Abstract: We present a method for the simultaneous Bayesian learning of the correlation matrix and graphical model of a multivariate dataset, using Metropolis-within-Gibbs inference. Here, the data comprises measurement of a vector-valued observable, that we model using a high-dimensional Gaussian Process (GP), such that, likelihood of GP parameters given the data, is Matrix-Normal, defined by a mean matrix and between-rows and between-columns covariance matrices. We marginalise over the between-row matrices, to achieve a closed-form likelihood of the between-columns correlation matrix, given the data. This correlation matrix is updated in the first block of an iteration, given the data, and the (generalised Binomial) graph is updated in the second block, at the partial correlation matrix that is computed given the updated correlation. We also learn the 95% Highest Probability Density credible regions of the correlation matrix as well as the graphical model of the data. The difference in the acknowledgement of measurement errors in learning the graphical model, is demonstrated on a small simulated dataset, while the large human disease-symptom network—with > 8,000 nodes—is learnt using real data. Data on the vino-chemical attributes of Portugese red and white wine samples are employed to learn the correlation structure and graphical model of each dataset, to then compute the distance between the learnt graphical models.

Keywords and phrases: Graphical models, Matrix-variate Normal, Metropolis-within-Gibbs, Hellinger metric.
is then modelled using a high-dimensional Gaussian Process, rendering the likelihood, \( k + 1 \)-variate Tensor Normal. However, a high-dimensional graph showing the correlation structure amongst the multiple components of a general tensor-shaped data set, would not be easy to visualise or interpret.

Instead, in this paper, we focus on making Bayesian inference on the correlation structure—and simultaneously learn the graphical model—of a multivariate, matrix-shaped data set. Our aim is to advance a method that treats the correlation matrix and graph, each as a random variable, and learn both given the data, along with well-defined uncertainties, namely, 95% Highest Probability Density credible regions, while acknowledging possible errors of measurement. It is to this effect that we perform a Metropolis-within-Gibbs-based Bayesian inference (Robert and Casella, 2004), on the correlation matrix given the data, and on the graph given the updated correlation.

Often, in real-life applications, different matrix-shaped data sets are realised under different experimental conditions. With the aim of learning the difference between the underlying correlation structures of a pair of such datasets, we will find the distance between pairs of the learnt graphical models, given the respective dataset. So if we consider a data that is a 3rd-ordered tensor, (i.e. is cuboid-shaped data) to be built of multiple measurements of a matrix-valued variable—where each such measurement is realised at a distinct experimental condition—we can compute the distance between pairs of graphical models learnt given the respective matrix-shaped data. This distance will then tell us about the independence of the probability density functions that each such data is sampled from. In particular, we implement the Hellinger distance (Banerjee et al., 2015; Matusita, 1953) between the graphical models; to be precise, the Hellinger metric computes the distance between two probability densities—in our implementation, we find the pairwise Hellinger distance between the posterior probability densities of the graphical models, given the respective matrix-shaped data.

Our learnt graphical model of the given data, comprises a set of random inhomogeneous graphs (Frieze and Karonski, 2016) that lie within the credible regions that we define in this paper, where each such graph is a generalisation of a Binomial graph (Frieze and Karonski, 2016), in which the probability of existence of the edge between a given pair of vertices is dependent on the partial correlation of the components of the observable vector corresponding to these vertices, where the partial correlation matrix is itself computed using the correlation matrix that is updated given the data at hand, within a Metropolis-within-Gibbs-based Bayesian inference scheme (Robert and Casella, 2004). We learn the between-columns correlation of the multivariate data, by modelling the latter using a high-dimensional Gaussian Process (GP), such that the likelihood of the parameters of this GP given the data, is matrix-normal. Thus, the inferred set of generalised Binomial random graphs that represent the graphical model given the data, manifests the uncertainty in the learnt graphical model, while acknowledging possible errors in measurement of the observable.

Bayesian learning of Gaussian undirected graphs typically involves invoking conjugacy. To be precise, a Hyper-Inverse-Wishart prior is imposed on the covariance matrix of the data, as this then allows for a Hyper-Inverse-Wishart posterior of the covariance, which in turn implies that the marginal posterior of of any clique is Inverse-Wishart—a known, closed-form density (Dawid and Lauritzen, 1993; Lauritzen, 1996). (This follows directly from the Inverse-Wishart conjugate prior on the covariance matrix, when the likelihood is Multivariate Normal with a known mean). Inference is then rendered easier, than when posterior sampling from a non-closed form posterior needs to be undertaken, using numerical techniques such as MCMC. Now, if the graph is not decomposable, and a Hyper-Inverse-Wishart prior is placed on the covariance matrix, the resulting Hyper-Inverse-Wishart joint posterior density that can be factorised into a set of Inverse-Wishart densities, cannot be identified as the clique marginals. Expressed differently, the clique marginals are not closed-form when the graph is not decomposable. However, this is not a worry in the MCMC-based inference scheme on random Binomial graphs that we use, because we are not making inference on the graph (writing its posterior) clique-by-clique, and neither are we reliant on the closed-form nature of the posteriors to sample from. Thus, our aim is to learn the graph, irrespective of validity of the decomposability assumption.

This paper is organised as follows. The following section deliberates upon the methodology that we use to learn the between-columns correlation matrix of a matrix-shaped dataset, and its graphical model, along with details of the Metropolis-within-Gibbs-based inference, and provides definition.
of the 95% HPD credible regions on the learnt graph. In Section 3 we demonstrate our learning on a low-dimensional, simulated dataset, to show the effect of acknowledgement of measurement uncertainties on the graphical model—of even such a low-dimensional data, and perform validation of our results and models (discussed in the supplementary section). At the same time, (in Section 6), we learn the large graphical model of a real, highly multivariate, matrix-shaped dataset, namely the human disease-phenotype dataset. In Section 5, we present empirical illustration of our inter-graph distance computation, by learning the vino-chemical graphical models of Portuguese white and red wine datasets (see Section 4), and finding the distance between the two. The paper is rounded up with a section that summarises the main findings and the conclusions.

2. Learning correlation matrix and graphical model given data, using Metropolis-within-Gibbs

Let \( X \in \mathbb{R}^p \) be a \( p \)-dimensional observed vector, with \( X = (X_1, \ldots, X_p)^T \). Let there be \( n \) measurements of \( X_j, j = 1, \ldots, p \), so that the \( n \times p \)-dimensional matrix \( D = [x_{ij}]_{i=1}^n_{j=1} \) is the data that comprises \( n \) measurements of the \( p \)-dimensional observable \( X \). Let the \( i \)-th realisation of \( X \) be \( x_i, i = 1, \ldots, n \).

We model \( X \) using a high-dimensional GP, so that the set of realisations of this variable that comprises the data \( D \), is jointly matrix-normal, i.e.

\[
\{x_1, \ldots, x_n\} \sim \mathcal{MN}(\mu, \Sigma_R, \Sigma_C),
\]

where this matrix-normal density is parametrised by an \( n \times p \)-dimensional mean matrix \( \mu \), an \( n \times n \)-dimensional covariance matrix \( \Sigma_R \), an element of which is the covariance between a pair of rows in \( D \), and a \( p \times p \)-dimensional covariance matrix \( \Sigma_C \) that manifests information about between-columns covariance in data \( D \). This is synonymous to saying that the likelihood of \( \mu, \Sigma_C \) and \( \Sigma_R \), given data \( D \), is matrix normal.

2.1. Learning the correlation structure in the data

We standardise the data \( D \) by the empirical mean and standard deviation, to then model this standardised data \( D_S \) using a high-dimensional GP with zero mean. Thus, the \( n \times p \)-dimensional matrix \( D_S = [z_{ij}] \), with \( z_{ij} = \frac{x_{ij} - \bar{x}_j}{\sqrt{\gamma_j}}, \) where \( \bar{x}_j := \frac{\sum_{i=0}^n x_{ij}}{n} \) and \( \gamma_j^2 := \frac{\sum_{i=0}^n x_{ij}^2}{n} - \left( \frac{\sum_{i=0}^n x_{ij}}{n} \right)^2 \). Then modelling the standardised observable \( Z = (Z_1, \ldots, Z_p)^T \) with a zero-mean high-dimensional GP, we get the joint probability distribution of the \( n \) values of \( Z \) that comprise \( D_S \) to be

\[
\{z_1, \ldots, z_n\} \sim \mathcal{MN}(0, \Sigma_R^{(S)}, \Sigma_C^{(S)}),
\]

i.e. the likelihood of the covariance matrices \( \Sigma_R^{(S)} \) and \( \Sigma_C^{(S)} \), given data \( D_S \), is matrix-normal:

\[
\ell(\Sigma_R^{(S)}, \Sigma_C^{(S)} | D_S) = \frac{1}{(2\pi)^{\frac{n^2}{2}} |\Sigma_C^{(S)}|^{\frac{1}{2}} |\Sigma_R^{(S)}|^{\frac{1}{2}}} \times \exp \left[ -\frac{1}{2} \text{tr} \left\{ \left( \Sigma_R^{(S)} \right)^{-1} D_S (\Sigma_C^{(S)})^{-1} (D_S)^T \right\} \right], \tag{2.1}
\]

Here \( \Sigma_R^{(S)} \) generates the covariance between the standardised variables \( Z_i \) and \( Z_{i'} \); \( i, i' = 1, \ldots, n \), (while \( \Sigma_R \) generates the covariance between \( X_i \) and \( X_{i'} \)). In other words, \( \Sigma_R^{(S)} \) generates the correlation between rows of the standardised data set \( D_S \). Similarly, \( \Sigma_C^{(S)} \) generates the correlation between columns of \( D_S \).

Importantly, we use uniform prior on \( \Sigma_C^{(S)} \), and Jeffry’s prior on \( \Sigma_R^{(S)} \): \( \pi_0(\Sigma_R^{(S)}) = |\Sigma_R^{(S)}|^{\alpha} \), \( \alpha = -\left( \frac{n}{2} + 1 \right) \).
Theorem 2.1. The joint posterior probability density of the correlation matrices $\Sigma_C^{(S)}, \Sigma_R^{(S)}$, given the standardised data $D_S$ is

$$\left[\Sigma_C^{(S)}, \Sigma_R^{(S)}|D_S\right] \propto \ell(\Sigma_R^{(S)}, \Sigma_C^{(S)}|D_S) \left[\Sigma_C^{(S)}, \Sigma_R^{(S)}\right],$$

where $\ell(\Sigma_R^{(S)}, \Sigma_C^{(S)}|D_S)$ is the likelihood of $\Sigma_R^{(S)}, \Sigma_C^{(S)}$ given data $D_S$. This can be marginalised over the $n \times n$-dimensional between-rows’ correlation $\Sigma_R^{(S)}$, to yield

$$\left[\Sigma_C^{(S)}|D_S\right] \propto \frac{1}{c\left(\Sigma_C^{(S)}\right)} \left\|D_S(\Sigma_C^{(S)})^{-1}(D_S)^T\right\|^{-\frac{n}{2}},$$

where the prior on $\Sigma_C^{(S)}$ is uniform; prior on $\Sigma_R^{(S)}$ is the non-informative $\pi_0(\Sigma_R^{(S)}) = \left|\Sigma_R^{(S)}\right|^{\alpha}$, $\alpha = -\frac{n}{2} - 1$, and $\Sigma_C^{(S)}$ is assumed invertible. Here, $c\left(\Sigma_C^{(S)}\right)$ is a function of $\Sigma_C^{(S)}$ that normalises the likelihood.

Proof. The joint posterior probability density of $\Sigma_C^{(S)}, \Sigma_R^{(S)}$, given data $D_S$:

$$\left[\Sigma_C^{(S)}, \Sigma_R^{(S)}|D_S\right] \propto \ell(\Sigma_R^{(S)}, \Sigma_C^{(S)}|D_S) \left[\Sigma_C^{(S)}, \Sigma_R^{(S)}\right],$$

i.e.

$$\left[\Sigma_C^{(S)}, \Sigma_R^{(S)}|D_S\right] \propto \frac{1}{(2\pi)^{\frac{n}{2}} \left|\Sigma_C^{(S)}\right|^\frac{n}{2} \left|\Sigma_R^{(S)}\right|^\frac{n}{2}} \times \exp\left[-\frac{1}{2} \operatorname{tr}\left\{(\Sigma_R^{(S)})^{-1}(D_S)(\Sigma_C^{(S)})^{-1}(D_S)^T\right\}\right] \left|\Sigma_R^{(S)}\right|^{-\frac{n}{2} - 1},$$

(2.2)

using the likelihood from Equation 2.1; using prior on $\Sigma_R^{(S)}$ to be $\pi_0(\Sigma_R^{(S)}) = \left|\Sigma_R^{(S)}\right|^{\alpha}$ where $\alpha = -\frac{n}{2} - 1$; using prior on $\Sigma_C^{(S)}$ to be uniform.

Marginalising $\Sigma_R^{(S)}$ out from the joint posterior $\left[\Sigma_C^{(S)}, \Sigma_R^{(S)}|D_S\right]$, we get:

$$\left[\Sigma_C^{(S)}|D_S\right] \propto \frac{1}{\left|\Sigma_C^{(S)}\right|^\frac{n}{2}} \int \frac{1}{\left|\Sigma_R^{(S)}\right|^\frac{n}{2}} \left|\Sigma_R^{(S)}\right|^{-\frac{n}{2} - 1} \times \exp\left[-\frac{1}{2} \operatorname{tr}\left\{(\Sigma_R^{(S)})^{-1}D_S(\Sigma_C^{(S)})^{-1}(D_S)^T\right\}\right] d(\Sigma_R^{(S)})$$

(2.3)

Here $\Sigma_R^{(S)} \in \mathcal{R} \subseteq \mathbb{R}^{(n \times n)}$. Now,

- let $Y := (\Sigma_R^{(S)})^{-1}$. Then $d(\Sigma_R^{(S)}) = |Y|^{-(n+1)}dY$ (Mathai and G.Pederzoli, 1997),
- let $V^{-1} := D_S(\Sigma_C^{(S)})^{-1}(D_S)^T$, $\Longrightarrow \operatorname{tr}\left[(\Sigma_R^{(S)})^{-1}D_S(\Sigma_C^{(S)})^{-1}(D_S)^T\right] = \operatorname{tr}\left[V^{-1}Y\right]$ (using commutativeness of trace),

so that in Equation 2.3, we get

$$\left[\Sigma_C^{(S)}|D_S\right] \propto \frac{1}{\left|\Sigma_C^{(S)}\right|^\frac{n}{2}} \int |Y|^\frac{n}{2} |Y|^\frac{n}{2 + 1} \times \exp\left[-\frac{1}{2} \operatorname{tr}\left\{V^{-1}Y\right\}\right] |Y|^{-(n+1)}dY.$$

(2.4)

The integral in the RHS of Equation 2.4 represents the unnormalised Wishart pdf $W_n(V,q)$, over all values of the random matrix $Y$, where the scale matrix and degrees of freedom of this pdf are $V$ and $q = n + 1$ respectively, i.e. $q > n - 1$. Thus, integral in the RHS of Equation 2.4 is the integral of the unnormalised pdf of $Y \sim W_n(V,q)$,
over the full support of $\mathbf{Y}' \equiv (\mathbf{\Sigma}_R^{(S)})^{-1}$, i.e. the integral in the RHS of Equation 2.4 is the normalisation of this pdf:

$$2^{\frac{n}{2}} \Gamma_n \left( \frac{n}{2} \right) |\mathbf{V}|^\frac{n}{2} = 2^{\frac{n+1}{2}} \Gamma_n \left( \frac{n+1}{2} \right) \left| (\mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T)^{-1} \right|^{-\frac{n+1}{2}},$$

i.e. integral on RHS of Equation 2.4 is proportional to $\left| (\mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T)^{-1} \right|^{-\frac{n+1}{2}}$, i.e.

$$\left[ \mathbf{\Sigma}_C^{(S)} | \mathbf{D}_S \right] \propto \frac{1}{\left| \mathbf{\Sigma}_C^{(S)} \right|^\frac{n}{2}} \left| (\mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T)^{-1} \right|^{-\frac{n+1}{2}}$$

(2.5)

Now, if $\mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T$ is invertible, $\left| (\mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T)^{-1} \right|^{-\frac{n+1}{2}} = \left| \mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T \right|^{\frac{n+1}{2}}$.

