WISDoM: a framework for the Analysis of Wishart distributed matrices

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WISDoM (Wishart Distributed Matrices) is a new framework for the characterization of symmetric positive-definite matrices associated to experimental samples, like covariance or correlation matrices, based on the Wishart distribution as a null model. WISDoM can be applied to tasks of supervised learning, like classification, even when such matrices are generated by data of different dimensionality (e.g. time series with same number of variables but different time sampling). In particular, we show the application of the method for the ranking of features associated to electro encephalogram (EEG) data with a time series design, providing a theoretically sound approach for this type of studies.

I. INTRODUCTION

High-dimensionality time-structured data are extremely common in fields such as finance, biophysics and complex systems. Very often, experimental limitations lead to uneven sampling (i.e. a different number of time points in terms of frequency or duration) and this poses problems for many types of analysis (e.g. sample classification). As a consequence, clipping or padding techniques are applied, altering the underlying temporal structure. In recent years, studies on such data have seen an increasing popularity in a wide range of fields, from functional magnetic resonance imaging (fMRI) [1–3] to time series exploration for critical transition prediction in clinical scenarios [4, 5]. The common goal of this type of research is to develop models and algorithms capable of reaching the highest possible classification and prediction performances, for diagnostic and real time applications, while unveiling underlying information about a system. Reproducibility and generalization issues of commonly applied methods are in part caused by ad-hoc preprocessing of data, due to the lack of simple null models, often substituted by reshuffling-based null models. We introduce a theoretically sound method based on the statistical distribution of symmetric positive-definite matrices (i.e. covariance and correlation matrices) extracted from data, using the Wishart distribution as a null model, as a possible way to overcome some of the aforementioned issues. Properties of distribution of random symmetric positive-definite matrices have proven to be useful in fields such as condensed matter, especially in the study of disordered systems [6]. The WISDoM method exploits the properties of the Wishart distribution in order to compute limit distributions for the classes of samples in a classification problem, and a log-likelihood based score is defined for the single variables to quantify their relevance in the classification task.

II. THE WISHART DISTRIBUTION

The Wishart distribution $W_p(n, \Sigma)$ is a probability distribution of random nonnegative-definite $p \times p$ matrices that is used to model random covariance matrices.

The parameter $n$ is the number of degrees of freedom (e.g. the number of points in the time series), and $\Sigma$ is a nonnegative-definite symmetric $p \times p$ matrix (with $p$ the number of variables, or features, of the time series) called the scale matrix.

Def. Let $X_1...X_n$ be $N_p(0, \Sigma)$ distributed vectors, forming a data matrix $p \times n$, $X = [X_1...X_n]$. The distribution of a $p \times p$, $M = XX^T = \sum_{i=1}^{n} X_i X_i^T$ random matrix is a Wishart distribution. [7]

We have then by definition:

$$M \sim W_p(n, \Sigma) \sim \sum_{i=1}^{n} X_i X_i^T \quad X_i \sim N_p(0, \Sigma)$$  (1)

so that $M \sim W_p(n, \Sigma)$ is the distribution of a sum of $n$ rank-one matrices defined by independent normal $X_i \in \mathbb{R}^p$ with $E(X) = 0$ and $\text{Cov}(X) = \Sigma$.

In particular, it holds for the present case:

$$E(M) = nE(X_i X_i^T) = n\text{Cov}(X_i) = n\Sigma$$  (2)

A. PDF Computation for Invertible $\Sigma$

In general, any $X \sim N(\mu, \Sigma)$ can be represented as

$$X = \mu + AZ, \quad Z \sim N(0, I_p)$$  (3)
so that
\[ \Sigma = \text{Cov}(X) = ACov(Z)A' = AA' \quad (4) \]

The easiest way to find A in terms of \( \Sigma \) is the LU-decomposition, which finds a unique lower diagonal matrix A with \( A_{ii} \geq 0 \) such that \( AA' = \Sigma \).

