clusters as well as the adjusted Rand. The original correlation structure had 3 clusters. A perfect allocation of points gives an adjusted Rand of 1.

Our results show that adding noise can create scenarios about which the algorithm is unable to determine the true structure (CC2 and CC3) and scenarios where the noise is not sufficient to decrease the performance of the algorithm (CC1 and CC4). CC1 and CC2 had reasonably low between cluster correlation but a high bound on the noise. CC3 and CC4 had high between cluster correlation and a low bound on the noise. In
Figure 2: Each histogram represents the distribution of entry-wise differences between the generated matrix and the template. The distribution of differences for GH3 is similar to the correlation matrix generated by sampling 250 random normal vectors.

CC1 we select the noise vectors from $\mathbb{R}^{25}$ which creates noise which is generally small in magnitude. In additional simulations (not shown), large within cluster correlations tend to be consistent with perfect clustering results; small within cluster correlations give rise to poor clustering results.
4.3 Toeplitz Correlation

The rapid off-diagonal decrease of the correlation values in the Toeplitz structure makes clustering difficult. Even with a base correlation of 0.9, observations 20 places away will be correlated at only $0.9^{20} = 0.12$. Our experience is that the PAM algorithm is only able to cluster Toeplitz structure data with quite small sample sizes or quite high correlations. However, we do recognize some structure to the results. Each final cluster has observations which are all correlated by at least 0.5. That is, the cluster sizes are determined by the base $\rho$ value and not the original sample size.

To assess simulating the Toeplitz correlation structure, we simulated three equal sized clusters with a given baseline $\rho$; all noise vectors were chosen randomly from $\mathbb{R}^2$. As before, for each scenario listed below, we simulate 1000 correlation matrices and use Algorithm 3 for adding noise to the correlation matrix. The cluster size, baseline $\rho$ and length of the noise vector ($\|\varepsilon_i\|$) are given in Table 3.

| cluster size | baseline $\rho$ ($\|\varepsilon_i\|$) |
|--------------|-------------------------------------|
| 20           | $0.8$ ($0.1$)                       |
| 50           | $0.9$ ($0.05$)                      |
| 100          | $0.95$ ($0.025$)                    |
|              | $0.99$ ($0.005$)                    |

Table 3: The twelve different simulation settings and their respective symbols used in Figure 3

Clustering Results

Figure 3 gives the results of the Toeplitz simulation. Each dot represents the average over all 1000 simulations of the median cluster size (on a natural log scale) and the average over all 1000 simulations of the reported number of clusters. The vertical lines represent the minimum and maximum cluster size of all 1000 simulations (on a natural log scale). The cluster size depends primarily on the baseline $\rho$ value, not the original cluster size. The horizontal line is the average of the cluster sizes over three simulation settings. Interestingly, the correlation cutoff for each cluster is reasonably constant. As seen in Table 4, the clustering results seem to be a function of the furthest observations being correlated by at least 0.5. Further analysis on this topic is suggested, but it is beyond the scope of the current work.

The case of $\rho = 0.99$ correlation warrants special consideration. For small sample sizes, the PAM algorithm finds the correct allocation of points each time. For the simulation with 100 observations in each cluster, PAM finds six clusters instead of three (resulting in clusters of size 50). Note that with such a strong correlation, there is very little noise we can add while ensuring that the resulting matrix is a correlation matrix. Therefore, the simulations for the $\rho = 0.99$ correlation setting are unsurprisingly similar across the 1000 replicates.
Figure 3: Each dot represents the average over all 1000 simulations of the median cluster size (on a natural log scale) and the average over all 1000 simulations of the number of clusters. The vertical lines represent the minimum and maximum cluster size of all 1000 simulations (on a natural log scale). The cluster size depends primarily on the baseline $\rho$ value, not the original cluster size. The horizontal line is the average of the cluster sizes over three simulation settings.