- It is given that $\mathbf{\Sigma}_C^{(S)}$ is invertible, i.e. $(\mathbf{\Sigma}_C^{(S)})^{-1}$ exists.
- The original dataset is examined to discard rows that are linear transformations of each other, leading to data matrix $\mathbf{D}_S$, no two rows of which are linear transformations of each other

$$\Rightarrow \mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T$$ is positive definite, i.e. $\mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T$ is invertible,

$$\Rightarrow \left| (\mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T)^{-1} \right|^{(n+1)/2} = \left| \mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T \right|^{-(n+1)/2}.$$  

Using this in Equation 2.5:

$$\left[ \mathbf{\Sigma}_C^{(S)} | \mathbf{D}_S \right] \propto \left| \mathbf{\Sigma}_C^{(S)} \right|^{-p/2} \left| \mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T \right|^{-(n+1)/2}.$$  

(2.6)

This posterior of the between-columns correlation matrix $\mathbf{\Sigma}_C^{(S)}$ given data $\mathbf{D}_S$, is normalised over all possible datasets, where the possible datasets abide by a column-correlation matrix of $\mathbf{\Sigma}_C^{(S)}$, as:

$$c \left( \mathbf{\Sigma}_C^{(S)} \right) = \prod_{z = 1}^{n'} \int \frac{1}{\left| (\mathbf{D}'(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}')^T)^{-1} \right|^{-\frac{n+1}{2}}} dz_1 dz_{11} \ldots dz_{n/p},$$  

(2.7)

where $\mathbf{D}' = [z_1, \ldots, z_{p}] = [z_{ij}]_{i = 1, j = 1}^{n', p}$ is a dataset with $n'$ rows and $p$ columns, comprising values of random standardised variables $Z_{ij} \in \mathbb{Z}$, simulated to bear between-column correlation matrix of $\mathbf{\Sigma}_C^{(S)}$, s.t. $\mathbf{D}'(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}')^T$ is positive definite $\forall \mathbf{D}' \in \mathcal{D}$. Choosing the same number of rows for all choices of the random data matrix $\mathbf{D}'$, i.e. for a constant $n'$, $\mathcal{D} \subseteq \mathbb{R}^{(n' \times p)}$. Then $c \left( \mathbf{\Sigma}_C^{(S)} \right)$ is a positive definite function of $\mathbf{\Sigma}_C^{(S)}$.

Using this normalisation on the posterior of $\mathbf{\Sigma}_C^{(S)}$ given $\mathbf{D}_S$, in Equation 2.6 we get

$$\pi \left( \mathbf{\Sigma}_C^{(S)} | \mathbf{D}_S \right) = \frac{1}{c \left( \mathbf{\Sigma}_C^{(S)} \right) \left| \mathbf{\Sigma}_C^{(S)} \right|^{\frac{n}{2}} \left| \mathbf{D}_S(\mathbf{\Sigma}_C^{(S)})^{-1}(\mathbf{D}_S)^T \right|^{\frac{n+1}{2}}},$$  

(2.8)

where $c \left( \mathbf{\Sigma}_C^{(S)} \right) > 0$ is defined in Equation 2.7. \( \square \)

The posterior $\left[ \mathbf{\Sigma}_C^{(S)} | \mathbf{D}_S \right]$ as given by Theorem 2.1, suggests that we have to compute the normalisation $c \left( \mathbf{\Sigma}_C^{(S)} \right)$, in every iteration, i.e. for every updated value of $\mathbf{\Sigma}_C^{(S)}$. We recall that this
normalisation is given by Equation 2.7, where the standardised \( Z'_{ij} \), \( i = 1, \ldots, n' \); \( j = 1, \ldots, p \) are simulated s.t. the column correlation between \( (Z'_{1m}, \ldots, Z'_{n'm})^T \) and \( (Z'_{1q}, \ldots, Z'_{n'q})^T \) is \( s_{mq} \), with \( \Sigma^{(S)} = [S_{mq}]_{m=1}^{p} = 1, q=1 \). However, it is hard to compute \( c(\Sigma^{(S)}) \), defined in Equation 2.7, as a closed-form integral. Instead, we define an estimator \( \hat{c} \) of the integral representing the all-data averaged normalisation, in the \( t \)-th iteration of the \( N \)-iteration long MCMC chain that we run, \( (t = 0, \ldots, N) \).

So, we estimate the integral in the RHS of Equation 2.7 using its unbiased estimator. We rephrase the integrand as \( h(Z'_{11}, \ldots, Z'_{n'p}, \Sigma^{(S)}_C) \), i.e.

\[
h(Z'_{11}, \ldots, Z'_{n'p}, \Sigma^{(S)}_C) := \frac{1}{\left| (D'(\Sigma^{(S)}_C)^{-1}(D')^T) \right|^{n/p}}.
\]

Then the estimator of the normalisation in Equation 2.7 is

\[
\hat{c}(\Sigma^{(S)}_C) = \mathbb{E}_{Z'_{n'p}} [h(Z'_{11}, \ldots, Z'_{n'p}, \Sigma^{(S)}_C)] = \mathbb{E}_{D'} [h(Z'_{11}, \ldots, Z'_{n'p}, \Sigma^{(S)}_C)].
\]

However, it is difficult to implement this estimator by sequentially computing expectations w.r.t. distribution of each of the elements of \( D' \). Instead, we compute the expectation w.r.t. the block \( D' \) of these elements, where \( D' \) abides by a column-correlation of \( \Sigma^{(S)}_C \), i.e., we compute

\[
\hat{c}'(\Sigma^{(S)}_C) = \mathbb{E}_{D'} [h(Z'_{11}, \ldots, Z'_{n'p}, \Sigma^{(S)}_C)].
\]

During the \( t \)-th iteration of the MCMC chain, let the column correlation matrix be \( \Sigma_t \) and the normalisation be \( \hat{c}_t \). Then \( \hat{c}_t \) is defined using \( \Sigma_t \) and the sample of \( n' \times p \)-dimensional data sets \( \{D_1^t, \ldots, D_K^t\} \), s.t. \( D_k^t(\Sigma_t)^{-1}(D_k^t)^T \) is positive definite \( \forall k = 1, \ldots, K \), at each \( t \). Then:

\[
\hat{c}_t := \frac{1}{K} \sum_{k=1}^{K} \frac{1}{\left| (D_k^t(\Sigma_t)^{-1}(D_k^t)^T) \right|^{n/p}}.
\]

2.2. Learning the graphical model

We perform Bayesian learning of the inhomogeneous, Generalised Binomial random graph, given the learnt \( p \times p \)-dimensional, between-columns correlation matrix \( \Sigma^{(S)}_C \), of the multivariate data set \( D_S := (Z_1, \ldots, Z_p)^T \), that results from the standardisation of the available data \( D := (X_1, \ldots, X_p)^T \).

Thus, the graph \( G(p, R) \) is a random variable that gets updated in every iteration of our Bayesian inference scheme (Metropolis-within-Gibbs), at the updated (partial) correlation matrix given the data. Here, the value \( G(p, R) \), has the vertex set \( V \) and the between-columns partial correlation matrix of data \( D_S \) is \( R = [R_{ij}] \), s.t. \( R_{ij} \) takes the value \( \rho_{ij} \), \( i \neq j \), and \( \rho_{ii} = 1 \). The vertex set is \( V = \{1, \ldots, p\} \) s.t. vertices \( i, j \in V \), \( i \neq j \), are joined by the edge \( G_{ij} \) that is a random binary variable taking values of \( g_{ij} \), where \( g_{ij} \) is either 1 or 0, and is the \( ij \)-th element of the edge matrix \( G = [G_{ij}] \).

Given a learnt value of the between-columns correlation matrix \( \Sigma^{(S)}_C \), to compute the value \( \rho_{ij} \) of the partial correlation variable \( R_{ij} \), we first invert \( \Sigma^{(S)}_C \) to yield: \( \Psi := \left( \Sigma^{(S)}_C \right)^{-1} ; \Psi = [\psi_{ij}] \), s.t.

\[
R_{ij} = -\frac{\psi_{ij}}{\sqrt{\psi_{ii}\psi_{jj}}}, \quad i \neq j,
\]

and \( \rho_{ii} = 1 \) for \( i = j \).
The posterior probability density of the graph $G(p, R)$ defined for the edge matrix $G$, is given as

$$
\pi(G_{11}, G_{12}, \ldots, G_{p,p-1} | R) \propto \ell(G_{11}, G_{12}, \ldots, G_{p,p-1} | R) \pi_0(G_{11}, G_{12}, \ldots, G_{p,p-1}),
$$

where $\pi_0(G_{11}, G_{12}, \ldots, G_{p,p-1})$ is the prior probability density on the edge parameters $[G_{ij}]_{i \neq j; i, j = 1}^p$, and $\ell(G_{12}, \ldots, G_{ip}, G_{21}, G_{23}, \ldots, G_{p,p-1} | R)$ is the likelihood of the edge parameters, given the partial correlation matrix $R$ (that is itself computed using the between-columns correlation matrix $\Sigma^{(S)}$, learnt given $D_S$, (see Equation 2.8)).

We choose a prior on $G_{ij}$ that is Bernoulli(0.5), i.e. $\pi_0(G_{11}, G_{12}, \ldots, G_{p,p-1}) = \prod_{i,j=1; i \neq j}^p 0.5^{g_{ij}} 0.5^{1-g_{ij}}$; thus, the prior is independent of the edge parameters.

We choose to define the likelihood of any edge parameter given the corresponding partial correlation, to be a Folded Normal density (Leone et al., 1961). Thus, likelihood of the edge parameters given $R$ is

$$
\prod_{i \neq j; i, j = 1}^p \frac{1}{\sqrt{2\pi\sigma_{ij}}} \exp \left[ -\frac{(G_{ij} - R_{ij})^2}{2\sigma_{ij}^2} - \frac{(G_{ij} + R_{ij})^2}{2\sigma_{ij}^2} \right],
$$

where the variance parameters $\{\sigma_{ij}\}_{i \neq j; i, j = 1}^p$ are indeed hyperparameters that are also learnt from the data; these variance parameters have uniform prior probabilities imposed on them.

In light of the fact that parameters that are learnt, are the edge parameters as well as the variance parameters, we rephrase the likelihood as:

$$
\ell(G_{12}, \ldots, G_{1p}, G_{21}, G_{23}, \ldots, G_{p,p-1}, \sigma_{12}, \ldots, \sigma_{1p}, \sigma_{21}, \sigma_{23}, \ldots, \sigma_{p,p-1} | R) = 
\prod_{i \neq j; i, j = 1}^p \frac{1}{\sqrt{2\pi\sigma_{ij}}} \exp \left[ -\frac{(G_{ij} - R_{ij})^2}{2\sigma_{ij}^2} - \frac{(G_{ij} + R_{ij})^2}{2\sigma_{ij}^2} \right].
$$

\(2.11\)

### 2.3. Inference using Metropolis-within-Gibbs

We model the $p$-dimensional vector-valued observable ($n$ realisations of which together comprise the standardised data $D_S$), using a Gaussian Process, s.t. the joint probability distribution of the $n$ realisations of this observable is Matrix-Normal with zero mean; while the between-row matrix can be marginalised out from this likelihood, the between-columns, $p \times p$-dimensional correlation matrix $\Sigma^{(S)}_C$ is learnt given data $D_S$. Upon learning $\Sigma^{(S)}_C$, using which the partial correlation matrix $R$ is computed—the graphical model comprising the credible-region defining set of random Binomial graphs $\{G(p, R)\}$ is learnt, where the vertex set of each graph in this set is fixed as $V$; the “credible region” in question is defined below in Section 2.4.

We perform Metropolis-within-Gibbs based inference on the unknowns. Then, at the beginning of any iteration, $\Sigma^{(S)}_C$ is updated given $D_S$, following which, $G(p, R)$ is updated at the newly updated $\Sigma^{(S)}_C$.

To be precise, by updating $\Sigma^{(S)}_C$, we imply updating the $\frac{p^2 - p}{2}$ non-diagonal terms of the upper (or lower) triangle of the symmetric $p \times p$ correlation matrix $\Sigma^{(S)}_C$, i.e. the parameters $S_{12}, S_{13}, \ldots, S_{1p}, S_{23}, \ldots, S_{p-1p}$. Given the nature of the likelihood of the $S_{ij}$ parameters, $i < j; i, j = 1, \ldots, p$, (see Equation 2.8), this updating involves inversion of $\Sigma^{(S)}_C$, and computing of the determinants of $\Sigma^{(S)}_C$ and $D_S \left(\Sigma^{(S)}_C\right)^{-1} (D_S)^T$. The inversion and determinant computation will need to be undertaken in every iteration. Such is possible with the computation of the square root of the column correlation matrix $\Sigma^{(S)}_C$, as well as the factorisation of $D_S \left(\Sigma^{(S)}_C\right)^{-1} (D_S)^T$ into two triangular matrices, since determinant of a triangular matrix is easily computed, as the product of the diagonal elements of such a matrix. Thus, in any iteration, we can compute the
$p \times p$-dimensional, (lower by choice) triangular matrix, that is the square root $L_C^{(S)}$ of $\Sigma_C^{(S)}$, i.e. $\Sigma_C^{(S)} = L_C^{(S)} (L_C^{(S)})^T$. Here $L_C^{(S)}$ is computed via Cholesky decomposition. Cholesky decomposition of $\Sigma_S = (\Sigma_C^{(S)})^{-1} (D_S)^T$ into the (lower) triangular matrix $L$ and $L^T$ is also undertaken, following the inversion of $\Sigma_C^{(S)}$ into $(\Sigma_C^{(S)})^{-1}$. Since the factors of $\Sigma_C^{(S)}$ are already computed (Cholesky decomposed) as $L_C^{(S)}$ and $(L_C^{(S)})^T$, the inversion of $\Sigma_C^{(S)}$ is undertaken using a forward substitution algorithm, i.e. we set $(\Sigma_C^{(S)})^{-1} = ((L_C^{(S)})^{-1} (L_C^{(S)})^{-1},$ where $(L_C^{(S)})^{-1}$ is computed using $L_C^{(S)}$ in a forward substitution scheme; here $(L_C^{(S)})^{-1} L_C^{(S)} = I$. Then $D_S ((L_C^{(S)})^T)^{-1} (L_C^{(S)})^{-1} (D_S)^T$ is Cholesky decomposed into $L$ and $L^T$. The underlying schemes for forward substitution and Cholesky Decomposition are discussed in Section 4 of the Supplementary Material.