Then by (1) and (4) with \( \mu = 0 \) we have:
\[ W_p(n, \Sigma) = \frac{1}{2^{p/2} \Gamma_p \left( \frac{n}{2} \right)} | \Sigma |^{-p/2} \exp \left[ -\frac{1}{2} tr(\Sigma^{-1} M) \right] \]
\[ f(M, n, \Sigma) = \frac{1}{2^{p/2} \Gamma_p \left( \frac{n}{2} \right)} | \Sigma |^{-p/2} \exp \left[ -\frac{1}{2} tr(\Sigma^{-1} M) \right] \]
so that \( f(M, n, \Sigma) = 0 \) unless \( M \) is symmetric and positive-definite. \( [8] \)

Note that in (6) we define \( \Gamma_p(\alpha) \) as the generalized gamma function:
\[ \Gamma_p(\alpha) = \pi^{\alpha p - \frac{1}{2} p(p-1)} \prod_{i=1}^{p} \Gamma \left( 2\alpha + 1 - \frac{i}{2} \right) \quad (7) \]

**B. Estimation of the Wishart Parameters from Empirical Covariance**

We justify the use of the Wishart distribution under the assumption of Multivariate Gaussian distributed data scenarios. This kind of assumption is indeed generally good for a wide range of problems. Furthermore, the use of the average covariance matrix (obtained for all the elements of one class) to compute the scale matrix for the class estimated distribution will be proven to be a good approximation of a complete Bayesian model.

This is done by showing that the Wishart Distribution is the conjugate prior of a multivariate Gaussian distribution, such as the Gamma distribution for the univariate Gaussian case. By considering a Gaussian model with known mean \( \mu \), so that the free parameter is the variance \( \sigma^2 \), in [9], the likelihood function is defined as follows:
\[ p(X_1...X_n | \sigma^2) \propto (\sigma^2)^{-\frac{n}{2}} \exp \left( -\frac{1}{2\sigma^2} n(X - \mu)^2 \right), \quad (8) \]
\[ (X - \mu)^2 = \frac{1}{n} \sum_{i=1}^{n} (X_i - \mu)^2 \quad (9) \]

The conjugate prior is an inverse Gamma distribution. Recall that \( \theta \) has an inverse Gamma distribution with parameters \((\alpha, \beta)\) when \( \frac{1}{\theta} \sim \text{Gamma}(\alpha, \beta) \).

The density then takes the form
\[ \pi_{\alpha, \beta}(\theta) \propto \theta^{-(\alpha+1)} e^{-\frac{\beta}{\theta}} \quad (10) \]

Using this prior, the posterior distribution of \( \sigma^2 \) is given by
\[ p(\sigma^2 | X_1...X_n) \sim \text{InvGamma}(\alpha + \frac{n}{2}, \beta + \frac{n}{2}(X - \mu)^2) \quad (11) \]

In the multidimensional setting, the inverse Wishart takes the place of the inverse Gamma. It has already been stated that the Wishart distribution is a distribution over symmetric positive semi-definite \( d \times d \) matrices \( W \). A more compact form of the density is given by
\[ \pi_{\nu_0, S_0}(W) \propto |W|^{-\frac{(nu_0 + d - 1)}{2}} \exp \left( -\frac{1}{2} tr(S_0^{-1} W) \right), \quad (12) \]
\[ |W| = \det(W) \quad (13) \]
where the parameters are the degrees of freedom \( \nu_0 \) and the positive-definite scale matrix \( S_0 \).

If \( W^{-1} \sim \text{Wishart}(\nu_0, S_0) \) we can then state that \( W \) has an Inverse Wishart Distribution, whose density has the form
\[ \pi_{\nu_0, S_0}(W) \propto |W|^{-\frac{(nu_0 + d - 1)}{2}} \exp \left( -\frac{1}{2} tr(S_0^{-1} W) \right), \quad (14) \]