4.4 hub-Toeplitz Correlation

To assess simulating the hub-Toeplitz correlation structure using the parameter settings below we use Algorithm 4. All simulations were done in the three cluster setting with sample sizes of $(n_1 = 100, n_2 = 50, n_3 = 80)$. Recall that with the hub-Toeplitz correlation, the correlation values descend according to some power (here linearly) from a specified maximum to a specified minimum correlation.

| Scenario | Parameters |
|----------|------------|
| hTC1     | $\rho_1 \in (0.7 \to 0)$, $\rho_2 \in (0.7 \to 0)$, $\rho_3 \in (0.4 \to 0)$, $\epsilon_i \in \mathbb{R}^2$, $\|\epsilon_i\| = 0.23$ |
| hTC2     | $\rho_1 \in (0.7 \to 0.5)$, $\rho_2 \in (0.7 \to 0.6)$, $\rho_3 \in (0.4 \to 0.2)$, $\epsilon_i \in \mathbb{R}^2$, $\|\epsilon_i\| = 0.29$ |
| hTC3     | $\rho_1 \in (0.7 \to 0.5)$, $\rho_2 \in (0.7 \to 0.6)$, $\rho_3 \in (0.4 \to 0.2)$, $\epsilon_i \in \mathbb{R}^{25}$, $\|\epsilon_i\| = 0.29$ |
| hTC4     | $\rho_1 \in (0.7 \to 0.5)$, $\rho_2 \in (0.7 \to 0.6)$, $\rho_3 \in (0.4 \to 0.2)$, $\epsilon_i \in \mathbb{R}^2$, $\|\epsilon_i\| = 0.1$ |
| hTC5     | $\rho_1 \in (0.8 \to 0)$, $\rho_2 \in (0.75 \to 0)$, $\rho_3 \in (0.7 \to 0)$, $\epsilon_i \in \mathbb{R}^2$, $\|\epsilon_i\| = 0.19$ |

Clustering Results

For each of the scenarios, we simulated 1000 correlation matrices. We then clustered the data using PAM; the clustering results were assessed by determining the number of clusters the algorithm produced (truth was three clusters) as well as the concordance between the clustering results and the truth (1 gives perfect concordance).

As with the constant correlation, using the hub-Toeplitz structure, we can add noise that keeps clustering structure intact or that obscures enough of the structure to
After finding the median cluster size for each simulation, the average is taken across different original cluster sizes and across the 1000 simulations. The average resulting cluster size is given by the horizontal lines in Figure 3.

Because PAM was able to find the correct clusters for small samples using $\rho = 0.99$, only the simulations with clusters of size 100 are reported for $\rho = 0.99$.

Table 4: The resulting clusters are composed of objects that are correlated by no less than about 0.5

| Scenario | hTC1 | hTC2 | hTC3 | hTC4 | hTC5 |
|----------|------|------|------|------|------|
| min # clusters | 3    | 3    | 3    | 3    | 3    |
| median # clusters | 11   | 8    | 3    | 3    | 3    |
| max # clusters | 20   | 13   | 3    | 3    | 3    |
| median adj Rand | 0.320 | 0.4142 | 1    | 1    | 1    |

Table 5: Results from optimal number of clusters as well as the adjusted Rand. The original correlation structure had 3 clusters. A perfect allocation of points gives an adjusted Rand of 1.

make clusters indistinguishable. Recall, in the hub-Toeplitz structure, the correlations within a cluster degrade linearly (as opposed to exponentially in the Toeplitz structure of Section 3). For correlation structures that degrade all the way to zero (hTC1 and hTC5), the algorithm is able to discern the structure if the original correlations are large (hTC5). For correlation structures that degrade only a small amount (hTC2, hTC3, hTC4), the results are based on the amount of error and the dimension from which the noise vectors are selected.

5 Conclusion

We have developed an algorithm for adding noise, in a highly controlled manner, to a template correlation matrix in order to obtain a more realistic correlation matrix. Moreover, we have demonstrated how our general procedure can be tailored to a number of different correlation models (e.g., constant correlation, Toeplitz structure).

