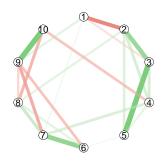
# BGGM: A R Package for Bayesian Gaussian Graphical Models

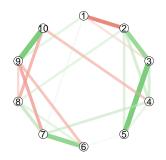
Donald R. Williams

25 May 2019

 Gaussian graphical models capture condition dependencies between random variables



- Gaussian graphical models capture condition dependencies between random variables
- Non-zero relations imply pairwise, conditional dependent relations, in which all other variables in the model have been controlled for



- Gaussian graphical models capture condition dependencies between random variables
- Non-zero relations imply pairwise, conditional dependent relations, in which all other variables in the model have been controlled for
- This powerful framework for learning the structure of multivariate data has been used across the sciences



- To date, the most common applications have been gene co-expression and functional connectivity "networks"
  - Common to have more variables p than observations n (i.e., high dimensional data)
  - Requires some form of regularization to make estimation possible (e.g., lasso)

- To date, the most common applications have been gene co-expression and functional connectivity "networks"
  - Common to have more variables p than observations n (i.e., high dimensional data)
  - Requires some form of regularization to make estimation possible (e.g., lasso)
- Numerous R packages-e.g., glasso, huge, and flare
  - Limited to *only* point estimates

- To date, the most common applications have been gene co-expression and functional connectivity "networks"
  - Common to have more variables p than observations n (i.e., high dimensional data)
  - Requires some form of regularization to make estimation possible (e.g., lasso)
- Numerous R packages-e.g., glasso, huge, and flare
  - Limited to *only* point estimates
- High-dimensional inference is an active area of research
  - Confidence intervals and p-values provided in SILGGM

 More recently, GGMs have become increasingly popular in the social-behavioral sciences

- More recently, GGMs have become increasingly popular in the social-behavioral sciences
  - Regularization is not only unnecessary, but actually has worse performance than non-regularized methods

- More recently, GGMs have become increasingly popular in the social-behavioral sciences
  - Regularization is not only unnecessary, but actually has worse performance than non-regularized methods
- Related publications:

- More recently, GGMs have become increasingly popular in the social-behavioral sciences
  - Regularization is not only unnecessary, but actually has worse performance than non-regularized methods
- Related publications:

MULTIVARIATE BEHAVIORAL RESEARCH https://doi.org/10.1080/00273171.2019.1575716





#### On Nonregularized Estimation of Psychological Networks

Donald R. Williams (a), Mijke Rhemtulla, Anna C. Wysocki, and Philippe Rast (b)
Department of Psychology, University of California, Davis, CA, USA

- More recently, GGMs have become increasingly popular in the social-behavioral sciences
  - Regularization is not only unnecessary, but actually has worse performance than non-regularized methods
- Related publications:

British Journal of Mathematical and Statistical Psychology (2019) © 2019 The British Psychological Society



www.wileyonlinelibrary.com

## Back to the basics: Rethinking partial correlation network methodology

Donald R. Williams\* oand Philippe Rast University of California, Davis, California, USA

• We need methods specifically for (p < n)

- We need methods specifically for (p < n)
  - Extend inference beyond point estimates

- We need methods specifically for (p < n)
  - Extend inference beyond point estimates
  - Testing for invariances—i.e., the null hypothesis of conditional independence

- We need methods specifically for (p < n)
  - Extend inference beyond point estimates
  - Testing for invariances—i.e., the null hypothesis of conditional independence
- Only one R package for Bayesian GGMs (BDgraph)
  - Limited to identifying non-zeros

- We need methods specifically for (p < n)
  - Extend inference beyond point estimates
  - Testing for invariances—i.e., the null hypothesis of conditional independence
- Only one R package for Bayesian GGMs (BDgraph)
  - Limited to identifying non-zeros
- **BGGM** includes many novel (Bayesian) methods, each of which goes beyond detecting non-zero effects

- We need methods specifically for (p < n)
  - Extend inference beyond point estimates
  - Testing for invariances—i.e., the null hypothesis of conditional independence
- Only one R package for Bayesian GGMs (BDgraph)
  - Limited to identifying non-zeros
- BGGM includes many novel (Bayesian) methods, each of which goes beyond detecting non-zero effects
  - Edge set identification