Let \( X_1...X_n \) be \( N(0, \Sigma) \) distributed observed data. Then an inverse Wishart prior multiplying the likelihood \( p(X_1...X_n | \Sigma) \) yields
\[ p(X_1...X_n | \Sigma) \pi_{\nu_0, S_0}(\Sigma) \propto \]
\[ |\Sigma|^{-\frac{n}{2}} \exp \left( -\frac{n}{2} tr(\Sigma^{-1} \mathbf{S}) \right) |\Sigma|^{-\frac{(nu_0+d+1)}{2}} \exp \left( -\frac{1}{2} tr(S_0^{-1} \Sigma) \right) \]
\[ = |\Sigma|^{-\frac{(nu_0+d+1)}{2}} \exp \left( -\frac{1}{2} tr((\mathbf{S} + S_0) \Sigma^{-1}) \right) \quad (16) \]
where \( \mathbf{S} \) is the empirical covariance:
\[ \mathbf{S} = \frac{1}{n} \sum_{i=1}^{n} X_iX_i^T \quad (18) \]

Thus, an posteriori distribution with the form
\[ p(\Sigma | X_1...X_n) \sim \text{InvWishart}(\nu_0 + n, n\mathbf{S} + S_0) \quad (19) \]

is obtained.

Similarly, it can be stated that for the inverse covariance (precision) matrix \( \Sigma^{-1} \) the conjugate prior is a Wishart distribution.

**III. FEATURE RELEVANCE ESTIMATION THROUGH LIKELIHOOD RATIOS**

**A. Class-Wise Estimated Distribution**

The core idea of the WISDoM method is to represent each element undergoing classification as a covariance
matrix of its features. Nominally, each element can be characterized by the covariance matrix extracted by the repeated observations of the vector of its features, for example derived by a time series. The aim is to use the free parameters of the Wishart distribution (the scale matrix \( S_0 \) and the number \( n \) of the degrees of freedom, as shown in (3)) to compute an estimation of the distribution for a certain class of elements, and then assign a single element to a given class by computing a log-likelihood between the element being analyzed and all the classes. Furthermore, a score can be assigned to each feature by estimating the variation in terms of log-likelihood, due to its removal from the feature set. If the removal of a feature causes significant increase (or decrease) in the log-likelihood, it can be stated that such feature is highly representative of the system analyzed. Thus, the WISDoM approach allows not only to assign a given element to a class, but also to identify the features with the highest relevance in the classification process.

Covariance matrices are a good choice for a distance metric in a classification task, both for the way they represent a system and for the property that the average of a set of covariance matrices is a covariance matrix itself. If each element of a given class \( C \) is represented by a covariance matrix \( \Sigma \) of its features, this property allows us to estimate a distribution for the class by choosing

\[ S_0 = \hat{\Sigma}_C = \frac{1}{N} \sum_{i=1}^{N} \Sigma_i \]  

The other necessary parameter for the estimation is the number of degrees of freedom \( n \). Assume that an \( X_i = (x_1, \ldots, x_p) \) vector of \( p \) features is associated to each element \( i \) of a given class, while having \( n \) observations for this vector. The covariance matrix \( \Sigma_i \) computed over the \( n \) observations will represent the interactions between the features of element \( i \). The number of degrees of freedom \( n \) of the Wishart distribution is then given by the number of times \( X_i \) is observed.

Let us give an example tied to functional MR brain imaging in order to further clarify the concepts being introduced. An image of patient \( i \)'s brain is acquired; as usual these images are divided in a certain number \( p \) of zones (voxel, pixel etc.), each zone being sampled \( n \) times over a given time interval in order to observe a certain type of brain activity and functionality. In this example, the features contained in vector \( X_i = (x_1, \ldots, x_p) \) associated to patient \( i \) are indeed the zones chosen to divide \( i \)'s brain image, each zone having been sampled \( n \) times during an acquisition interval. The correlation \( p \times p \) matrix \( \Sigma_i \) computed for \( i \)'s observation is then representative of the functional correlation between the \( p \) zones of \( i \)'s brain. Repeating this procedure for the \( N \) patients of a known class \( C \) (i.e. a diagnostic group) and computing the \( \hat{\Sigma}_C \) scale matrix for the class, will allow us to estimate a Wishart distribution for that class and draw samples from it.

### B. Log-Likelihood Ratio Score

After defining how to represent classes distribution, WISDoM allows to compute the log-likelihood of each element to belong to one of the classes. Moreover, if dimensionality reduction is needed, WISDoM allows to compute the variation of log-likelihood ratio scores due to the removal of features, singularly or in groups, thus estimating how much the classification performance changes. Uninformative features can thus be pruned. The whole process can be seen as a feature transformation, mapping the covariance matrix \( \Sigma \) of subject \( i \) to a score vector formed by the change in log-likelihood for each feature.