Our method allows for noisy correlation matrices which differ more from the initial template than the estimated correlation matrix based on simulated normal data. Using normal data produces a sample correlation matrix with limited and well-behaved (possibly unrealistic) differences from the original template correlation if the generated sample is large. If the generated sample is small, then the sample correlation matrix is not positive definite (i.e., most of the eigenvalues will be zero). Using uniform $[-1,1]$ deviates as random correlation values produces a matrix that is in general not even positive semidefinite. It can also create relationships between observations that are meaningless (e.g., a trio of observations where the first is highly correlated to the other two but the other two are negatively correlated).
Using a standard clustering algorithm, we have shown that simulated correlation matrices can be used to assess existing or novel statistical methodology. We provide the user with detailed algorithms to use on several standard clustering structures, as well as a general algorithm to apply to any correlation matrix for which the smallest eigenvalue can be reasonably estimated.

A Appendix

In this section we justify the crucial inequalities (15) and the limits (16). First observe that the Toeplitz matrix $T_n$ from (14) is simply the upper-left corner of the infinite Toeplitz matrix

$$T = \begin{pmatrix} 1 & \rho & \rho^2 & \rho^3 & \cdots \\ \rho & 1 & \rho & \rho^2 & \cdots \\ \rho^2 & \rho & 1 & \rho & \cdots \\ \rho^3 & \rho^2 & \rho & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

(25)

which induces a linear operator $T$ on the Hilbert space $\ell^2$ of all square-summable infinite sequences. Since the $ij$th entry of $T$ is the $(i-j)$th complex Fourier coefficient of the function $P_\rho(\theta) : [-\pi, \pi] \to \mathbb{R}$ defined by

$$P_\rho(\theta) = \sum_{n=-\infty}^{\infty} \rho^{|n|} e^{in\theta} = \frac{1 - \rho^2}{1 - \rho \cos \theta + \rho^2},$$

we conclude from [4, Thm. 1.9] that $T$ is a bounded selfadjoint operator whose spectrum equals the range of $P_\rho$ [11, Pr. 250] (note that $P_\rho(\theta)$ is the so-called Poisson kernel from the study of harmonic functions).

A short calculus exercise reveals that $P_\rho(\theta)$ achieves its maximum value $\frac{1+\rho}{1+\rho}$ at $\theta = 0$ and its minimum value $\frac{1-\rho}{1+\rho}$ at $\theta = \pm \pi$ (see Figure 4) from which we conclude

![Figure 4: The Poisson kernel $P_\rho(\theta)$ for $\rho = 0.2, 0.5, 0.8$. As $\rho \to 1^-$, the graphs spike sharply at $\theta = 0$ while tending rapidly to zero for $\theta$ away from 0. Intuitively, the functions $P_\rho(\theta)$ approximate a point mass (i.e., Dirac $\delta$-function) at $\theta = 0$ as $\rho \to 1^-$.](image-url)
that the spectrum of $T$ is precisely the closed interval $\left[\frac{1-\rho}{1+\rho}, \frac{1+\rho}{1-\rho}\right]$. By [4, Prop. 2.17], it follows that the spectrum (i.e., the set of eigenvalues) of $T_n$ is also contained in this interval. This establishes the inequalities (15). The limiting behavior (16) follows immediately from [4, Thm. 5.14].

References

[1] D. B. Allison, X. Cui, G. P. Page, and M. Sabripour, Microarray data analysis: from disarray to consolidation and consensus, Nature Reviews Genetics 7 (2005), no. 1, 55–65.

[2] John Barnard, Robert McCulloch, and Xiao-Li Meng, Modeling covariance matrices in terms of standard deviations and correlations, with application to shrinkage, Statistica Sinica 10 (2000), 1281–1311.