As mentioned above, we assume that at every iteration, the proposed $\Sigma_C^{(S)}$ and $D_S ((\Sigma_C^{(S)})^{-1} (D_S)^T$ are positive definite—to implement which, we start by identifying rows in the original data set that are linearly dependent; for each set of rows that are identified as linearly dependent, only one row is retained and the rest discarded from the original data set. While this is undertaken prior to the initiation of the MCMC chain, it is still possible that during an iteration, a proposed $\Sigma_C^{(S)}$ is s.t. its square root $L_C^{(S)}$ is not positive definite, within some pre-set numerical threshold. One possible solution to this problem is numerical, for example, implementing ridge adjustment (Wothke, 1993), i.e. adding a “small” number to the diagonal elements of $L_C^{(S)}$, where “small” is typically $\lesssim 10^{-14}$ times a diagonal element of the matrix in our implementation. Another, less ad hoc solution is to propose $L_C^{(S)}$ in any iteration—instead of $\Sigma_C^{(S)}$—where the diagonal elements of $L_C^{(S)}$ are proposed as positive definite, while ensuring that the $\Sigma_C^{(S)}$ generated as $L_C^{(S)} (L_C^{(S)})^T$ abides by the constraints of a correlation matrix, i.e. the diagonal elements are 1 and non-diagonal elements are $\in [-1, 1]$. Adhering to such constraints is as difficult a numerical challenge as the original one. Given this, we opt to propose $\Sigma_C^{(S)}$ in every iteration and perform its Cholesky decomposition, while implementing the ridge adjustment discussed above.

As we saw in Section 2, the joint posterior probability density of the elements $S_{ij}$ of the $(p^2-p)/2$ upper/lower triangle of the correlation matrix, given data $D_S$, is normalised, with the normalisation factor that needs updating at each update of $\Sigma_C^{(S)}$: $i < j$; $i, j = 1, \ldots, p$. This normalisation factor is $c(\Sigma_C^{(S)})$ defined in Equation 2.7. An estimator $\hat{c}$ of this normalisation in the $t$-th iteration is given in Equation 2.9—as the arithmetic mean of $K$ number of random realisations of the integrand in the integral representing the normalisation $c(\Sigma_C^{(S)})$. Each such realisation results from a sampled data set $D_k^{(t)}$ that bears the column correlation matrix that is the column correlation updated in this $t$-th iteration of the MCMC chain; $t = 0, \ldots, N$, $k = 1, \ldots, K$. Here, each of the $K$ sampled data sets is generated with $n^t$ rows (and the $p$ columns, as $\Sigma_C^{(S)}$ is $p \times p$-dimensional). To generate $D_k^{(t)}$ as a randomly sampled $n^t \times p$-sized data set with column correlation as in the $t$-th iteration, we use established sampling techniques for sampling data given a correlation structure.

The algorithm followed for our Metropolis-within-Gibbs-based inference is the following.

1(i) At the 0-th iteration, we choose a seed value $\Sigma_0$ of the correlation matrix $\Sigma_C^{(S)}$. To be precise, we choose a seed value $s_{ij}^{(0)}$ of the parameter $S_{ij}$; $i < j$; $i = 1, \ldots, p$. At this iteration—as at every iteration—Cholesky decomposition of the column correlation matrix is undertaken. Thus, in the 0-th iteration, we compute the $p \times p$-dimensional, lower (by choice) triangular matrix that is the square root $L_0$ of $\Sigma_0$, i.e. $\Sigma_0 = L_0 L_0^T$. The Cholesky decomposition of $\Sigma_0$ is performed as delineated in Section 4 of the Supplementary Material. This allows for $\Sigma_0$ to be computed as square of the product of the diagonal elements of $L_0$. Using $L_0$, its inverse $L_0^{-1}$ is computed using the forward substitution algorithm delineated in Section 4 of the Supplementary Material, and the inverse $\Sigma_0^{-1}$ of $\Sigma_0$ is then $\Sigma_0^{-1} = (L_0^{-1})^T L_0^{-1}$. Next, $D_S \Sigma_0^{-1} (D_S)^T$ is Cholesky decomposed, to allow for the determinant of this matrix to be computed. Using the computed precision matrix $\Sigma_0^{-1}$ in the 0-th iteration, the partial correlation matrix $R_0$ in this iteration
is computed, i.e. $\rho_{ij}^{(0)}$ is computed $\forall i \neq j$; $i, j = 1, \ldots, p$, where $R_0$ takes the value $[\rho_{ij}^{(0)}]$. For this seed correlation $\Sigma_0$, the estimator of the normalisation factor $c_0$ is computed using Equation 2.9, following the random selection of $K$ number of $n'/p$-dimensional data sets $D_0^{(p)}$ with column correlation $\Sigma_0, k = 1, \ldots, K$. We use $n'/n$. We compute the joint posterior probability density $\pi(s_{12}^{(0)}, \ldots, s_{p-1,p}^{(0)}|D_S)$ of the non-diagonal, upper triangle elements of $\Sigma_0$, given data $D_S$, using Equation 2.8.

1(ii) In the 0-th iteration, seed values $(g_{ij}^{(0)} = 1)$ of the edge parameter $G_{ij}$, are assigned. In addition, seed values $\sigma_{ij}^{(0)}$ are assigned to the $\sigma_{ij}$ parameter; $i < j$; $i, j \in V$. The joint posterior probability density of $(g_{ij}^{(0)}$ and $\sigma_{ij}^{(0)}$, $\forall i, j = 1, \ldots, p$; $i < j$, is given as the product of the likelihood in Equation 2.11, the uniform prior on each variance parameter and the Bernoulli prior with rate parameter 0.5 on each edge parameter.

2(i) As the $t$-th iteration begins, $t = 1, \ldots, N$, we propose a value $s_{ij}^{(t)}$ for the $ij$-th element of the correlation matrix $\Sigma_C^{(S)}$, such that the proposed value of this matrix is $\Sigma_C^{*}$ in the $t$-th iteration. This is done by proposing $s_{ij}^{(t)}$ from a Truncated Normal density that is left truncated at $-1$ and right truncated at $1$, i.e.

$$s_{ij}^{(t)} \sim \mathcal{TN}(s_{ij}^{(t-1)}, v_{ij}, -1, 1), \quad \forall i, j = 1, \ldots, p; \ i \neq j,$$

where $v_{ij}$ is the experimentally chosen variance of the Truncated Normal proposal density, and the mean of this density is the value $s_{ij}^{(t-1)}$ that is the current value of the parameter $S_{ij}$ at the end of the $t - 1$-th iteration. Here the current correlation matrix is $\Sigma_{t-1}$, and we in fact use $v_0 = v_{ij} \forall i, j$. We refer to the estimator of the normalisation at the proposed $\Sigma_C^{*}$ as $\hat{c}_t$, and compute it using the generated sample $\{D_1^{(t)}, \ldots, D_K^{(t)}\}$ in Equation 2.9. The current normalisation $\hat{c}_{t-1}$ at the current correlation matrix $\Sigma_{t-1}$ is computed using the generated sample $\{D_1^{(t-1)}, \ldots, D_K^{(t-1)}\}$ in Equation 2.9. Then we accept the proposed $\Sigma_C^{*}$, at a probability of

$$a(\Sigma_C^{*}, \Sigma_{t-1}) := \min \left(1, \frac{\hat{c}_{t-1} \times \pi(\Sigma_C^{*} | D_S) \mathcal{TN}(\Sigma_{t-1}; \Sigma_C^{*}, v_0, -1, 1)}{\hat{c}_t \times \pi(\Sigma_C^{(S)} | D_S) \mathcal{TN}(\Sigma_{t-1}; \Sigma_C^{(S)}, v_0, -1, 1)} \right),$$

where $\pi(\cdot|D_S)$ is given in Equation 2.6, as

$$\pi(\Sigma_C^{(S)} | D_S) \propto \left| \Sigma_C^{(S)} \right|^{-p/2} \left| D_S(\Sigma_C^{(S)})^{-1}(D_S)^T \right|^{-(n+1)/2}.$$

(2.10)

2(ii) At the 2nd stage of the $t$-th iteration, the graph variable $G(p, R)$ is updated, given the current partial correlation matrix $R_t$. To be precise, we propose $g_{ij}^{(t)} ~ \text{Bernoulli}(g_{ij}^{(t)}, \rho_{ij}^{(t)})$ pmf, $\forall i, j = 1, \ldots, p; i < j$. Also, for each $i, j$, we propose $\sigma_{ij}^{(t)}$ from a Normal density $\mathcal{N}(\sigma_{ij}^{(t)}; \sigma_{ij}^{(t-1)}, w_{ij}^2)$, where $w_{ij}^2$ are the experimentally chosen variance of the proposal density and the mean of this density is the value of $\sigma_{ij}$ that is current at the end of the $t - 1$-th iteration. Then we accept the proposed $g_{ij}^{(t)}$, $\sigma_{ij}^{(t)}$, $\forall i < j; i, j = 1, \ldots, p$, at the probability of

$$\min \left(1, \frac{\prod_{i < j; i, j = 1}^p \mathcal{TN}(g_{ij}^{(t)}; \rho_{ij}^{(t)}, \sigma_{ij}^{(t)}) \text{Bernoulli}(g_{ij}^{(t-1)}; \rho_{ij}^{(t)})}{\prod_{i < j; i, j = 1}^p \mathcal{TN}(g_{ij}^{(t-1)}; \rho_{ij}^{(t-1)}, \sigma_{ij}^{(t-1)}) \text{Bernoulli}(g_{ij}^{(t)}; \rho_{ij}^{(t)}, \sigma_{ij}^{(t)})} \right),$$

where $\mathcal{TN}(g_{ij}^{*}, \rho_{ij}, \sigma_{ij}) = \frac{1}{\sqrt{2\pi\sigma_{ij}}} \exp \left[ -\frac{(g_{ij}^{*} - \rho_{ij})^2}{2\sigma_{ij}^2} - \frac{(g_{ij}^{*} + \rho_{ij})^2}{2\sigma_{ij}^2} \right]$. If the acceptance probability $> w'$, where $w' \in [0, 1]$, we accept the proposed values of the edge and variance parameters, i.e. set $g_{ij}^{(t)} = g_{ij}^{(t)}$ and $\sigma_{ij}^{(t)} = \sigma_{ij}^{(t)}$, $\forall i < j; i, j \in V$. Otherwise, the proposed values of the parameters are rejected and we set the current values in iteration $t$ to be those
of the previous iteration. The graph at the end of the $t$-th iteration is $G^{(t)}(p, R_t)$, where $R_t$ is the updated partial correlation matrix in the $t$-iteration.

3 Stop if $t = N$; else repeat Steps 2.

2.4. Definition of 95% HPD credible regions on the random graph variable and the learnt graphical model

We perform Bayesian inference on the random graph variable $G(p, R)$, leading to one sampled graph at the end of each of the $N + 1$ iterations of our inference scheme (Metropolis-within-Gibbs). The sample of graphs obtained from the post-burnin part of the MCMC chain then encompasses our learning of the graphical model of the data $D_S$. In order to acknowledge uncertainties in the Bayesian learning of this graphical model, we need to include in its definition, only those sampled graphs that lie within an identified 95% HPD credible region. How can we model this uncertainty, and in particular, present a single representation of the learnt graphical model of $D_S$, inclusive of such learnt uncertainties?

We address this concern by defining the fraction $N_{ij}$ of the post-burnin number $N_{post}$ of iterations (where $N_{post} < N + 1$), in which the $ij$-th edge exists, i.e. $G_{ij}$ takes the value $1$, $\forall i, j = 1, 2, \ldots, p$, $i \neq j$. Thus, we define the variable $N_{ij}$ that takes the value

$$n_{ij} := \frac{\sum_{t=N-N_{post}+1}^{N} I_1(g_{ij}^{(t)})}{N_{post}}, \quad i < j; \ i, j = 1, \ldots, p,$$  \hspace{1cm} (2.12)

where the indicator function

$$I_1(g_{ij}^{(t)}) = 1 \quad \text{if} \quad g_{ij}^{(t)} = 1$$

$$I_1(g_{ij}^{(t)}) = 0 \quad \text{if} \quad g_{ij}^{(t)} = 0$$

Then $N_{ij}$ is the fractional number of sampled graphs, in which an edge exists between vertices $i$ and $j$. This leads us to interpret $\{N_{ij}\}_{i,j \in V; i < j}$ as carrying information about the uncertainty in the graph learnt given data $D_S$; in particular, $n_{ij}$ approximates the probability of existence of the edge between the $i$-th and $j$-th nodes in the graphical model of the data at hand. Indeed the $N_{ij}$ parameters are functions of the partial correlation matrix $R$ that is learnt given this data, but for the sake of notational brevity, we do not include this explicit $R$ dependence in our notation to denote the edge probability parameters.

So we view the set $\{G(p, R_t)\}_{t=N-N_{post}+1}^N$ of graphs on vertex set $V = \{1, \ldots, p\}$ and edge matrix $G_t$ that is updated given $R_t$, equivalently as the post-burnin sample $\{g_{12}^{(t)}, g_{13}^{(t)}, \ldots, g_{1p}^{(t)}, g_{23}^{(t)}, \ldots, g_{pp}^{(t)}\}_{t=N-N_{post}+1}^N$ of edge parameters. We include only those edge parameters in our defined 95% HPD credible region, that occur with probability $\geq 0.05$ in this sample. In other words, only for $ij$ pairs s.t. $N_{ij} \geq 0.05$, define the $g_{ij}$ parameters included in the set that comprises the 95% HPD credible region on the edge parameters, in our definition. Indeed, the graphical model of the data is then the set of those graphs on vertex set $V = \{1, \ldots, p\}$, the existing edges of which are those $G_{ij}$ parameters that lie within this defined 95% HPD credible region.

Definition 2.1. The graphical model of data $D_S$ for which the between-column partial correlation matrix is $R$, is the $R$-dependent set or family $G_{p, \Phi(R)}$ of all inhomogeneous Binomial graphs $G(p, R)$, the edge probabilities in which is given by the matrix $\Phi(R) = [\phi_{ij}(R_{ij})]$, s.t. probability of the edge between the $i$-th and $j$-th nodes ($i \neq j; \ i, j \in V$) is

$$\phi_{ij}(R_{ij}) = [H(n_{ij} - 0.05)]n_{ij},$$  \hspace{1cm} (2.13)

Here, $n_{ij}$ is the value of the parameter $N_{ij}$ defined in Equation 2.12, and $H(\cdot)$ is the Heaviside function (Duff and Naylor, 1966) s.t. the Heaviside or step-function of $A \in \mathbb{R}$ is

$$H(a) = 1 \quad \text{if} \quad a \geq 0$$

$$= 0 \quad \text{if} \quad a < 0.$$
Only edges with non-zero edge probability \( \phi_{ij}(R_{ij}) \), are marked on the learnt graphical model, and the corresponding value of \( N \) is written next to each such marked edge. Then by this definition, any graph \( G(p, R) \in G_{p, \Phi(R)} \) is sampled from within the 95% HPD credible region on inhomogeneous random Binomial graphs given the partial correlation matrix \( R \) of the data.

Thus, in our approach, the binary edge parameter \( G_{ij} \) between the \( i \)-th and \( j \)-th nodes, takes the value 1 (i.e. the edge exists), with a learnt probability—in fact, we learn the joint posterior of all \( G_{ij} \) parameters given the learnt correlation structure of the data, while acknowledging the propagation of uncertainties in our learning of the correlation given the data, into our learning of the distribution of the \( G_{ij} \) parameters given this learnt partial correlation matrix \( R \). A summary of this learnt distribution is then the edge probability parameter \( \phi_{ij}(R_{ij}) \), the value of which is marked on the visualisation of the graphical model of the data against the edge between the \( i \)-th and \( j \)-th nodes, as long as \( \phi_{ij}(R_{ij}) > 0 \), i.e. \( n_{ij} \geq 0.05 \); \( i \neq j \); \( i, j \in V \). In other words, only edges occurring with posterior probabilities in excess of 5% are included in this graphical model.