**Complete Matrix Score**

The scoring system introduced for the WISDoM Classifier relies upon computing the log-likelihood of a matrix \( \Sigma_i \) with respect to the Wishart distribution estimated for a class \( C \), using \( \hat{\Sigma}_C \) as the scale matrix. If a problem concerning two given classes \( A \) and \( B \) is taken into account, the score assigned to each \( \Sigma_i \) can be defined as follows:

\[
score_i = \log P_W(\Sigma_i | n, \hat{\Sigma}_A) - \log P_W(\Sigma_i | n, \hat{\Sigma}_B) \tag{21}
\]

Where \( \hat{\Sigma}_{A,B} \) are the scale matrix computed for the classes \( A, B \) and \( \log P_W(\Sigma_i | n, \hat{\Sigma}_{A,B}) \) can be seen as the logarithm of the probability of \( \Sigma_i \) belonging to the Wishart distribution estimated for one of the two classes \( A, B \).

**Single Feature Score**

WISDoM allows to obtain information about the features used for classification by reducing the matrix \( A \) to its principal submatrices. A resume on principal submatrix algebra for positive-definite matrices can be found in the Appendix. An important property for the principal submatrices of a symmetric positive definite matrix is that any \((n-k) \times (n-k)\) partition is also symmetric and positive definite.

Such properties can be used to reduce both a class scale matrix \( \Sigma_C \) and any \( \Sigma_i \) matrix, in order to study its deviation from a class’s estimated Wishart distribution derived from the removal of one of its components (the features contained in vector \( X_i = (x_1, \ldots, x_p) \), from which the matrix \( \Sigma_{i,p \times p} \) is computed). Iterating this process over all the features (i.e. analyzing all the \((p-1) \times (p-1)\) principal submatrices of \( \Sigma_i \) and \( \Sigma_C \)) allows the method to assign a score to each feature, representing its weight in the decision for \( \Sigma_i \) to be assigned to one class or another. Note that for such an order of principal submatrices, the process will reduce the \( \Sigma_{i,p \times p} \) matrix to a score vector of length \( p \) for each element \( i \) undergoing
the classification. Let us now introduce the following notation in order to define the score assigned for each of the \(x_p\) features of the vector \(X_i = (x_1, ..., x_p)\). Let \(\Sigma_j\) be a principal submatrix of order \((p - 1)\), of the matrix \(\Sigma\) computed on the observation of \(X_i = (x_1, ..., x_p)\) for subject \(i\), obtained by the deletion of the \(j^{th}\) row and the \(j^{th}\) column, with \(1 \leq j \leq p\). Let \(\hat{\Sigma}_{C_j}\) be a principal submatrix of order \((p - 1)\), of the matrix \(\hat{\Sigma}_C\) computed for the class \(C\) obtained by the deletion of the \(j^{th}\) row and the \(j^{th}\) column, with \(1 \leq j \leq p\). The score assigned to each feature of \(X_i = (x_1, ..., x_p)\) is then given by eq. (23).

\[
\text{Score}_j(C) = \Delta \log P_{W_j}(C) = \log P_{W}(\Sigma, n | \hat{\Sigma}_{C}, n) - \log P_{W}(\Sigma_j, n | \hat{\Sigma}_{C_j}, n) \tag{23}
\]

In other terms, each partition \(\Sigma_j\) represents the matrix \(\Sigma\) without the elements tied to feature \(x_j\) (the elements in row \(j\) and column \(j\) of \(\Sigma\)). Computing the variation in terms of log-likelihood between the estimated Wishart distribution for the class and the estimated wishart distribution for the class without component \(j\), allows to gain information about which feature is more relevant. Note that this kind of scoring is class-dependent. Computing this score vector with respect to all the classes \(C_1, ..., C_n\) of a given problem and computing a score ratio will allow element \(i\), after a suitable training, to be assigned to the most likely of the classes while retaining information on which features are the most important.