- We need methods specifically for (p < n)
  - Extend inference beyond point estimates
  - Testing for invariances—i.e., the null hypothesis of conditional independence
- Only one R package for Bayesian GGMs (BDgraph)
  - Limited to identifying non-zeros
- BGGM includes many novel (Bayesian) methods, each of which goes beyond detecting non-zero effects
  - Edge set identification
  - Exploratory and Confirmatory hypothesis testing

- We need methods specifically for (p < n)
  - Extend inference beyond point estimates
  - Testing for invariances—i.e., the null hypothesis of conditional independence
- Only one R package for Bayesian GGMs (BDgraph)
  - Limited to identifying non-zeros
- BGGM includes many novel (Bayesian) methods, each of which goes beyond detecting non-zero effects
  - Edge set identification
  - Exploratory and Confirmatory hypothesis testing
  - Bayesian measures of prediction error

- We need methods specifically for (p < n)
  - Extend inference beyond point estimates
  - Testing for invariances—i.e., the null hypothesis of conditional independence
- Only one R package for Bayesian GGMs (BDgraph)
  - Limited to identifying non-zeros
- BGGM includes many novel (Bayesian) methods, each of which goes beyond detecting non-zero effects
  - Edge set identification
  - Exploratory and Confirmatory hypothesis testing
  - Bayesian measures of prediction error
  - Methods to compare any number of GGMs

- We need methods specifically for (p < n)
  - Extend inference beyond point estimates
  - Testing for invariances—i.e., the null hypothesis of conditional independence
- Only one R package for Bayesian GGMs (BDgraph)
  - Limited to identifying non-zeros
- BGGM includes many novel (Bayesian) methods, each of which goes beyond detecting non-zero effects
  - Edge set identification
  - Exploratory and Confirmatory hypothesis testing
  - Bayesian measures of prediction error
  - Methods to compare any number of GGMs
  - etc. described in 3 first-author papers (in review): Journal of Mathematical Psychology, Psychological Methods,...

This remainder of this talk will describe these methods (Overview of an (in prep) Journal of Statistical Software paper)

## Psychological "Networks"

## Psychological "Networks"

- The undirected graph is G = (V, E)
  - Vertex set  $V = \{1, 2, ..., p\}$  (i.e., nodes or variables)
  - Edge set  $E \subset V \times V$

## Psychological "Networks"

- The undirected graph is G = (V, E)
  - Vertex set  $V = \{1, 2, ..., p\}$  (i.e., nodes or variables)
  - Edge set  $E \subset V \times V$
- Let  $\mathbf{Y} = (\mathbf{y}_1, ..., \mathbf{y}_p)'$  be a  $n \times p$  matrix
  - Each  $\mathbf{y}$  is a n dimensional vector that is indexed by the graphs vertices.

## Psychological "Networks"

- The undirected graph is G = (V, E)
  - Vertex set  $V = \{1, 2, ..., p\}$  (i.e., nodes or variables)
  - Edge set  $E \subset V \times V$
- Let  $\mathbf{Y} = (\mathbf{y}_1, ..., \mathbf{y}_p)'$  be a  $n \times p$  matrix
  - Each  $\mathbf{y}$  is a n dimensional vector that is indexed by the graphs vertices.
- ullet Assume that  $\mathbf{Y} \sim \mathcal{N}(oldsymbol{\mu}, oldsymbol{\Sigma})$ 
  - Mean vector  $\boldsymbol{\mu}=(0_1,...,0_p)'$
  - $p \times p$  positive definite covariance matrix  $\Sigma$

## Psychological "Networks"

- The undirected graph is G = (V, E)
  - Vertex set  $V = \{1, 2, ..., p\}$  (i.e., nodes or variables)
  - Edge set  $E \subset V \times V$
- Let  $\mathbf{Y} = (\mathbf{y}_1, ..., \mathbf{y}_p)'$  be a  $n \times p$  matrix
  - Each  $\mathbf{y}$  is a n dimensional vector that is indexed by the graphs vertices.
- ullet Assume that  $\mathbf{Y} \sim \mathcal{N}(oldsymbol{\mu}, oldsymbol{\Sigma})$ 
  - Mean vector  $\boldsymbol{\mu}=(0_1,...,0_p)'$
  - $-p \times p$  positive definite covariance matrix  $\Sigma$
- Denote the precision matrix  $\mathbf{\Theta} = \mathbf{\Sigma}^{-1}$

#### **Conditional Relations**

The graph, or the underlying conditional (in)dependence structure, is obtained from the off-diagonal elements—i.e.,  $\theta_{ij} \in \Theta_{ij}, 1 \le i < j \le p$ .