2.5. Incorporating measurement uncertainties in the learnt graphical model

If measurement errors affect the values of the \( i \)-th component \( Z_i \) of the \( p \)-dimensional vector-valued observable \( Z \), where measurements of \( Z_i \) comprise the \( i \)-th column of data \( D_S \), \( (i = 1, \ldots, p) \), the variance of the probability distribution of such errors—if unknown—can be learnt given the data. So let the error in \( Z_i \) be \( \epsilon_i \) that we assume is Normally distributed with variance \( v_{\epsilon_i} \), i.e. \( \epsilon_i \sim \mathcal{N}(0, v_{\epsilon_i}) \). Then if the unknown error variance \( v_{\epsilon_i} \) is proposed in the \( t \)-th iteration of our MCMC chain to be \( v_{\epsilon_i}^{(t)} \), the correlation \( s_{ij}^{(t)} \) has to be adjusted by the factor \( 1/\sqrt{1 + v_{\epsilon_i}^{(t)}} \), \( \forall j \neq i \).

3. Empirical illustration: simulated data

The simulated data that we use in this section, is a 5-columned data set \( D_{\text{orig}} \) with number of rows \( n_{\text{orig}} = 4000 \), where \( D_{\text{orig}} \) is simulated to bear a chosen between-columns correlation matrix \( \Sigma_C^{(\text{true})} \) that is given as:

\[
\begin{pmatrix}
1 & 0.9914 & -0.8964 & 0.02526 & 0.0656 \\
0.9914 & 1 & 0.01981 & 0.6647 \\
-0.8964 & 0.01981 & 1 & -0.009747 & -0.06140 \\
0.02526 & 0.6647 & -0.009747 & 1 & 0.03622 \\
0.0656 & -0.06140 & 0.03622 & 1 & 1
\end{pmatrix}
\]

which when inverted, allows for the computation of the empirical partial correlation matrix, following Equation 2.10. This empirical partial correlation matrix is \( R^{(\text{true})} \):

\[
\begin{pmatrix}
1 & 0.9574 & -0.2114 & 0.004786 & 0.005037 \\
0.9574 & 1 & -0.04897 & 0.03900 & 0.01206 \\
-0.2114 & -0.04897 & 1 & 0.02736 & -0.006288 \\
0.004786 & 0.03900 & 0.02736 & 1 & 0.03527 \\
0.005037 & 0.01206 & -0.006288 & 0.03527 & 1
\end{pmatrix}
\]

We randomly sample \( n \) (=300 typically) rows from this simulated data set \( D_{\text{orig}} \), to define our toy data set \( D_T \), that we will implement in our method, to

- learn the between-columns correlation matrix \( \Sigma_C^{(S)} = [S_{ij}]_{i=1;j=1}^{n \times p} \) given the standardised version \( D_T^{(S)} \) of \( D_T \), and thereafter, learn the graphical model of data \( D_T^{(S)} \), as defined in Definition 2.1 with \( p=5 \) and partial correlation matrix \( R = [R_{ij}]_{i=1;j=1}^{n \times p} \), where elements of \( R \) are computed using the learnt \( \Sigma_C^{(S)} \) in Equation 2.10. Here \( D_T^{(S)} \) comprises \( n \) simulated values of the variables \( Z_1, \ldots, Z_5 \).
– perform model checking using $D_T^{(S)}$. To be precise, we predict the distribution of $Z_i$ when in the identified test data, $Z_j$ is restricted to take values in the chosen, narrow interval $[z_j^{(0)} - \delta_j, z_j^{(0)} + \delta_j]$, for $j \neq i; i, j = 1, \ldots, 5$–and then compare the empirical distribution of $Z_i$ in the test data, with the posterior predictive distribution of $Z_i$, given the correlation matrix learnt using $D_T^{(S)}$. Also, given $D_T^{(S)}$ and $Z_j$, we perform MCMC-based sampling from the joint posterior of $\{\bar{Z}_{i}^{\mu} = p\}$ and $\Sigma_C^{(S)}$. This is discussed in Section 1 of the Supplementary Section.

– learn the correlation matrix and graphical model of the data, where a chosen measurement error is placed on $Z_i, i = 1, \ldots, p$; the unknown variance $\nu_i$ of this error density is also learnt.

Plots of $Z_i$ against $Z_1$ are included in Figure 1; $i = 2, 3, 4, 5$.

3.1. Learning correlation matrix & graph given toy data $D_T^{(S)}$

We learn the between-columns correlation matrix $\Sigma_C^{(S)}$ given the standardised toy data $D_T^{(S)}$ by employing the algorithm discussed in Section 2.3. We use $n = 300$, $p = 5$, and with the aim of estimating the normalisation $\hat{c}_i$ of the posterior in the $t$-th iteration, we choose $K = 20$ number of sampled data sets with $n'$ rows and $p$ columns, generated in each iteration, to bear the column-correlation matrix proposed in that iteration. Indeed, we set $n' = n$. Here $t = 0, \ldots, N$.

In the $t$-th iteration of our MCMC chain, the first block update in our Metropolis-within-Gibbs inference scheme, leads to the updating of the column correlation matrix to $\Sigma_t$ given the data $D_T^{(S)}$, using which we compute the value of the partial correlation matrix $R_t = [\rho_{ij}^{(0)}]$ in this iteration. Then the second block update leads to the updating of the values of the binary graph edge parameters to $g_{ij}^{(t)}$ and variance parameters to $\sigma_{ij}^{(t)}$, given $R_t$. Traces of the marginal posterior probability of five of the $S_{ij}$ parameters given data $D_T^{(S)}$ are shown in the top left panel Figure 2, while the joint posterior of all $G_{ij}$ and $\sigma_{ij}$ parameters given the learnt partial correlation matrix, is shown in the top left panel Figure 3. Histograms representing approximations of marginals of individual $R_{ij}$ and $\sigma_{ij}$ parameters, given the data and the learnt partial correlation respectively, occupy other panels of Figure 2 and Figure 3 respectively. Here $i < j; i, j = 1, \ldots, p$.

The graphical model of the data $D_T^{(S)}$ is presented in Figure 4. The fraction $n_{ij}$ of post-burnin samples of $g_{ij}$ with a value of 1, i.e. an approximation to the probability of existence of the edge joining nodes $i$ and $j$, is marked next to each edge of the graph, as long as $n_{ij} \geq 0.05$, i.e. the edge probability parameter $\phi_{ij}(R_{ij})$ is non-zero.

We note that the column correlation matrix $\Sigma_C^{(S)}$ of the Gaussian Process that models the data, is such that the partial correlation $\rho_{12}$ between $Z_1$ and $Z_2$ is learnt to be in the 95% HPD credible region of $\in [0.86, 0.95]$ approximately, which is close to the empirical value of 0.96. Again, the empirical value of $\rho_{13}$ is about -0.2, and the learnt value is $\in [-0.44, -0.27]$ approximately; empirical value of $\rho_{23}$ is about 0.04, and the learnt value is $\in [-0.11, 0.05]$ approximately. The other
partial correlation parameters have smaller values in the chosen correlation structure that the data is simulated to bear—each of which is close to the corresponding learnt value. This offers confidence in our method of learning the correlation matrix $\Sigma_C^{(S)}$ of the standardised toy data $D_T^{(S)}$.

### 3.2. Effect of measurement uncertainties in learning of correlation and graph

As we discussed in Section 2.5, in our approach, we are able to incorporate measurement errors in one or more of the variables $Z_1, \ldots, Z_p$, into the learning of the between-columns correlation structure given the toy data set $D_T^{(S)}$, that then affects the learning of the graphical model of this data. Let the unknown variance of the error distribution of $Z_i$ be $v_{\epsilon_i}$, ($i = 1, \ldots, p$). Then, one model of the total variance of $Z_i$ is $s^2_{ii} + v_{\epsilon_i}$, where $s^2_{ii}$ would be the variance of $Z_i$, had $Z_i$ been free of any measurement errors. However, $Z_i$ results from standardising the $i$-th observable $X_i$, by its empirical variance, i.e. $s^2_{ii}$ is unity by design. Thus, when measurement error is no longer absent, the variance of $Z_i$ increases to $1 + v_{\epsilon_i}$ assuming $Z_i$ to be independent of the error in $Z_i$, so that the variances add
Fig 3. Top left: trace of joint posterior probability density of the graph edge parameters $g_{ij}$ and variance parameters $\sigma_{ij}^2$, given the partial correlation matrix learnt in the first block update of our Metropolis-within-Gibbs inference scheme, given the 5-columned toy data set $D_5^{(S)}$. Other panels: histogram approximations to the marginal posterior probability density of three of the variance parameters.

Fig 4. Figure showing graphical model of toy data $D_5^{(S)}$—learnt in our Metropolis-within-Gibbs inference scheme in which we learn the correlation matrix $\Sigma^{(S)}_C$ of the data, simultaneously with the graph. The observables $Z_1, \ldots, Z_5$, measurements of which comprise the data, are marked by filled red circles, as the 5 nodes in this graph. The probability of the edge parameter $g_{ij}$ to exist (i.e. for $g_{ij}$ to be 1) for $i \neq j$, $i, j = 1, \ldots, 5$—is approximated by the fraction $n_{ij}$ of post-burnin iterations in which the current value of $g_{ij}$ is 1. This value of $n_{ij}$ is marked against the edge joining the $i$-th and $j$-th nodes, as long as $n_{ij} > 0.05$.

linearly. Indeed, in the presence of measurement error in $X_i$, the absolute value of the correlation $s_{ij}$ between $Z_i$ and $Z_j$ decreases (by a factor of $\sqrt{1 + \epsilon}$, in the model in which variances add linearly). On the other hand, the partial correlation $\rho_{ij}$ may increase or decrease (Liu, 1988). That such
is a possibility, is corroborated in the correlation and partial correlation structures of an example data set that comprises measurements of a 3-dimensional observable vector \((Z_1, Z_2, Z_3)^T\). Then, 
\[
\rho_{ij} = \frac{s_{ij} - s_{ik}s_{jk}}{\sqrt{(1 - s_{ik}^2)(1 - s_{jk}^2)}}, \quad i \neq j, i \neq k, k \neq j; i, j, k = 1, 2, 3.
\]
It follows that if \(|s_{ij}|\) and \(|s_{ik}|\) decrease, \(\rho_{ij}\) can either increase or decrease. But \(\rho_{ij}\) is the probability for the edge between the \(i\)-th and \(j\)-th nodes of the graph of this data, to exist, i.e. \(\rho_{ij} = \Pr(g_{ij} = 1)\). Then it is possible that while in the absence of measurement errors, \(g_{ij} = 1\) during a fraction \(n_{ij} < 0.05\) of the number of post-burnin iterations, in the presence of measurement error in \(X_i\), \(\rho_{ij}\) increases sufficiently to ensure that the fraction of iterations during which this edge exists is in excess of 0.05. If this happens, the edge between the \(i\)-th and \(j\)-th nodes will be included in the graphical model of the data when measurement error in \(X_i\) is acknowledged, but not when such error is not. In other words, ignoring measurement uncertainties can lead to a potential misrepresentation of the graphical model of the data at hand.

In our work, it is possible to produce graphs while ignoring, as well as acknowledging the measurement uncertainty in one or more components of the \(p\)-dimensional observable vector, \(n\) measurements of which results in the matrix-shaped data at hand. In fact, it is also possible to learn the variance of the error density of the components of this observable. We demonstrate this in the experiment discussed here.

In this implementation, we add measurement error to the 2nd component \(X_2\) of the 5-dimensional observable vector, \(n\) standardised measurements of which comprise data \(D^{(S)}_T\). We choose to impose
Gaussian measurement errors on \( Z_2 \), s.t. this Gaussian error density is \( \epsilon_2 \sim \mathcal{N}(0, 0.01) \). We then define a data set that is the same as \( D_T^{(S)} \), except that the 2nd column of this data is now sampled from a Gaussian with zero mean and variance given by \( 1+0.01 \), i.e. sampled from the convolution of a standard Normal, with the density \( \mathcal{N}(0, 0.01) \). The resulting data set is referred to as \( D_T^{(err)} \). Thus, the true value of the variance \( v_\epsilon \) of the 2nd column of the data \( D_T^{(err)} \) is 0.01. We will treat this variance as an unknown and in fact, learn this value using \( D_T^{(err)} \).

We learn the column-correlation matrix of this data using the method delineated in Section 2.3 above, using an MCMC chain that we run with this data \( D_T^{(err)} \). The only exception to the method of learning the \( s_{ij} \) parameters is that the correlation between the \( Z_i \) and \( Z_j \) is given by \( s_{ij} \sqrt{(1+v_\epsilon_i)(1+v_\epsilon_j)} \) in the model in which the variances are assumed to add linearly; \( i \neq j; i,j = 1, \ldots, p \). Thus, in addition to the \( p(p-1)/2 \) number of \( s_{ij} \) parameters, we now also learn the \( p \) number of \( v_\epsilon_i \) parameters, where the latter is the variance of the error distribution of \( Z_i \). We actually learn the standard deviation of the error density on \( Z_i \), namely \( \gamma_i \), i.e. \( v_\epsilon_i = \gamma_i^2 \).

In the \( t \)-th iteration, we propose \( \gamma_i \) from a Gaussian proposal density that has the mean given by the current value of the parameter in this iteration, and an experimentally chosen variance. Here \( t = 0, \ldots, N \). This is undertaken \( \forall i = 1, \ldots, p \). The \( S_{ij} \) parameters are always proposed from Truncated Normal proposal densities that are left and right truncated at -1 and 1 respectively and have mean given by the current parameter value, while the variance is fixed. Then the correlation parameters that define the correlation matrix in the \( t \)-th iteration, are \( s_{ij}^{(t*)} = s_{ij} \sqrt{(1+(\gamma_i^{(t*)})^2)(1+(\gamma_j^{(t*)})^2)} \), \( i \neq j; i,j = 1, \ldots, p \). We use Gaussian priors on the \( S_{ij} \) parameters, where such a Gaussian is centred on the empirical correlation between \( Z_i \) and \( Z_j \) in the data, while uniform priors are used on all other parameters. Using the proposed and current correlation matrices in our Metropolis-Hastings inferential scheme, we compute the marginals of the individual \( S_{ij} \) parameters as well as the \( \gamma_i \) parameters (\( \gamma_i^2 = v_\epsilon_i \)).

Histogram representations of the marginals (normalised to 1 at the mode), of some of these parameters are displayed in Figure 5. The 95% HPD credible region on \( \gamma_2 \) that we learn given this data is \([-0.2,0.2]\) approximately. The learnt standard deviations of the error densities of variables
other than $Z_2$, are 0 approximately. We also note from this figure that the changes in the partial correlations introduced by the introduction of the measurement error in one variable, can be both an increase and decrease—this is discussed above. The effect on introducing this measurement error on $Z_2$, on the graphical model of the data $D_T^{(err)}$, is presented in Figure 6. In this graphical model, the edge $G_{23}$ between the 2-nd and 3-rd nodes takes the value 1, with probability of about 0.16, while $n_{23}$ was less than 0.05 in the graphical model of data $D_T$—which differs from $D_T^{(err)}$ only in that the 2nd column is imposed with a Gaussian error of variance 0.01. Thus, the effect of introducing this error to measurements of the variable $Z_2$ propagates into the (partial) correlation structure of the data, to then affect the graphical model. Comparing this learnt graph to the graph of the toy data $D_T^{(S)}$, we recognise that measurement errors can distort the graphical model of a data.