Let us introduce a 2-class example, in order to show how this kind of result might be obtained. Let \(C_1\) and \(C_2\) be the two classes of a given problem. Let a set of \(N\) matrices \(\Sigma_i\) be a set of correlation matrices computed for \(N\) subjects whose class is known. Let \(\hat{\Sigma}_{C1}\) and \(\hat{\Sigma}_{C2}\) be the scale matrices computed as seen in eq. (20), used to estimate the Wishart distribution for both classes \(C_1\) and \(C_2\), and \(\hat{\Sigma}_{C1j}\) and \(\hat{\Sigma}_{C2j}\) their \((p - 1)\) order partitions, as in eq. (23).

If from each matrix \(\Sigma_i\) the score vector is computed as in eq. (22), with respect to both classes \(C_1, C_2\), an inter-class log-likelihood ratio vector can be obtained by assigning to each feature a score defined as follows:

\[
\text{Ratio}_j = \Delta \log P_{W_j}(C_1) - \Delta \log P_{W_j}(C_2) \tag{24}
\]

Training a classifier on a set of \(N\) elements whose classes are known, after each matrix \(\Sigma_i\) (and as a consequence each feature vector \(X_i\)) has undergone the transformations defined in eq. (23) and (24), yields an improvement in performance for certain problems, as it will be shown later.

A new element will be classified according to its transformed ratio vector given by eq. (24), thus simultaneously retaining information about its class’s most significant features: the score assigned to each feature is a measure of how much its removal impacts on the decision to assign each matrix \(\Sigma_i\) to one class or another. A generalization to \((p - n)\) order transformations can be found in the Appendix.

IV. WISDOM FOR EEG EYE STATE DETECTION

An application of the WISDoM method to electroencephalogram (EEG) time series data for eye state detection will be shown in this section.

A. Dataset

The dataset used was downloaded from the UCI Machine Learning Repository (http://archive.ics.uci.edu/ml/). This dataset has been chosen for many reasons: it’s openly accessible, contains records from 14 electrodes with standard headset placement (fig. 1), thus making the features of our problem directly linked to brain topology and a published classification performance benchmark on the dataset exists [10]. The data consisted in a series of 14980 time points, sampled for each one of the 14 electrodes and labelled with a 1 or a 0 to mark whether the eyes of the subject are open or closed at that time point.

To make data suitable for the WISDoM pipeline, the time series has been split into batches according to eye state changes. In this way, a correlation matrix can be extracted for each batch (the "elements" for this classification problem) interpreting each time point as an observation. The length of each batch is thus used when computing the degrees of freedom of each class Wishart distribution during training. A total of 140 batches with various lengths, 70 with eye state 1 and 70 with eye state 0, were obtained from the dataset.
B. Pipeline

The representative matrix for each class is computed as the average (weighted on the length of each batch) of matrices of the elements belonging to eye state 0 or eye state 1, excluding the element to be predicted in a Leave One Out fashion in order to avoid overfitting. By doing this, we verify that the method is independent from the sampling window chosen when applied to time series data, with the only constraint that the length of such window cannot be less than the number of the features of the system.

After undergoing feature score computation, a stochastic grid search on a set of classifiers has been performed in order to obtain the best prediction performance with the transformed features. All the classification tasks are validated through a 10-fold crossvalidation. Versions and references for all Python packages used can be found in Appendix and at [11–18].

C. Results

We first tried to assess eye state using complete matrix score, as in eq. (21). Classifiers reported in fig. 2 were trained and tuned, with the aim of obtaining the best performance possible. However, in this scenario the resulting classification performances were poor, reaching an accuracy of ~60% in the best cases. We then proceeded to compute single feature scoring, as in eq.(23), obtaining a feature transformation. As in fig. 2, different classifiers belonging to two main categories (decision trees and linear classifiers) have been trained on the transformed features. The best performance has been achieved with a C-support Vector Machine (Python 3.6 SciKitLearn implementation) resulting in a 84.6% ROC AUC score and an accuracy score of 84.3%, better than the benchmark of 83.5% accuracy set by Rajesh Kanna et al.[10].

To assess which features contain the largest amount of useful information for prediction, a set of single feature C-SVM classifications has been performed (fig.3).