#### **Conditional Relations**

The graph, or the underlying conditional (in)dependence structure, is obtained from the off-diagonal elements—i.e.,  $\theta_{ij} \in \Theta_{ij}$ ,  $1 \le i < j \le p$ .

- Conditional Independence
  - $-\mathbf{Y}_{u}\perp \!\!\!\perp \mathbf{Y}_{k}\mid \mathbf{Y}_{V_{\setminus \{u,k\}}}\notin E$

#### **Conditional Relations**

The graph, or the underlying conditional (in)dependence structure, is obtained from the off-diagonal elements-i.e.,  $\theta_{ij} \in \Theta_{ij}, 1 \le i < j \le p$ .

- Conditional Independence
  - $-\mathbf{Y}_{u}\perp \!\!\!\perp \mathbf{Y}_{k}\mid \mathbf{Y}_{V\setminus\{u,k\}}\notin E$
  - Evidence for the null hypothesis!

#### **Conditional Relations**

The graph, or the underlying conditional (in)dependence structure, is obtained from the off-diagonal elements-i.e.,  $\theta_{ij} \in \Theta_{ij}, 1 \le i < j \le p$ .

- Conditional Independence
  - $-\mathbf{Y}_{u}\perp \mathbf{Y}_{k}\mid \mathbf{Y}_{V\setminus\{u,k\}}\notin E$
  - Evidence for the null hypothesis!
- Conditional Dependence
  - $-\mathbf{Y}_{u} \not\perp \!\!\!\!\perp \mathbf{Y}_{k} \mid \mathbf{Y}_{V_{\setminus \{u,k\}}} \in E$

#### **Conditional Relations**

The graph, or the underlying conditional (in)dependence structure, is obtained from the off-diagonal elements-i.e.,  $\theta_{ij} \in \Theta_{ij}, 1 \le i < j \le p$ .

- Conditional Independence
  - $-\mathbf{Y}_{u}\perp \mathbf{Y}_{k}\mid \dot{\mathbf{Y}}_{V_{\setminus\{u,k\}}}\notin E$
  - Evidence for the null hypothesis!
- Conditional Dependence
  - $-\mathbf{Y}_{u} \not\perp \!\!\!\perp \mathbf{Y}_{k} \mid \mathbf{Y}_{V_{\setminus \{u,k\}}} \in E$
- Partial Correlations:

#### **Conditional Relations**

The graph, or the underlying conditional (in)dependence structure, is obtained from the off-diagonal elements-i.e.,  $\theta_{ij} \in \Theta_{ij}, 1 \le i < j \le p$ .

- Conditional Independence
  - $-\mathbf{Y}_{u} \perp \mathbf{Y}_{k} \mid \mathbf{Y}_{V_{\setminus \{u,k\}}} \notin E$
  - Evidence for the null hypothesis!
- Conditional Dependence

$$-\mathbf{Y}_{u} \not\perp \!\!\!\perp \mathbf{Y}_{k} \mid \mathbf{Y}_{V_{\setminus \{u,k\}}} \in E$$

Partial Correlations:

$$\rho_{ij} = \frac{-\theta_{ij}}{\sqrt{\theta_{ii}\theta_{jj}}} \tag{1}$$

#### **Conditional Relations**

The graph, or the underlying conditional (in)dependence structure, is obtained from the off-diagonal elements-i.e.,  $\theta_{ij} \in \Theta_{ij}, 1 \le i < j \le p$ .