4. Implementation on real data

In this section we discuss a real-data application of our Bayesian learning of the between-columns correlation matrix of a multivariate data set, and simultaneously learning the graphical model of the data at hand, given the updated correlation structure. We use the relatively well-known data sets on 11 different chemical attributes and “quality” classes of red and white wines, grown in the Minho region of Portugal (referred to a “vinho verde”); these data sets have been considered before by Cortez et al. (1998) and discussed in the website https://onlinecourses.science.psu.edu/stat857/node/223. The data consists of information on 1599 red wines and 4898 white wines. Each of these data sets consists of 12 columns that contain information on physiochemical attributes of the sampled wines; these properties are assigned the following names: “fixed acidity” ($X_1$), “volatile acidity” ($X_2$), “citric acid” ($X_3$), “residual sugar” ($X_4$), “chlorides” ($X_5$), “free sulphur dioxide” ($X_6$), “total sulphur dioxide” ($X_7$), “density” ($X_8$), “pH” ($X_9$), “sulphates” ($X_{10}$), “alcohol” ($X_{11}$) and “quality” ($X_{12}$). Then the $n$-th row and $i$-th column of the data matrix carries measured/assigned value of the $i$-th property of the $n$-th wine in the sample, where $i = 1, \ldots, 12$ and $n = 1, \ldots, n_{\text{orig}} = 1599$ for the red wine data $D_{\text{orig}}^{(red)}$, while $n = 1, \ldots, n_{\text{orig}} = 4898$ for the white wine data $D_{\text{orig}}^{(white)}$. We refer to the $i$-th vinous property to be $X_i$. Then $X_i \in \mathbb{R}_{\geq 0}$ $\forall i = 1, \ldots, 11$, while $X_{12}$ that denotes the perceived “quality” of the wine is a categorical variable. Each wine in these samples was assessed by at least three experts who graded the wine on a categorical scale of 0 to 10, in increasing order of excellence. The resulting “sensory score” or value of the “quality” parameter was a median of the expert assessments (Cortez et al., 1998). We seek the graphical model given each of the wine data sets, in which the relationship between any $X_i$ and $X_j$ is embodied, $i \neq j$; $i, j = 1, \ldots, 12$. Thus, we seek to find out how the different vino-chemical attributes affect each other, as well as the quality of the wine, in the sample at hand.

Here, $X_1, \ldots, X_{11}$ are real-valued, while $X_{12}$ is a categorical variable, and our methodology allows for the learning of the graphical model of a data set that in its raw state bears measurements of variables of different types. In fact, we standardise our data, s.t. $X_i$ is standardised to $Z_i$, $i = 1, \ldots, p$, $p = 12$. We work with only a subset data set, (comprising only $n < n_{\text{orig}}$ rows of the available $D_{\text{orig}}^{(c)}$: $n = 300$ typically). Thus, the data sets with $n$ rows, containing $Z_i$ values, ($i = 1, \ldots, p = 12$), are $n \times p$-dimensional matrices each; we refer to these data sets that we work with, as $D_S^{(white)}$ and $D_S^{(red)}$, respectively for the white and red wines.

Our aim is to learn the between-column correlation matrix $\Sigma_S^{(m)}$ given data $D_S^{(m)}$, and simultaneously learn the graphical model of this data using the methodology that we have developed above; $m = \text{white}, \text{red}$.

The motivation behind choosing these data sets are basically three-fold. Firstly, we sought multivariate, matrix-shaped, real-life data, that would admit graphical modelling of the correlations between the different variables in the data. Also, we wanted to work with data, results from—at least a part of—which exists in the literature. Comparison of these published results, with our independent results can then illustrate strengths of our method. Thirdly, treating the red and white wine data as data realised at different experimental conditions, we would want to address the question of the distance between these data, and we propose to do this by computing the distance between the graphical models of the two data sets. Hence our choice of the popular Portuguese red and white
wine data sets, as the data that we implement to illustrate our method on. It is to be noted that a rigorous vinaceous implications of the results, is outside the scope and intent of this paper. However, we will make a comparison of our results with the results of the analysis of white wine data that is reported in https://onlinecourses.science.psu.edu/stat857/node/223 precludes analysis of the red wine data.

4.1. Results given data \( D_{\text{white}}^{(\text{white})} \)

As per the underlying principle of our Bayesian learning methodology discussed above (Section 2), we model the observable vector \((Z_1, \ldots, Z_p)^T\) using a Gaussian Process. Within a Metropolis-within-Gibbs inferential scheme (discussed in Section 2.3), we first perform the updating of the \(p(p-1)/2\) parameters \(S_{12}, \ldots, S_{p-1\,p}\) that are the elements of the upper triangle of the between-column correlation matrix \( \Sigma_{S}^{(\text{white})} \), given data \( D_{\text{white}}^{(\text{white})} \) that has \(n = 300\) number of rows and \(p = 12\) number of columns. The proposal and prior densities on the \(S_{ij}\) parameters are as discussed in Section 2.2. The posterior probability density of the unknowns given the data is computed using these chosen priors and likelihood that is given in Equation 2.8. The updated correlation matrix is then used to compute the updated partial correlation matrix, given which, we update the binary graph edge parameters \(G_{ij}\) and the parameters \(\sigma_{ij}^2\) that provide the variance of the likelihood function defined in Equation 2.11. Priors and proposal densities of the unknowns are as discussed in Section 2.2. Marginals of all unknowns are computed, and traces of the joint posterior probability density in each of the two block updates in our MCMC chain, are examined. The graph edge probability parameter \(\phi_{ij}(R_{ij})\) is also computed from the graphs sampled in the post-burnin part of the MCMC chain.

The top-left panel of Figure 7 presents the trace of the joint posterior probability density of the correlation parameters \(S_{ij}\) given the data \( D_{\text{white}}^{(\text{white})} \). All the other panels of this figure include marginal posterior probabilities of some of the partial correlation parameters, with value \(\rho_{ij}\), where the \(i\)-th variable is the \(i\)-th vinous parameter listed above, with \(i = 1, \ldots, 12\); \(j \neq i, j = 1, \ldots, 12\). Figure 8 presents the trace of the joint posterior of the \(G_{ij}\) and \(\sigma_{ij}^2\) parameters, updated in the 2nd block of each iteration of our MCMC chain, at the updated (partial) correlation matrix. The other panels of this figure depict the histogram representation of the marginals of some of the \(\sigma_{ij}^2\) parameters. Thus we obtain the sample of graphs, \( \{G^{(i)}(p, R_i)\}_{i=N-N_{\text{post}}+1}^N \), where each graph is on the vertex set \( V = \{1, \ldots, p\} \) and is learnt given the partial correlation matrix \( R_i \) in the \(i\)-th iteration of our MCMC chain. We compute the graph edge probability parameter \(\phi_{ij}(R_{ij})\) for each \(ij\)-pair of nodes in this sample, and include only those edges in the graphical model of the \( D_{\text{white}}^{(\text{white})}\) data, that have non-zero \(\phi_{ij}(R_{ij})\), i.e. \(n_{ij} \geq 0.05\) (see Section 2.4). For these edges, the value \(n_{ij}\) is marked against the edge between the \(i\)-th and \(j\)-th nodes in the representation of this graphical model of this white wine data set, that is shown in Figure 9. Here \(i \neq j\), \(i, j = 1, \ldots, p = 12\).

4.1.1. Comparing against previous work done with white wine data

The graphical model of the white wine data presented in Figure 9 is strongly corroborated by the simple empirical correlations between pairs of different vino-chemical properties–this correlation structure is apparent in the “scatterplot of the predictors” included as part of the results of the “Exploratory Data Analysis” reported in https://onlinecourses.science.psu.edu/stat857/node/223 on the white wine data. They use the full white wine data set \( D_{\text{orig}}^{(\text{white})} \), to construct a matrix of scatterplots of \(X_i\) against \(X_j\), where \(i \neq j\); \(i, j = 1, \ldots, 11\). It is to be noted that in the data analysis reported in https://onlinecourses.science.psu.edu/stat857/node/224, the matrix of scatter-plots of pairs of variables \(i\) and \(j\) was included, where this set of variables excluded the last column of the white wine data—the column that informs us of the assessed “quality” of the wine.

When we compare our learnt graphical model with the results of this reported “Exploratory Data Analysis”, we remind ourselves that partial correlation (that drives the probability of the edge between the \(i\)-th and \(j\)-th nodes), is often smaller than the correlation between the \(i\)-th and \(j\)-th
variables, computed before the effect of a third variable has been removed (Sheskin, 2004). If this is the case, then an edge between nodes $i$ and $j$ in the learnt graphical model, is indicative of a high correlation between the $i$-th and $j$-th variables in the data. However, in the presence of a suppressor variable (that may share a high correlation with the $i$-th variable, but low correlation with the $j$-th), the absolute value of the partial correlation parameter can be enhanced to exceed that of the correlation parameter. In such a situation, the edge between the nodes $i$ and $j$ in our learnt graphical model may show up (within our defined 95% HPD credible region on edge probabilities, i.e. at probability higher than 0.05), though the empirical correlation between these variables is computed as low (Sheskin, 2004). So, to summarise, if the empirical correlation between two variables reported for a data set is high, our learnt graphical model should include an edge between the two nodes. But the presence of an edge between pair of nodes is not necessarily an indication of high empirical correlation between a pair of variables—as in cases where suppressor variables are involved. Guessing the effect of such suppressor variables via an examination of the scatterplots is difficult in this multivariate situation. Lastly, it is appreciated that empirical trends are only indicators as to the Gaussian-process based model of the learnt correlation structure (and the graphical model learnt thereby) given the data at hand.

As mentioned above, in this comparative exercise, $i \neq j$; $i, j = 1, \ldots, 11$. (Existence of edges to/from $Z_{12}$, i.e. the “quality” variable is corroborated by examining results reported in https://onlinecourses.science.psu.edu/stat857/node/225 on regressing this variable against the others). Indeed, these empirical scatterplots visually appear to suggest stronger correlations between fixed acidity and pH; residual sugar and density; free sulphur dioxide and total sulphur dioxide; density and total sulphur dioxide; density and alcohol; alcohol and density—than amongst other pairs of variables. In our learnt graphical model, these are in fact
Fig 8. Top left panel: trace of the joint posterior probability of the graph edge parameters $G_{ij}$ and the variance parameters $\sigma^2_{ij}$ that are the variances used in the likelihood function defined in Equation 2.11; these parameters are updated within the 2nd block update of our Metropolis-within-Gibbs inferential scheme, at the correlation matrix that is updated given the data $D_S^{(white)}$ of Portuguese white wine samples. Here $i \neq j; i, j = 1, \ldots, 12$. All other panels: histogram representations of marginal posterior probability densities of some of the variance parameters learnt given the correlation matrix that is itself learnt, given data $D_S^{(white)}$.

the very node pairs that are identified to have edges (at probability in excess of 0.05) between them. Also, in [https://onlinecourses.science.psu.edu/stat857/node/225](https://onlinecourses.science.psu.edu/stat857/node/225), the multiple and polynomial regression analysis of the predictors $X_1, \ldots, X_{11}$ on the response variable termed “quality”, i.e. $X_{12}$, suggested the variables alcohol and volatile acidity to have maximal effect on quality; again, alcohol and volatile acidity are the two variables included in this work for further attempts at classification of the white wines in the sample (using tree-based regression and random forests). Indeed, this is corroborated in our learning of the graphical model that manifests edges between the nodes corresponding to variables: alcohol-quality, and volatile acidity-quality.

### 4.2. Results given data $D_S^{(red)}$

The $D_S^{(red)}$ data is the standardised version of a subset of the original red wine data set $D_{orig}^{(red)}$. $D_S^{(red)}$ comprises $n = 300$ rows and $p = 12$. Thus, the $D_S^{(red)}$ data comprises $n$ measurements of the $p$-dimensional observable vector $(Z_1, \ldots, Z_p)^T$, where $Z_i$ is the standardised $X_i$, where $X_i$ has been described above in Section 2; $i = 1, \ldots, p = 12$. As with the white wine data, we implement data $D_S^{(red)}$ in our Metropolis-within-Gibbs-based inference scheme to learn the between-column correlation matrix $\Sigma_S^{(red)}$ of the red wine data, and learn the graphical model of data $D_S^{(red)}$, given the learnt correlation $\Sigma_S^{(red)}$.

The marginal posterior of some of the partial correlation parameters $\rho_{ij}$ computed using the elements of the correlation matrix $\Sigma_S^{(red)}$ that is updated in the first block of Metropolis-within-Gibbs, are presented in Figure 3 of the Supplementary Section. In the second block, we update the
edge parameters $G_{ij}$ of the graph $G(p, R)$ given the newly updated $R$. Figure 4 of the Supplementary Section presents the trace of the joint posterior probability of the $G_{ij}$ parameters and the variance parameters $\sigma_{ij}^2$ (of the Folded Normal likelihood). The marginal of some of the variance parameters are also shown in the other panels of this figure. The inferred graphical model of the red wine data is included in Figure 10.

4.2.1. Comparing against empirical work done with red wine data

To the best of our knowledge, analysis of the red wine data has not been reported in the literature. In lieu of that, we present a matrix of pairwise scatterplots of the first 11 columns of the red wine data in Figure 5 of the Supplementary Material. Firstly, we compare the learnt correlations (see plots of $R_{1j}$, for $j = 2, \ldots, 9$, as displayed in Figure 3 of the Supplementary Section), to the correlations manifest in this matrix of scatterplots, to check for compatibility between the learnt and empirical results. We note that all moderately correlated variable pairs, as represented in these scatterplots, are joined by edges in our learnt graphical model of the red wine data—as is to be expected if the learning of the graphical model is correct. Such pairs include fixed acidity-citric acid,
fixed acidity-density, fixed acidity-pH, volatile acidity-citric acid, free sulphur dioxide-total sulphur dioxide, density-alcohol. However, an edge may exist between a pair of variables even when the apparent empirical correlation between these variables is low (see Section 4.1.1); this owes to the effect of other variables. Such effects give rise to the remaining edges seen in our learnt graphical model of the red wine data, namely, the edges between residual sugar-density and residual sugar-alcohol. Indeed, we examine this more closely by regressing residual sugar against the remaining 10 variables (other than quality); the results of this Ordinary Least Squares regression exercise are included in Figure 6 of the Supplementary Material. It shows that in this regression model, $Z_7$ (density) and $Z_{10}$ (alcohol) affect residual sugar more than any of the other covariates—indeed, in our learnt graphical model of the red wine data, it is density and alcohol that residual sugar has edges with, respectively.

We further undertook a modelling of the relationship between the response variable “quality” ($Z_{12}$) and the other 11 covariates ($Z_1$ to $Z_{11}$), via an OLS regression in which quality is regressed over the other vino-chemical attributes. This modelling suggests the strongest effect of alcohol and volatile-acidity on quality (see Figure 7 of Supplementary Material); this trend is replicated in our learnt graphical model of the red wine data.