This allows to immediately identify which electrodes are the most useful in the eye state prediction task; the ranking obtained can be further exploited to evaluate prediction performance as a function of the number of ranked features used for classification. A performance of 75% accuracy is obtained by using only the top three ranked electrodes, unveiling that it is possible to retain an acceptable amount of accuracy while greatly reducing the dimensionality of the classification task. In fig. 4 we report an effect-size based ranking of the features, to evaluate classification performances at an increasing number of ranked features used by the C-SVM. It can be seen that the first two features ranked (electrodes T8 and F8) are the same obtained by the ranking in fig.3, contributing to big jumps in the performance landscape. This highlights the importance of the information recorded by these two electrodes about the state of the whole system.

Figure 2: Performance comparison of different classifiers on the WISDoM transformed features. The classifiers are reported as follows: RFC: Random Forest Classifier [19], DTC: Decision Tree Classifier[20, 21], ADA: ADA Boosting Tree Classifier [22, 23], LDA: Linear Discriminant Analysis Classification [24], LogReg: Logistic Regression Classifier [25], Perc: Perceptron Classifier [26], SVM: C-Support Vector Machine [27, 28]. All classifiers are SciKitLearn implementations.

Figure 3: Feature ranking based on each feature SVM classification capability in terms of ROC AUC score. Temporal (T8) and outer frontal (F8, F7) electrodes seems to convey the most important signals for eye state prediction.
V. DISCUSSION

The WISDoM framework is introduced: a system for modelling symmetric positive definite matrices, such as covariance and correlation matrices, used in a wide array of problems, especially prediction and classification tasks with a variety of data typologies. Representing each element to be classified as the covariance/correlation matrix of its features allows for the Wishart distribution to be used as a null model, allowing to compare datasets with same number of features but of different sampling size. This property makes the WISDoM method suitable for problems with non-homogeneous data size, for example time series with uneven lengths, missing points or irregularly sampled data. We show that a feature transformation based on WISDoM scores can be used for feature dimensionality reduction, sometimes allowing for enhanced classification and prediction performances. The method has been tested on the EEG eye state prediction dataset of the open UCI Machine Learning Repository, surpassing the previous classification benchmark and giving useful insights on the minimum number and location of electrodes needed to record sufficient information for the task.

Author contribution

EG, CM and DR designed the research. CM and EG analyzed the data and implemented the method. CM, DR and EG wrote the paper.
VI. APPENDIX

A. Visualizing the Wishart Distribution

The Wishart distribution is a generalization to multiple dimensions of the chi-squared distribution, or in the case of non-integer degrees of freedom, of the gamma distribution.

We show in fig. 5 that for a 1-dimensional and equal to 1 Σ scale matrix, the Wishart distribution \( W_1(n, 1) \) is equivalent to the \( \chi^2(n) \) distribution.

![Figure 5: Monodimensional Wishart Distribution and \( \chi^2(n) \) distribution comparison](image)

Save for this simple case, being the Wishart a distribution over matrices, it is a generally hard task to visualize it as a density function. Samples can be however drawn from it and the eigenvectors and eigenvalues of the resulting sampled matrix can be exploited to define an ellipse.

An example of this technique is shown in fig. 6. A set of five sampled matrices is drawn for each plot. The upper plots show sampling for Wishart distributions with \( n \) \( \text{degfreedom} = 80 \), while the lower plots show sampling for Wishart distributions with \( n \) \( \text{degfreedom} = 10 \) in order to show the effects of varying both the scale matrix and the number of degrees of freedom. Note that for \( \Sigma = I_2 \) (left plot in fig. 6) the sample would look on average like circles. The scale matrix for the right-most plot is \( \Sigma = \begin{bmatrix} 4 & 3 \\ 3 & 4 \end{bmatrix} \).

![Figure 6: Plot of eigenvalue and eigenvectors defined ellipses, drawn from different Wishart distributions.](image)

B. Principal Submatrices

**Def.** Let \( A \) be an \( n \times n \) matrix. A \( k \times k \) submatrix of \( A \) formed by deleting \( n-k \) rows of \( A \), and the same \( n-k \) columns of \( A \), is called principal submatrix of \( A \). The determinant of a principal submatrix of \( A \) is called a principal minor of \( A \).