[3] Albrecht Böttcher and Sergei M. Grudsky, Spectral properties of banded Toeplitz matrices, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2005. MR 2179973 (2006k:47054)

[4] Albrecht Böttcher and Bernd Silbermann, Introduction to large truncated Toeplitz matrices, Universitext, Springer-Verlag, New York, 1999. MR 1724795 (2001b:47043)

[5] Kun Chen, Kehui Chen, Hans-Georg Müller, and Jane-Ling Wang, Stringing high-dimensional data for functional analysis, Journal of the American Statistical Association 106 (2011), 275–284.

[6] YounJeong Choi and Christina Kendziorski, Statistical methods for gene set co-expression analysis, Bioinformatics 25 (2009), 2780–2786.

[7] Alan R. Dabney and John D. Storey, Optimality driven nearest centroid classification from genomic data, PLoS ONE 10 (2007), e1002.

[8] PI Davies and NJ Higham, Numerically stable generation of correlation matrices and their factors, BIT 40 (2000), 640–651.

[9] Yaqian Guo, Trevor Hastie, and Robert Tibshirani, Regularized linear discriminant analysis and its application in microarrays, Biostatistics 8 (2007), no. 1, 86–100.

[10] Adam Hafdahl, Combing correlation matrices: simulation analysis of improved fixed-effects methods, Journal of Educational and Behavioral Statistics 32 (2007), 180–205.

[11] Paul Richard Halmos, A Hilbert space problem book, second ed., Graduate Texts in Mathematics, vol. 19, Springer-Verlag, New York, 1982, Encyclopedia of Mathematics and its Applications, 17. MR 675952 (84e:47001)

[12] J. Hardin, A. Mitani, L. Hicks, and B. VanKoten, A robust measure of correlation between two genes on a microarray, BMC Bioinformatics 8 (2007), no. 220, 220.
[13] J. Hardin and J. Wilson, A note on oligonucleotide expression values not being normally distributed, Biostatistics 10 (2009), 446–450.

[14] L. J. Heyer, S. Kruglyak, and S. Yooseph, Exploring expression data: Identification and analysis of coexpressed genes, Genome Research 9 (1999), 1106–1115.

[15] R. B. Holmes, On random correlation matrices ii the toeplitz case, Communications in Statistics - Simulation and Computation 18 (1989), 1151–1537.

[16] ______, On random correlation matrices, SIAM Journal of Matrix Analysis Applications 12 (1991), 239–272.

[17] Sehee Hong, Generating correlation matrices with model error for simulation studies in factor analysis: A combination of the tucker-koopman-linn model and wijsman’s a1 algorithm, Behavior Research Methods, Instruments & Computers 31 (1999), 727–730.

[18] Roger A. Horn and Charles R. Johnson, Matrix analysis, Cambridge University Press, Cambridge, 1990, Corrected reprint of the 1985 original. MR MR1084815 (91i:15001)

[19] Rui Hu, Xing Qiu, and Galina Glazko, A new gene selection procedure based on the covariance distance, Bioinformatics 25 (2010), 348–354.

[20] Song Huang, Tiejun Tong, and Hongyu Zhao, Bias-corrected diagonal discriminant rules for high-dimensional classification, Biometrics 66 (2010), 1096–1106.

[21] Harry Joe, Generating random correlation matrices based on partial correlations, Journal of Multivariate Analysis 97 (2006), 2177–2189.

[22] L. Kaufman and P. Rousseeuw, Finding groups in data, Wiley, New York, 1990.

[23] Kyung In Kim and Mark A van de Wiel, Effects of dependence in high-dimensional multiple testing problems, BMC Bioinformatics 9 (2008), 114.

[24] Piotr Kraj, Ashok Sharma, Nikhil Garge, Robert Podolsky, and Richard A. McIndoe, ParaKMeans: Implementation of a parallelized K-means algorithm suitable for general laboratory use, BMC Bioinformatics 9 (2008), 200.