5. Hellinger distance between posterior probability densities of graphs given white and red wine datasets

We are interested in answering the question of whether two multivariate datasets $D_1$ and $D_2$, are independent of each other or not; in effect, the question addresses the possible independence of the
pdfs that the two data sets at hand are sampled from. This is of course a hard question to address when the data comprise unequal, but large number of measurements \((n_1 \text{ and } n_2 \text{ respectively})\) of two high-dimensional vector-valued observables, s.t. \(D_m\) comprises measurements of the standardised variable \(Z_m \in \mathbb{Z}_m \subseteq \mathbb{R}^p, m = 1, 2\). We address this question by learning the graphical model of each dataset as per the methodology discussed above, and then by computing the Hellinger distance between the posterior probability density of the graphical model \(G_{p,\Phi_m(R)}\) of data \(D_1\), the between-columns partial correlation matrix of which is \(R^{(p \times p)}\), and the posterior of the graphical model \(G_{p,\Phi_m(R)}\) given the other data set, the partial correlation matrix–that is updated given the data during the first block update. So we marginalise the \(\sigma\) parameters, given the partial correlation matrix–that is updated given the data during the first block update. Thus we see that the Hellinger distance is closely related to the Bhattacharyya distance between two densities: 

\[
D^2_H(g, f) = \int \left( \sqrt{g(x)} - \sqrt{h(x)} \right)^2 dx
\]

\[
= \int g(x)dx + \int h(x)dx - 2 \int \sqrt{g(x)} \sqrt{h(x)}dx
\]

\[
= 2 \left( 1 - \int \sqrt{g(x)} \sqrt{h(x)}dx \right). \tag{5.1}
\]

Thus we see that \(D^2_H(\cdot, \cdot)\) takes values in \([0, 2]\), where the value of 0 is attained when the two densities are equal, and the value of 2 is attained when the densities are singular. The Hellinger distance is closely related to the Bhattacharyya distance between two densities: 

\[
D_B(g, f) = -\log \left[ \int \left( \sqrt{g(x)} \sqrt{h(x)} \right)^2 dx \right]
\]

(Bhattacharyya, 1943).

For the standardised wine data \(D_S^{(m)}\) where \(m = \text{red, white}\), the posterior probability density of the graph edge parameters \(G_{ij}^{(m)}\) is \(\pi(G_{11}^{(m)}, G_{12}^{(m)}, \ldots, G_{p-1}^{(m)} | R_m)\), where we learn the partial correlation matrix \(R_m\), given this data. Indeed, during the second block update of our Metropolis-within-Gibbs inference, we compute the value of the joint posterior probability of all the \(G_{ij}\) and \(\sigma^2_{ij}\) parameters, given the partial correlation matrix–that is updated given the data during the first block update. So we marginalise the \(\sigma^2_{ij}\) out of this joint posterior of all edge and variance parameters, i.e. marginalise out all \(\sigma^2_{ij}\) for all \(i, j = 1, \ldots, p i \neq j\), to achieve the joint posterior probability density of the graph edge parameters given the partial correlation matrix of the data at hand.

So, at the end of the \(t\)-th iteration, we compute the value of the posterior \(\pi(G_{11}^{(mt)}, G_{12}^{(mt)}, \ldots, G_{p-1}^{(mt)} | R_{mt})\), \(t = 0, \ldots, N_{iter}\). Given the availability of the posterior at discrete points in its support, implementation of the integral of the relevant posterior probability density in the definition of the Hellinger distance is replaced by the discretised version of this definition. So the square of the Hellinger distance \(D^2_H(\text{white, red})\) between the posterior probability densities

\[
p_{\text{white}} := \pi(G_{11}^{(\text{white})}, G_{12}^{(\text{white})}, \ldots, G_{p-1}^{(\text{white})} | R_{\text{white}})
\]

and

\[
p_{\text{red}} := \pi(G_{11}^{(\text{red})}, G_{12}^{(\text{red})}, \ldots, G_{p-1}^{(\text{red})} | R_{\text{red}})
\]
is discretised as

$$D_H^2(p_{\text{white}}, p_{\text{red}}) = \sum_{t=N_{\text{burnin}}+1}^{N_{\text{iter}}} \frac{(\sqrt{p_{\text{white}}^{(t)}} - \sqrt{p_{\text{red}}^{(t)}})^2}{N_{\text{iter}} - N_{\text{burnin}}},$$

(5.2)

where for the \( m \)-th data set, \( m = \text{white, red} \), \( p_m^{(t)} \) is the value of the posterior of the graph edge parameters given the partial correlation matrix, in the \( t \)-th iteration, and we consider only post-burnin posterior samples for the computation of the Hellinger distance. In other words, \( p_m^{(t)} := \pi(G_{\text{white}}^{(mt)}, G_{\text{red}}^{(mt)}, \ldots, G_{p-1}^{(mt)} \mid \mathbf{R}_{ml}) \). The Bhattacharyya distance can be similarly discretised.

However, MCMC does not provide normalised posterior probability densities—as we employ uniform priors on the variance parameters, the marginalised posterior probability of the edge parameters is known only up to an unknown scale. In fact, what we record at the end of the \( t \)-th iteration, is the logarithm \( \ln(p_m^{(t)}) \) of the un-normalised posterior of the edges of the graph given the \( m \)-th data (\( m = \text{red, white} \)). Hence the Hellinger distance between the red and white wine graphs that we compute is only known upto a constant normalisation \( S \) that we use to scale \( p_{\text{white}}^{(t)} \) and \( p_{\text{red}}^{(t)} \), \( \forall t, 0, \ldots, N_{\text{iter}} \). We choose this scale parameter \( S \) to ensure that the scaled, log posterior of the graph in the \( t \)-th iteration, is easily exponentiable, as in \( \exp(\ln(p_m^{(t)})/s) \). One way of achieving this is to choose the global scale \( S \) as: \( \max\{\ln(p_{\text{white}}^{(0)}), \ln(p_{\text{white}}^{(1)}), \ldots, \ln(p_{\text{white}}^{(N_{\text{iter}})}), \ln(p_{\text{red}}^{(0)}), \ldots, \ln(p_{\text{red}}^{(N_{\text{iter}})})\} \).

Indeed, this definition yields the value of the global scale \( S \) to be \( S = \ln(p_{\text{red}}^{(1474)}) \approx 142.7687 \); we then use \( \exp(\ln(p_m^{(t)})/s) \) in Equation 5.2. The computed Hellinger distance will of course be affected by the global scaling parameter that we use. We also compute the Bhattacharyya distance using the (similarly scaled) logarithm of the posterior values as obtained from MCMC; again the Bhattacharyya distance is unnormalised given our incomplete knowledge of the posterior of the graph at any iteration.

Alternatively, we could define a (discretised version of the) odds ratio of unscaled logarithm of the unnormalised posterior densities of the graphical models learnt using MCMC, given the two real wine data sets, as \( \int (\log(g(x)) - \log(h(x))) \, dx \); such is then a divergence measure that we define as

$$O_p(p_{\text{white}}, p_{\text{red}}) := \sum_{t=N_{\text{burnin}}+1}^{N_{\text{iter}}} \left[ \log(p_m^{(t)} - \log(p_m^{(t)}) \right].$$

(5.3)

Then scaling the log posterior given either data set, at any iteration, by the scale value of \( s = 142.7687 \) approximately—which is the maximal value of the log posterior of the graph in the 1474-th iteration, given the red wine data—we get \( D_H(p_{\text{white}}, p_{\text{red}}) \approx 0.1153 \), so that the logarithm of this value of the Hellinger distance is \( \ln(0.1153) \approx -2.1602 \). Similarly, using the same scale, the Bhattacharyya distance is \( D_B(p_{\text{white}}, p_{\text{red}}) \approx -1.7623 \), where we recall that this measure is a logarithm of the distance. Indeed, values of these distances are affected by our choice of the scale \( S \).

However, what is of interest is the comparison of the ratio of the Hellinger distance between posterior probability of graphical models given two datasets, for a given choice of the scale \( S \), to the uncertainty inherent in the graphical model of either data, as computed at that chosen \( S \). This uncertainty inherent to the graphical model given the \( m \)-th data can be computed as the difference

$$D_{max,s}(m) := \max\{\exp(\ln(p_m^{(0)})/s), \exp(\ln(p_m^{(1)})/s), \ldots, \exp(\ln(p_m^{(N_{\text{iter}})})/s)\} - \min\{\exp(\ln(p_m^{(0)})/s), \exp(\ln(p_m^{(1)})/s), \ldots, \exp(\ln(p_m^{(N_{\text{iter}})})/s)\},$$

computed for this choice of \( S \). By this definition, \( D_{max,s}(m) \) provides the separation between the maximal and minimal posteriors of graphs scaled by a chosen scale \( S \), generated in the MCMC run using the \( m \)-th data; \( m = \text{white, red} \). So for a chosen scale, we compute the ratio of the distance between the two graphical models, to the uncertainty inherent in a graphical model, namely \( \sqrt{D_H^2(p_{\text{white}}, p_{\text{red}})/D_{max,s}(red)} \), and compare that with \( \sqrt{D_H^2(p_{\text{white}}, p_{\text{red}})/D_{max,s}(white)} \).

This comparison is depicted in the left panel of Figure 11 that shows that the difference \( D_{max,s}(white) \) between the scaled posterior of graphs given the white wine data is about 0.0694 while
$D_{\text{max},s}(\text{red})$ given the red wine data is about 0.05521. These values are compared to the Hellinger distance (between scaled posteriors) of about 0.1153, between graphs given the red and white wine data. Thus, $D_H(p_{\text{red}}, p_{\text{white}})$ is about $1.66D_{\text{max},s}(\text{white})$ and about $2.1D_{\text{max},s}(\text{red})$, i.e. the distance between the graphical models given the two data sets is higher than the internal uncertainties within the graphs inferred upon, given either data set. Then intuitively speaking, the Hellinger distance between the graphical models given the red and white wine datasets, may suggest independence of the data sets, but the question of interpretation of the computed values of distance/divergence between a pair of graphs, cannot be properly addressed unless a test of hypothesis can be undertaken to test if the computed distance is different from 0, i.e. the two graphical models (given the real red and white wine Portugese data sets in our work), are different.

Compared to these, the sample mean of the log odds of the posterior of the graphs generated in the post-burnin iterations, given the two data is 18.9273, which is about 1.9 times the maximal difference between the log posterior values of graphs achieved in the MCMC run with the white wine data, and about 2.4 times that for the red wine data (see Figure 11). Again, this suggests that the log odds as a measure of distance between the graphical models given these two wine data sets, is significantly higher than the uncertainty internal to the results for each data.

![Figure 11](image-url)

**Fig 11.** Left: minimum and maximum values of the scaled posterior probability density of the graph sampled in an iteration in the MCMC chain run with the red wine data, plotted in dotted lines against the number of the iteration. The difference between these values is depicted within the band delineated by these lines. The broken lines show the same for the results obtained from the MCMC chain run using the white wine data. The value of the Hellinger distance $D_H(p_{\text{red}}, p_{\text{white}})$ computed using the scaled posterior probabilities of the graphical models given the two wine data sets, is also marked, as about 0.1153. All log posterior values are scaled by a chosen global scale and exponentiated (as discussed in the text). Right: similar to the left panel, except that here, the ratio of the logarithm of the unscaled posteriors is used; the value of the log odds between the posteriors of the red and white wine data sets is marked to be about 18.927.

This work shows a simple and easily calculable method for comparing multiple, high-dimensional data sets, for their independence.

6. Learning the human disease-symptom network

Our methodology for learning the graphical model of a given data, can be implemented even for a highly multivariate data, i.e. one that generates a graph with a very large number of nodes. In this section, we discuss such a graph (with $\gtrsim 8000$ nodes) that describes the correlation structure of the human disease-symptom network.

Hoehndorf et al. (2015) (HSG hereon) learn this network by considering the similarity parameter for each pair of diseases that are elements of an identified set of diseases in the Human Disease Ontology (DO), that contains information about rare and common diseases, and spans heritable, developmental, infectious and environmental diseases. Here, the “similarity parameter” between one
disease and another, is computed using the ranked vectors of "normalised pointwise mutual information" (NPMI) parameters for the two diseases, where the NPMI parameter describes the relevance of a symptom (or rather, a phenotype), to the disease in question. HSG define the NPMI parameter semantically, as the normalised number of co-occurrences of a given phenotype and a disease in the titles and abstracts of 5 million articles in Medline. To do this, they make use of the Aber-OWL: Pubmed infrastructure that performs such semantical mining of the Medline abstracts and titles. The disease-disease pairwise semantic similarity parameters–computed using the degree of overlap in the relevance ranks of phenotypes associated with each disease–result in a similarity matrix, which HSG turn into a diseasedisease network based on phenotypes. To do this, they only choose from the top-ranking 0.5% of disease-disease similarity values. The phenotypes associated with the diseases, and the corresponding scoring functions (such as the NPMI), exist in the file “doid2hpo-fulltext.txt.gz” at http://aber-owl.net/aber-owl/diseasephenotypes. In fact, this file contains information about \( N_{\text{dis}} \) diseases, and the semantic relevance of each of the \( N_{\text{pheno}} \) phenotypes to each disease, as quantified by NPMI parameter values, in addition to other scores such as \( t \)-scores and \( z \)-scores. In this file, \( N_{\text{dis}} = 8676 \) and \( N_{\text{pheno}} = 19323 \).

In the phenotypic similarity network between diseases that HSG report, diseases are the nodes, and the edge between two nodes exists in this undirected graph, if the similarity between the nodes (diseases) is in the highest-ranking 0.5% of the 38,688,400 similarity values. They remove all self-loops from the network and all nodes with a degree of 0. Their network is presented in http://aber-owl.net/aber-owl/diseasephenotypes/network/. The network analysis was performed using standard softwares and they identify multiple clusters in their network, with agglomerates of some clusters (of diseases), found to correspond to known disease-classes. The "Group Selector" function on their visualisation kit, allows for the identification of 19 such clusters in their disease-disease network, with each cluster corresponding to a disease-class. This function also allows identification of the number of diseases (i.e. nodes) in each disease-class (see left panel of Figure 13). The sum of the number of nodes over their identified 19 clusters, is 5059. The number of edges in their network is reported to be 65,795. The average node degree is then about 26.2. The right panel of Figure 13 displays the ratio of intra-class variance to the inter-class variance of each disease-class; the value of the area under the Receiver Operating Characteristic curve (ROCAUC) for each cluster is opverplotted, where the ROCAUC value for the \( i \)-th cluster can be interpreted as the probability that a randomly chosen node is ranked as more likely to be in the \( i \)-th class than in the \( j \)-th class, with \( i \neq j \); \( i,j = 1,\ldots,19 \) (Hajian-Tilaki, 2013).

HSG’s network then manifests a similarity-structure that is computed using the available NPMI parameter values. Our interest is in learning the disease-disease graphical model, with each edge of such a graphical model learnt to exist at a learnt probability. We perform such learning using the NPMI semantic-relevance data that is made available for each of the \( N_{\text{dis}} \) number of diseases, by HSG–we refer to this data as the human disease-phenotype data \( D_{\text{DPH}} \). Using \( D_{\text{DPH}} \), we first compute the partial correlation between any pair of diseases, for each of which, information on the ranked (semantic) relevance of each of the \( N_{\text{pheno}} \) phenotypes exist, in this given dataset. Upon computation of the pairwise partial correlations, the graphical model for the \( D_{\text{DPH}} \) data is learnt.