Note that the definition does not specify which \( n-k \) rows and columns to delete, only that their indices must be the same.

Let us introduce a \( 3 \times 3 \) example.

For a general matrix \( A_{3 \times 3} \)

\[
A = \begin{bmatrix}
  a_{11} & a_{12} & a_{13} \\
  a_{21} & a_{22} & a_{23} \\
  a_{31} & a_{32} & a_{33}
\end{bmatrix}
\]

there are three **first order principal minors**:

- \( |a_{11}| \) formed by deleting the last two rows and columns
- \( |a_{22}| \) formed by deleting the first and third rows and columns
- \( |a_{33}| \) formed by deleting the first two rows and columns

There are three **second order principal minors**:

- \( \begin{vmatrix}
  a_{11} & a_{12} \\
  a_{21} & a_{22}
\end{vmatrix} \) formed by deleting column 3 and row 3
- \( \begin{vmatrix}
  a_{11} & a_{13} \\
  a_{31} & a_{33}
\end{vmatrix} \) formed by deleting column 2 and row 2
- \( \begin{vmatrix}
  a_{22} & a_{23} \\
  a_{32} & a_{33}
\end{vmatrix} \) formed by deleting column 1 and row 1

There’s one **third order principal minor**, namely \( |A| \).
For the sake of completion, we also recall the following definition.

**Def.** Let $A$ by an $n \times n$ matrix. The $k^{th}$ order principal sub-matrix of $A$ obtained by deleting the last $n - k$ rows and columns of $A$ is called the $k^{th}$ order **leading principal submatrix** of $A$, and its determinant is called the $k^{th}$ order **leading principal minor** of $A$.

C. Generalizing to $(p - n)$ Order Transformations

As previously seen, transforming all the $(p - 1) \times (p - 1)$ principal submatrices of $\Sigma_i$ by eq.(23), yields a vector of score of length $p$ for each element $i$. Anyway, for any $n < p$, a number of principal submatrices of $\Sigma_i$ can be obtained. These kind of submatrices can be used to gain information about the weight of $n$ simultaneously deleted features on the system structure and classification. Let us introduce an example for $(p - 2)$ order submatrices. Let $\Sigma_{jk}$ be a principal submatrix of order $(p - 2)$, of the matrix $\Sigma_i$ computed on the observation of $X_i = (x_1, ..., x_p)$ for subject $i$, obtained by the deletion of the $j^{th}$ row and the $j^{th}$ column and the $k^{th}$ row and the $k^{th}$ column, with $1 \leq j, k \leq p$. Let $\Sigma_{Cjk}$ be a principal submatrix of order $(p - 2)$, of the matrix $\Sigma_{Cjk}$ computed for the class $C$ obtained by the deletion of the $j^{th}$ row and the $j^{th}$ column and the $k^{th}$ row and the $k^{th}$ column, with $1 \leq j, k \leq p$.

Then, eq.(23) becomes:

\[
\text{Score}_{jk}(C) = \Delta \log P_{W|jk}(C) = \\
\log P_{W}(\Sigma, n | \Sigma_{C}, n) - \log P_{W}(\Sigma_{jk}, n | \Sigma_{Cjk}, n)
\]

(27)

in this case, a score is assigned to each coupling of the features $j, k$, and transformation (27) will yield not a vector, but a $p \times p$ matrix with diagonal elements equals to the scores obtained by (23), being the iteration with $j = k$ the coupling of the $j$ feature with itself. Non-diagonal elements represent the score of the coupling of feature $j$ with feature $k$. A notable characteristic of $(p - 2)$ order transformations for correlation matrices, is that the informative content after such an order of transformation is comparable to that of the original correlation matrix. It can thus be stated that the $(p - 2)$ order transformed correlation matrix seems to be equivalent to the original correlation matrix under an affine transformation.

D. Software Versions

References: [11–18]

- Python Version 3.6.2
- SciPy Version 0.19.14
- Pandas Version 0.25.3
- MatPlotLib Version 3.0.3
- NumPy Version 1.13.3
- SimPy Version 3.0.11
- Seaborn Version 0.9.0