[25] Johann Kraus and Hans Kestler, A highly efficient multi-core algorithm for clustering extremely large datasets, BMC Bioinformatics 11 (2010), 169.

[26] Peter Langfelder and Steve Horvath, Wgcna: an r package for weighted correlation network analysis, BMC Bioinformatics 9 (2008), 559.

[27] Peter Langfelder, Bin Zhang, and Steve Horvath, Defining clusters from a hierarchical cluster tree: the dynamic tree cut package for r, Bioinformatics 24 (2008), no. 5, 719–720.
[28] Daniel Lewandowski, Dorota Kurowicka, and Harry Joe, *Generating random correlation matrices based on vines and extended onion method*, Journal of Multivariate Analysis **100** (2009), 1989–2001.

[29] Xuefeng Li and Michael J. Daniels, *A new algorithm for simulating a correlation matrix based on parameter expansion and reparametrization*, Journal of Computational and Graphical Statistics **15** (2006), 897–914.

[30] George Marsaglia and Ingram Olkin, *Generating correlation matrices*, SIAM Journal of Scientific and Statistical Computing **5** (1984), 470–475.

[31] Robb Muirhead, *Aspects of multivariate statistical theory*, Wiley, New York, 1982.

[32] Barry L. Nelson and David Goldsman, *Comparisons with a standard in simulation experiments*, Management Science **47** (2001), 449–463.

[33] Chi Tim Ng and Harry Joe, *Generating random ar(p) and ma(q) toeplitz correlation matrices*, Journal of Multivariate Analysis **101** (2010), 1532–1545.

[34] Herbert Pang, Tiejun Tong, and Hongyu Zhao, *Shrinkage-based diagonal discriminant analysis and its applications in high-dimensional data*, Biometrics **65** (2009), 1021–1029.

[35] Gordon Rae, *A FORTRAN 77 program for generating sample correlation matrices*, Educational and Psychological Measurement **57** (1997), 189–192.

[36] W.M. Rand, *Objective criteria for the evaluation of clustering methods*, Journal of the American Statistical Association **66** (1971), 846–850.

[37] D. M. Rocke, R. Ideker, O. Troyanskaya, J. Quackenbush, and J. Dopazo, *Papers on normalization, variable selection, classification or clustering of microarray data*, Bioinformatics **25** (2009), no. 6, 701–702.

[38] Feng Tai and Wei Pan, *Incorporating prior knowledge of gene functional groups into regularized discriminant analysis of microarray data*, Bioinformatics **23** (2007), 3170–3177.

[39] David Tritchler, Elena Parkhomenko, and Joseph Beyene, *Filtering genes for cluster and network analysis*, BMC Bioinformatics **10** (2009), 193.

[40] M. J. van der Laan and K. S. Pollard, *A new algorithm for hybrid hierarchical clustering with visualization and the Bootstrap*, Journal of Statistical Planning and Inference **117** (2003), 275–303.

[41] Daniela M. Witten and Robert Tibshirani, *Covariance-regularized regression and classification for high dimensional problems*, Journal of the Royal Statistical Society, B **71** (2009), 615–636.

[42] K.Y. Yeung and W.L. Ruzzo, *An empirical study on principal component analysis for clustering gene expression data*, Bioinformatics **17** (2001), 763–774.
[43] Bin Zhang and Steve Horvath, *A general framework for weighted gene co-expression network analysis*, Statistical Applications in Genetics and Molecular Biology 4 (2005), no. 1, Article 17.

[44] Xiao Zhang, W. John Boscardin, and Thomas R. Belin, *Sampling correlation matrices in Bayesian models with correlated latent variables*, Journal of Computational and Graphical Statistics 15 (2006), 880–896.

[45] Verena Zuber and Korbinian Strimmer, *Gene ranking and biomarker discovery under correlation*, Bioinformatics 25 (2009), 2700–2707.

Partially supported by National Science Foundation Grants DMS-0638789 and DMS-1001614.