We compute the partial correlation \( R_{ij} \) between the \( i \)-th and \( j \)-th diseases in the \( D_{\text{DPH}} \) data, \((i,j = 1,\ldots,N_{\text{dis}}, i \neq j)\), in the following way. We rank the NPMI parameter values for the \( i \)-th disease and each of the \( N_{\text{pheno}} \) phenotypes, with the phenotype of the highest semantic relevance to the \( i \)-th disease assigned a rank 1. Let the rank vector of phenotypes, by semantic relevance to the \( i \)-th disease take the value \( \eta_i \) and similarly, the rank vector of phenotypes relevant to the \( j \)-th disease is \( \eta_j \). We compute the Spearman rank correlation \( \rho_{ij}^{(\text{rank})} \) of vectors \( \eta_i \) and \( \eta_j \). Then we compute the partial correlation \( R_{ij} \forall i,j = 1,\ldots,N_{\text{dis}}; i \neq j \), between the \( i \)-th and \( j \)-th nodes of our undirected graph, using the computed values of the Spearman rank correlation in \( \{\rho_{ij}^{(\text{rank})}\} \). It is useful to define the partial correlation using the Spearman rank correlation, rather than the correlation between the vector of normalised NPMI values, since we intend to correlate the \( i \)-th disease with the \( j \)-th disease depending on how relevant a given list of phenotypes is, to each disease, i.e. depending on the ranked relevance of the phenotypes.

To learn the graphical model given this partial correlation structure in \( R = [R_{ij}] \) (that is itself computed from the data \( D_{\text{DPH}} \), in the previous sections, we have delineated an MCMC-based
inference strategy, that helps us learn the edge parameters, as well as the variance of the likelihood. However, the data that we want to learn the graphical model for, is so highly multivariate−i.e. there are so many edges in the proposed graph−that we forego iterating over the multiple samples of edge and variance parameter values, and compute the graphical model for this data, by computing the posterior probability for each edge, given the computed partial correlation structure. In fact, the graphical model of data $D_{DPH}$ that we present, comprises only those edge parameters, the posterior probability of which exceeds 0.9.

Here, the posterior probability density of the edge $G_{ij}$ (=0 or 1) between the $i$-th and $j$-th diseases, is proportional to the likelihood and prior:

$$
\pi(G_{ij}|R_{ij}) \propto \ell(G_{ij}|R_{ij})\pi_0(G_{ij}),
$$

where the prior on $G_{ij}$ is $Bernoulli(0.5) \forall i, j$, and the likelihood is the Folded-Normal likelihood that we chose to work with in our learning, as discussed before in Section 2.2, i.e. likelihood given $R = [R_{ij}]$ is

$$
\prod_{i \neq j, i=1}^{N_{dis}} \frac{1}{\sqrt{2\pi}\sigma_{ij}} \exp \left[ -\frac{(G_{ij} - R_{ij})^2}{2\sigma_{ij}^2} - \frac{(G_{ij} + R_{ij})^2}{2\sigma_{ij}^2} \right],
$$

where the variance parameters $\{\sigma_{ij}^2\}_{i \neq j, i=1}^{N_{dis}}$ are defined as $\sigma_{ij}^2 = R_{ij}(1 - R_{ij})$.

**Definition 6.1.** Our visualised graph is a sub-graph of the full graph $G(N_{dis}, R)$ of data $D_{DPH}$, the between-columns partial correlation matrix of which is $R = [R_{ij}]$, $i \neq j$, $i, j = 1, \ldots, N_{dis}$, such that this visualised graph is defined to consist only of edges in the set: $E' := \{G_{ij} = 1\mid \pi(G_{ij}|R_{ij}) \geq 0.9; i \neq j, i, j = 1, \ldots, N_{dis}\}$. This visualised graph has 6052 number of nodes (diseases) and 145210 edges, so that the average node degree is about 24. It is a random undirected graphical model and represents our learning of the human disease phenotype graph (displayed in Figure 12).

7. Conclusion

In this work, we present a methodology that allows for the simultaneous learning of the inter-column correlation of a matrix-shaped dataset, and the graphical model of such data, where this undirected graphical model comprises random edge variables that can take values of either 1 or 0. Thus, the between-columns correlation matrix and the graph of the data, are both treated as random variables, and learnt within a Metropolis-within-Gibbs inference scheme in which the correlation matrix is first updated given the data, and the graph is then updated at the freshly updated correlation, without requiring to resort to the assumption of decomposability. We marginalise over all between-row correlation matrices, to achieve a closed-form likelihood for the between-column correlation matrix, given the data. The likelihood of an edge parameter of the graph, given the between-columns correlation, is chosen to be the Folded Normal density with mean given by the corresponding partial correlation (computed using the updated correlation matrix) and variance that is also learnt.

Consequently, the method is capable of acknowledging errors in the measurement of any observable−repeated measurement of which comprise a column in the dataset. The effect of ignoring such existent measurement errors, on the learning of the between-columns correlation matrix, and ultimately on the graphical model of the data, is demonstrated using a simple, low-dimensional simulated dataset. Even in such a low-dimensional example, the difference made to the graph, by the inclusion of measurement errors, is clear.

In addition, the method allows for the learning of the correlation matrix and the graphical model with objective uncertainties, namely the 95% HPD credible regions. On the graphical model, these uncertainties are imposed by choosing to compose the model with only those edges, the probability of existence of which (within the post-burnin part of the MCMC run), is $\geq 0.05$. Each included edge is presented with this probability of existence marked against the graph.

Upon learning the graphical model given a data set, we can then compute the distance between the graphs. We demonstrated this by computing the distance between the learnt graphical model of 11 different vino-chemical parameters of a sample of Portugese white wines, and that of Portugese red wines.
Fig 12. The human disease phenotype graphical model that we learn using the disease-disease partial correlation obtained using the computed Spearman rank correlation between the rank vectors of a list of phenotypes, where the phenotype ranking reflects semantic relevance of a phenotype to the disease in question (quantified by HSG as the NPMI parameter in the D\textsubscript{DPH} dataset). Only edges with posterior probability ≥ 0.9 are included in this graph, and nodes that have edges with posterior less than 0.9, are discarded, resulting in 6052 diseases (nodes) remaining in this graph. There are 145210 edges in the displayed graph. All diseases identified by name by HSG, to belong to one of the 19 given disease class, are presented above in the same colour; the colour key identifying these classes, is attached. To draw the graph, we used a Python-based code that implements the Fruchterman-Reingold force-directed algorithm.

wines. The Hellinger distance between the posterior probability of the graphical models, given the red and white wine datasets, was expressed in units of the uncertainty in learning either graphical model. This inter-graphical-model distance is sufficiently higher than the intra-graphical-model distance, for both the red-wine and the white wine datasets, to intuitively suggest inequality of the pdfs that the red and white wine vino-chemical datasets are sampled from.

While in our learning of the correlation structure and graphical model of a given dataset, we have in general employed MCMC-based inference methods, (Metropolis-within-Gibbs, to be precise), we can avoid such inference, when faced with the task of learning very large graphs, i.e. a graphical model of a highly multivariate dataset. We learnt such a graphical model that comprised ≥ 8000 nodes, without resorting to MCMC-based inference. This was the human disease-symptom network that expresses correlation between the i-th and j-th diseases based on the (rank) correlation of the vector of symptoms, where the symptoms for the i-th disease is ranked by relevance, ∀ i, j =
The ranking of a given vector of symptoms was performed based on the frequency of co-occurrences of the text for that symptom, with the \( i \)-th disease, in a documented set of titles and abstracts of medical science articles. This existing text-mined information was converted into a vector of ranks for a given set of symptoms. We then computed the Spearman rank correlation between the (symptom) vector of ranks for the \( i \)-th and \( j \)-th diseases, to then compute the partial correlation structure of this disease-symptom dataset. The likelihood of the \( ij \)-th edge of the sought disease-symptom graphical model was defined as Folded Normal density with mean given by the partial correlation \( \rho_{ij} \) computed from the rank correlation between the \( ij \)-th disease pair, and variance that we fixed to \( \rho_{ij}(1 - \rho_{ij}) \). (In contrast, in the MCMC chain we ran, this variance was treated as an unknown, and learnt). Bernoulli priors with rate 0.5 was imposed on the edge between these diseases, and the posterior probability of each edge in this graphical model was computed. Only edges with posterior in excess of 0.9 were retained in the final graphical model. Diseases belonging to the same medically-recognised disease-class are displayed in our learnt network in the same colour and symbol-type.

This is a very useful and practical way of learning very large networks, in real time, as long as the correlation structure is empirically known. This is often possible when the problem of learning the correlation can be cast into a semantic context—as was done in the example we consider, in learning the disease-disease correlation in terms of the associated symptoms, ordered by relevance. Other situations also admit such possibilities, for example, the product-to-product, or service-to-service correlation in terms of associated emotion, (or some other response parameter), can be semantically gleaned from the corpus of customer reviews uploaded to a chosen internet facility, and the same used to learn the network of products/services. Importantly, this method of probabilistic learning of small to large networks, is useful for the construction of networks that evolve with time, i.e. of dynamic networks.
Throughout, we refer to our main manuscript as WMC.

S1. Model checking

In the Section 3 of WMC, we discussed the learning of $\Sigma_C^{(S)}$ using the $n$ rows of the standardised toy data $D_T^{(S)}$, which is a 300-row subset from the 5-columned simulated dataset $D_{\text{orig}}$, discussed in that section of the main paper, where $D_{\text{orig}}$ is generated to abide by a chosen correlation matrix $\Sigma_{\text{true}}$ that is defined in Section 3 of WMC. Then $D_T^{(S)}$ comprises 300 different measurements of the 5-columned vector $Z := (Z_1, Z_2, Z_3, Z_4, Z_5)^T$, where $Z_i$ is a standardised variable $i = 1, \ldots, 5$. Having learnt the parameters of the Gaussian Process in Section 3 of WMC–of which the standardised observable $Z \in \mathbb{R}^5$ is a realisation–we want to predict values of $Z_i$ for values of $Z_j$ as given in a new or test data, $(j \neq i; i, j = 1, \ldots, 5)$; for our purposes, $p=5$. This test data $D_{\text{test}}$ is built to be independent of the training data $D_T^{(S)}$, as $q$ rows of the standardised version of the bigger data set $D_{\text{orig}}$–of which $D_T^{(S)}$ is also a subset–although the $q$ rows of $D_{\text{orig}}$ that comprise $D_{\text{test}}$, are chosen as distinct from the $n$ rows of the training data $D_T^{(S)}$. Our standardised test data $D_{\text{test}}$ has $p = 5$ columns and $q$ rows; in fact, we set $q = n$. We will predict $Z_2, Z_3, Z_4$ at each of the known $q$ ($=n$) values of $Z_1$ in the test data $D_{\text{test}}$, given the GP parameters (i.e. the between-columns covariance matrix $\Sigma_C^{(S)}$) that we learn using the training data. No prediction of $Z_5$ is undertaken. In fact, we will sample from the posterior predictive density of $Z_2, Z_3, Z_4$, given the correlation matrix learnt using training data $D_T^{(S)}$, and values of $Z_1$ in the test data $D_{\text{test}}$. We compare the predicted values of $Z_2, Z_3, Z_4$ against their empirical values in the test data. Such a comparison constitutes the checking of our models as well as the results (of the learning of $\Sigma_C^{(S)}$ given the training data $D_T^{(S)}$). We clarify this prediction now.

As we learn the marginal posterior probability density of each correlation parameter $S_{ij}$ given $D_T^{(S)}$, we need to choose a summary of this marginal distribution, at which the prediction of the $z_{ik}$ is undertaken, $i = 2, 3, 4, k = 1, \ldots, n$. We choose the mode of the marginal as this summary. Denoting the value of $Z_i$ in the $k$-th row of the test data as $z_{ik}$, $(k = 1, \ldots, q = n)$, we undertake the learning of $\{z_{2k}, z_{3k}, z_{4k}\}_{k=1}^n$ in the test data $D_{\text{test}}$, given values of $\{z_{1k}\}_{k=1}^n$ in $D_{\text{test}}$ and the modal values of $S_{ij}$ learnt using the training data $D_T^{(S)}$. In our Bayesian, MCMC-based inferential approach, this learning is equivalent to sampling from the posterior predictive of the unknowns, i.e. performing MCMC-based posterior sampling from

$$
\pi(z_{21}, z_{31}, z_{41}, \ldots, z_{2n}, z_{3n}, z_{4n}|z_{11}, \ldots, z_{1n}; s_{12}^{(M)}, \ldots, s_{1p}^{(M)}, s_{23}^{(M)}, \ldots, s_{2p}^{(M)}, \ldots, s_{p-1}^{(M)}, p),
$$

where $s_{ij}^{(M)}$ represents the modal value of the correlation parameter $S_{ij}$ that we learn given the training data $D_T^{(S)}$. We define the learnt “modal” correlation matrix to be $\Sigma_C^{(M)} = \{s_{ij}^{(M)}\}$.

In the $t$-iteration, we propose a value $z_{ik}^{(ts)}$ from a Gaussian proposal density with mean given by the current value $z_{ik}^{(t-1)}$ of this variable, and fixed variance $\nu_{ik}$, i.e. the proposed value is $z_{ik}^{(ts)} \sim \mathcal{N}(z_{ik}^{(t-1)}; \nu_{ik})$; we do this for $i = 2, 3, 4$ and $\forall k = 1, \ldots, n$, at each $t = 0, \ldots, N$. Then the proposed data in the $t$-th iteration is $D^{(ts)} = \{z_1, z_2^{(ts)}, z_3^{(ts)}, z_4^{(ts)}, z_5\}$, where $z_i = (z_{i1}, \ldots, z_{in})^T$, $i = 1, \ldots, 5$. The posterior of the unknowns is then given as in Equation 2.8, with the data given by $D^{(ts)}$ and the modal correlation matrix given by $\Sigma_C^{(M)}$ learnt using the training data set $D_T^{(S)}$. The
normalisation of the posterior is computed in the $t$-th iteration in the way described in Section 2.3 of WMC, at the $\Sigma_C^{(M)}$. We use uniform priors on all unknowns. So in each iteration, we (use Random-Walk Metropolis to) sample from the posterior of the unknown variables, given $\Sigma_C^{(M)}$ and the data on the $q = n$ number of $Z_1$ values in the test data $D_{\text{test}}$. We implement such posterior sampling to compute marginal predictive of each of the unknowns. We compare this marginal predictive of $Z_2, Z_3, Z_4$, to the empirical distribution of $Z_2, Z_3, Z_4$ in the test data $D_{\text{test}}$. We also compare the plots of the predicted $Z_i$ and the known $Z_1$ values, to the corresponding plot of empirical value of $Z_i$ and $Z_1; i = 2, 3, 4$. The results of this comparison for $Z_2, Z_3$ and $Z_4$ are included in Figure 14.

Figure 14 shows that the plots of the predicted values of $Z_i, i = 2, 3, 4$, against $Z_1$ (in red filled circles in the electronic version, and grey circles in the monochrome version), compare favourably–visually speaking–to the plots of the empirical $Z_i$ (in the test data), against $Z_1$. To be precise, the red (or grey) circles comprise predicted (or learnt) pair $(z_{1k}, z_{ik}^{(\text{mode})})$ for $k = 1, \ldots, q = n$, where $z_{ik}^{(\text{mode})}$ is the modal value of the marginal posterior density of $Z_{ik}$ given known values of $Z_1$ in the test data, and the (modal) correlation matrix $\Sigma_C^{(M)}$ (itself learnt given the training data). The black circles represent the empirical values $(z_{1k}, z_{ik})$ for $k = 1, \ldots, n$, i.e. the pair in the $k$-th row of the test data. We also plot the marginal of the learnt values of $Z_i$ given the data, superimposed on the frequency distribution of the empirical value of $Z_i$ in the test data–we do this for each $i = 2, 3, 4$. Again, the overlap between the results is encouraging. Thus, the predictions offer confidence in our model, as well as the results of our learning of the correlation structure of the data.

![Figure 14](image-url)

**Fig 14.** Top panels: figures comparing plots of empirical and predicted values of $Z_i$ against values of $Z_1$, for $i = 2, 3, 4$ moving from left to the right panel. Grey (red in the electronic version) circles depict pairs of $(z_{1k}, z_{ik})$ in the test data $D_{\text{test}}$, while black circles depict $Z_i$ values learnt given the first column of the test data and the modal correlation matrix $\Sigma_C^{(M)}$ that is itself learnt using the training data set $D_{\text{T}}^{(S)}$. Lower panels: marginal of $Z_i$ given 1st column of test data and $\Sigma_C^{(M)}$, plotted as a histogram in grey (or red in the electronic version), over its empirical distribution in black, i.e. the histogram of the $i$-th column of the test data. Here, $i = 2, 3, 4$ as we move from left to right.

However, conditioning the posterior predictive of $Z_i$ on a summary–modal in our earlier implementation–correlation matrix learnt given training data $D_{\text{T}}^{(S)}$ is restrictive in that this approach ignores the learnt distribution of the correlation matrices. After all, our learning of the correlation matrix given $D_{\text{T}}^{(S)}$ is MCMC-based, generating a value of $\Sigma_C^{(S)}$ in each iteration. In light of this, the marginal posterior of $Z_i$ obtained by marginalisation over the joint posterior probability density of all unknown components of $Z$ and $\Sigma_C^{(S)}$ is a possibility. Thus, we learn $\Sigma_C^{(S)}$ simultaneously with $Z_2, Z_3, Z_4$, i.e. the 2nd, 3rd and 4th columns of the test data, given the training data and the 1st column of the test
data. We will then perform MCMC-based posterior sampling from the joint posterior probability density:

\[
\pi \left( s_{12}, \ldots, s_{1p}, s_{23}, \ldots, s_{2p}, \ldots, s_{p-1}p, z_{21}, \ldots, z_{2n}, z_{31}, \ldots, z_{3n}, z_{41}, \ldots, z_{4n} | z_{11}, z_{1n}, D_T^{(S)} \right). \tag{7.1}
\]

In order to implement this, we propose \(z_{21}^{(t*)}, \ldots, z_{2n}^{(t*)}, z_{31}^{(t*)}, \ldots, z_{3n}^{(t*)}, z_{41}^{(t*)}, \ldots, z_{4n}^{(t*)}\) in each of the \(t\) iterations, \(t = 0, \ldots, N\). Each of these parameters is proposed from a Gaussian proposal density (with mean given by the current value and an experimentally chosen variance). At the same time, we propose the \(s_{ij}\) parameters, \(i \neq j\), \(i, j = 1, \ldots, p\) from a Truncated Normal proposal density, truncated at -1 and 1, with mean given by the current value of the parameter, and chosen variance.

For this implementation, at the \(t\)-th iteration, we need to define the augmented data \(D_A^{(t*)}\), which is the training data \(D_T^{(S)}\), augmented by the data set \(D^{(t*)}\) proposed in the \(t\)-th iteration, (defined above), where the 1st and 5th columns of \(D^{(t*)}\) are the known 1st and 5th columns of the test data \(D_{test}\), and the \(i\)-th column is the proposed vector \((z_{i1}^{(t*)}, \ldots, z_{in}^{(t*)})^T\), \(i = 2, 3, 4\). Thus, as the proposed \(D^{(t*)}\) varies from one iteration to the next, the augmented data \(D_A^{(t*)}\) also varies. This augmented data then has \(p\) columns nd \(n + q\) rows, i.e. \(2n\) rows, given our choice of \(q = n\). In the \(t\)-th iteration, the posterior probability density of the unknowns given this augmented data \(D_A^{(t*)}\) is computed, using the posterior defined in Equation 2.8 of WMC in which the generic data \(D_S\) is now replaced by \(D_A^{(t*)}\). While we impose uniform priors on the \(z_{ik}\) parameters, we place Gaussian priors on \(s_{ij}\), with such a prior centred at the empirical value of the correlation between the \(i\)-th and \(j\)-th columns of the data, \((i, j = 1, \ldots, p)\); the variance of these Gaussian priors are experimentally chosen.

Some results of sampling from the joint defined in Equation 7.1 are shown in Figure 15. These include comparison of the histogram representations of the marginals of 3 correlation parameters.
$S_{12}, S_{13}, S_{23}$, learnt in this implementation given the augmented data, with the marginal of the same correlation parameter learnt given training data $D_T^{(S)}$. The figure also includes a comparison of the empirical and predicted marginals of $Z_2$ and $Z_3$.

S2. Results of learning given the red wine data set

Figure 16 presents histogram representations of marginal posterior probability densities of some partial correlation parameters learnt given the standardised red wine data; the trace of the joint posterior of all the partial correlation parameters is also included. Figure 16 on the other hand presents the marginals of some of the variance parameters.

![Graph showing joint posterior probability densities](image_url)

**Fig 16.** The marginal posterior of some of the partial correlation parameters $\rho_{ij}$ computed using the elements of the correlation matrix $\Sigma_{S}^{(\text{red})}$ that is updated in the first block of our MCMC chain, run with the red wine data $D_S^{(\text{red})}$ of Portuguese red wine samples; $i \neq j$; $i, j = 1, \ldots, p = 12$. The top left hand panel of this figure presents the trace of the joint posterior probability density of the elements of the upper triangle of $\Sigma_S^{(\text{red})}$. 
S3. Empirical and regression analysis of red-wine data

The data on 1599 samples of Portugese red wines is discussed by Cortez et al. (1998) and considered in the main paper (Section 4.2). The between-columns correlation structure and graphical model of this data are reported in this section. These results are reviewed in light of independent data analysis of the red wine data that we undertook. The original red wine data is $D_{\text{orig}}^{(\text{red})}$, of which $D_{S}^{(\text{red})}$ is a standardised subset. The dataset has 12 columns, each containing information on vino-chemical attributes of the sampled wines; these properties are assigned the following names: “fixed acidity” ($X_1$), “volatile acidity” ($X_2$), “citric acid” ($X_3$), “residual sugar” ($X_4$), “chlorides” ($X_5$), “free sulphur dioxide” ($X_6$), “total sulphur dioxide” ($X_7$), “density” ($X_8$), “pH” ($X_9$), “sulphates” ($X_{10}$), “alcohol” ($X_{11}$); the 12-th column is the assessed “quality” ($X_{12}$) of a wine in the sample. The standardised version of variable $X_i$ is $Z_i$, $i = 1, \ldots, 12$.

A matrix of scatterplots of $X_j$ against $X_i$ is shown in Figure 18, for $i = 1, \ldots, 11$. These scatterplots visually indicate moderate correlations between the following pairs of variables: fixed acidity-citric acid, fixed acidity-density, fixed acidity-pH, volatile acidity-citric acid, free sulphur dioxide-total sulphur dioxide, density-alcohol. All these variables share an edge at probability $\geq 0.05$ in our learnt graphical model of data $D_{S}^{(\text{red})}$ (Figure 14 of main paper). However, an edge may exist between a pair of variables even when the apparent empirical correlation between these variables is low (see Section 4.1.1 of main paper), owing to the effect of other variables. Noticing such edges from the residual-sugar variable, we undertake a regression analysis (ordinary least squares) with residual-sugar regressed against the other remaining 10 vino-chemical variables. The MATLAB output of that analysis is included in Figure 19. The analysis indicates that the covariates with maximal (near-equal) effect on residual-sugar, are density and alcohol; residual-sugar is learnt to enjoy an edge with both density and alcohol in our learnt graphical model of the red wine data (Figure 14 of the main paper).

We also undertook a separate ordinary least squares analysis with the response variable quality, regressed against the vino-chemical variables as the covariates. The MATLAB output of this regression analysis is in Figure 20. We notice that the strongest (and nearly-equal) effect on quality is from the variables volatile-acidity and alcohol—the very two variables that share an edge at probability...
Fig 18. Matrix of scatterplots of the 11 different vino-chemical variables $X_1, \ldots, X_{11}$ that form the first 11 columns of the red wine data $D_{\text{orig}}^{(\text{red})}$. Here $X_j$ is plotted against $X_i$, $i \neq j$, $i,j = 1, \ldots, 11$. The $X_i$ relevant to the $i$-th row is named in the diagonal element of the $i$-th row; $j$ increases from 1 to 11 from left to right.
S4. Cholesky Factorisation and Matrix Inversion by Forward Substitution

Let a $p \times p$-square positive-definite (correlation) matrix be $\Sigma_C^{(S)} = L_C^{(S)} (L_C^{(S)})^T$. The Cholesky factorisation of $\Sigma_C^{(S)} = [s_{ij}]$ into its unique square root $L_C^{(S)} = [l_{ij}]$ can be shown to be defined by

\[
C = L \cdot L^T = \begin{bmatrix}
  l_{11} & 0 & \cdots & 0 \\
  l_{21} & l_{22} & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  l_{p1} & l_{p2} & \cdots & l_{pp}
\end{bmatrix}
\]

### OLS Regression Results

| Dep. Variable: | y | R-squared: | 0.401 |
|---------------|---|-----------|-------|
| Model: OLS    | Adj. R-squared: | 0.396 |
| Method: Least Squares | F-statistic: | 89.48 |
| Date: Tue, 02 May 2017 | Prob (F-statistic): | 3.45e-141 |
| Time: 06:53:50 | Log-Likelihood: | -1914.0 |
| No. Observations: | 1350 | AIC: | 3850. |
| Df Residuals: | 1339 | BIC: | 3907. |
| Df Model: | 10 |
| Covariance Type: | nonrobust |

|   | coef  | std err  | t  | P>|t| [95.0% Conf. Int.] |
|---|------|----------|----|---------------------|
| const | -766.3330 | 28.797 | -26.611 | 0.000 | -822.825 | -709.841 |
| x1   | -0.6843 | 0.041 | -16.824 | 0.000 | -0.764 | -0.604 |
| x2   | -0.3570 | 0.202 | -1.771 | 0.077 | -0.752 | 0.038 |
| x3   | 0.3193 | 0.251 | 1.271 | 0.204 | 0.173 | 0.812 |
| x4   | -1.7821 | 0.703 | -2.534 | 0.011 | -3.162 | -0.403 |
| x5   | 0.0081 | 0.004 | 2.163 | 0.031 | 0.001 | 0.015 |
| x6   | 0.0036 | 0.001 | 2.882 | 0.004 | 0.001 | 0.006 |
| x7   | 781.9845 | 29.412 | 26.587 | 0.000 | 724.286 | 839.683 |
| x8   | -3.9047 | 0.299 | -13.042 | 0.000 | -4.492 | -3.317 |
| x9   | -1.2234 | 0.185 | -6.622 | 0.000 | -1.586 | -0.861 |
| x10  | 0.8462 | 0.037 | 22.567 | 0.000 | 0.773 | 0.920 |

Omnibus: 1023.119 | Durbin-Watson: 1.782 |
Prob(Omnibus): 0.000 | Jarque-Bera (JB): 25392.413 |
Skew: 3.290 | Prob(JB): 0.00 |
Kurtosis: 23.202 | Cond. No. 9.18e+04 |

Fig 19. Output of ordinary least square analysis of regressing residual sugar on the other 10 vino-chemical attributes in the red wine data.
OLS Regression Results

| Dep. Variable: y | R-squared: 0.365 |
|------------------|------------------|
| Model: OLS       | Adj. R-squared: 0.360 |
| Method: Least Squares | F-statistic: 76.89 |
| Date: Mon, 01 May 2017 | Prob (F-statistic): 1.74e-124 |
| Time: 02:14:11 | Log-Likelihood: -1318.0 |
| No. Observations: 1350 | AIC: 2658.0 |
| Df Residuals: 1339 | BIC: 2715.0 |
| Df Model: 10 | Covariance Type: nonrobust |

| coef | std err | t | P>|t| | [95.0% Conf. Int.] |
|------|---------|---|------|------------------|
| const | 4.2567 | 0.653 | 6.523 | 0.000 | 2.977 | 5.537 |
| x1 | 0.0059 | 0.018 | 0.335 | 0.738 | -0.029 | 0.041 |
| x2 | -1.0993 | 0.128 | -8.558 | 0.000 | -1.351 | -0.847 |
| x3 | -0.1662 | 0.162 | -1.029 | 0.304 | -0.483 | 0.151 |
| x4 | -0.0013 | 0.014 | -0.091 | 0.927 | -0.029 | 0.027 |
| x5 | -1.7190 | 0.449 | -3.832 | 0.000 | -2.599 | -0.839 |
| x6 | 0.0033 | 0.002 | 1.371 | 0.171 | -0.001 | 0.008 |
| x7 | -0.0035 | 0.001 | -4.319 | 0.000 | -0.005 | -0.002 |
| x8 | -0.4105 | 0.167 | -2.463 | 0.014 | -0.738 | -0.084 |
| x9 | 0.8068 | 0.118 | 6.855 | 0.000 | 0.576 | 1.038 |
| x10 | 0.2939 | 0.018 | 15.975 | 0.000 | 0.258 | 0.330 |

Omnibus: 20.370 Durbin-Watson: 1.761
Prob(Omnibus): 0.000 Jarque-Bera (JB): 28.835
Skew: -0.161 Prob(JB): 5.48e-07
Kurtosis: 3.640 Cond. No: 2.40e+03

Here X1 to X10 are: 1.'fixed acidity'; 2.'volatile acidity'; 3.'citric acid'; 4.'residual sugar'; 5.'chlorides'; 6.'free sulphur dioxide'; 7.'total sulphur dioxide'; 8.'pH'; 9.'sulphate'; 10.'alcohol'

Fig 20. Output of ordinary least square analysis of regressing quality on the vino-chemical attributes of red wine samples in the red wine data.

the following scheme:

\[ l_{11} = \sqrt{s_{11}}, \]
\[ l_{ii} = \frac{s_{ii}}{l_{11}}, \quad i = 1, \ldots, p, \]
\[ l_{ij} = \frac{1}{l_{jj}} \sqrt{s_{ij} - \sum_{k=1}^{j-1} l_{ik}l_{kj}}, \quad j = 1, \ldots, i - 1; \quad i = 1, \ldots, p, \]
\[ l_{ii} = \sqrt{s_{ii} - \sum_{k=1}^{i-1} l_{ik}^2}, \quad i = 2, \ldots, p. \]
while forward substitution seeks $L_{C}^{-1}$ s.t. $L_{C}L_{C}^{-1} = I$, where $I$ is the $p \times p$-dimensional identity matrix. Then the scheme for forward substitution is the following:

$$m_{11} = \frac{1}{l_{11}},$$
$$l_{1i} = \frac{s_{1i}}{l_{11}}, \quad i = 1, \ldots, p,$$
$$l_{ij} = \sqrt{s_{ij} - \sum_{k=1}^{j-1} l_{ik}l_{kj}} \quad j = 1, \ldots, i - 1; \quad i = 1, \ldots, p,$$
$$l_{ii} = \sqrt{s_{ii} - \sum_{k=1}^{i-2} l_{ik}^2} \quad i = 2, \ldots, p,$$

(7.3)

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