- Conditional Independence
  - $\mathbf{Y}_u \perp \!\!\!\perp \mathbf{Y}_k \mid \mathbf{Y}_{V_{\setminus \{u,k\}}} \notin E$
  - Evidence for the null hypothesis!
- Conditional Dependence

$$-\mathbf{Y}_{u} \not\perp \!\!\!\perp \mathbf{Y}_{k} \mid \mathbf{Y}_{V_{\setminus \{u,k\}}} \in E$$

Partial Correlations:

$$\rho_{ij} = \frac{-\theta_{ij}}{\sqrt{\theta_{ii}\theta_{jj}}} \tag{1}$$

• E via hypothesis testing-e.g.,

$$\mathcal{H}_0: \rho_{ij} = 0 \tag{2}$$

$$\mathcal{H}_1:
ho_{ij}
eq 0$$

## **Method Organization**

**BGGM** is built around two approaches for Bayesian inference: estimation and hypothesis testing

**BGGM** is built around two approaches for Bayesian inference: estimation and hypothesis testing

- Estimation
  - Similar to frequentist methods, but allow for probabilistic inference
  - e.g., Credible interval exclusion of zero, or directional posterior probabilities  $p(\rho_{ij}>0|\mathbf{Y})$

**BGGM** is built around two approaches for Bayesian inference: estimation and hypothesis testing

#### Estimation

- Similar to frequentist methods, but allow for probabilistic inference
- e.g., Credible interval exclusion of zero, or directional posterior probabilities  $p(\rho_{ij} > 0|\mathbf{Y})$
- Prior distributions (often) play little role in inference, especially as  $n \to \infty$

**BGGM** is built around two approaches for Bayesian inference: estimation and hypothesis testing

- Estimation
  - Similar to frequentist methods, but allow for probabilistic inference
  - e.g., Credible interval exclusion of zero, or directional posterior probabilities  $p(\rho_{ij} > 0|\mathbf{Y})$
  - Prior distributions (often) play little role in inference, especially as  $n \to \infty$
- Hypothesis Testing
  - Bayesian model comparison with the Bayes factor
  - (relative) Evidence between competing models-e.g.,  $\mathcal{M}_0$  vs.  $\mathcal{M}_1$

**BGGM** is built around two approaches for Bayesian inference: estimation and hypothesis testing

- Estimation
  - Similar to frequentist methods, but allow for probabilistic inference
  - e.g., Credible interval exclusion of zero, or directional posterior probabilities  $p(\rho_{ij}>0|\mathbf{Y})$
  - Prior distributions (often) play little role in inference, especially as  $n \to \infty$
- Hypothesis Testing
  - Bayesian model comparison with the Bayes factor
  - (relative) Evidence between competing models–e.g.,  $\mathcal{M}_0$  vs.  $\mathcal{M}_1$
  - Prior distributions play a critical role (for all n), as they capture scientific expectations—i.e., actual predictions

**BGGM** is built around two approaches for Bayesian inference: estimation and hypothesis testing

#### Estimation

- Similar to frequentist methods, but allow for probabilistic inference
- e.g., Credible interval exclusion of zero, or directional posterior probabilities  $p(\rho_{ij} > 0|\mathbf{Y})$
- Prior distributions (often) play little role in inference, especially as  $n \to \infty$

#### **Estimation based methods**

These following methods are described in Williams (2018).

Williams, D. R. (2018). Bayesian Inference for Gaussian Graphical Models: Structure Learning, Explanation, and Prediction. PsyArXiv

#### **Estimation based methods**

These following methods are described in Williams (2018).

Williams, D. R. (2018). Bayesian Inference for Gaussian Graphical Models: Structure Learning, Explanation, and Prediction. PsyArXiv

The joint posterior density for the precision matrix follows

$$p(\Theta|\mathbf{Y}) \propto p(\mathbf{Y}|\Theta)p(\Theta),$$
 (3)

where  $\mathbf{Y}$  is a  $n \times p$  matrix drawn from a multivariate normal distribution—i.e.,

$$\mathbf{Y} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Theta}^{-1}).$$
 (4)

When using the conjugate Wishart prior,  $W(k, \mathbf{I}_p)$ , with k degrees of freedom and identity matrix  $\mathbf{I}_p$ , the posterior distribution also has a Wishart distribution—i.e.,

$$\Theta|\mathbf{Y} \sim \mathcal{W}(k+n, (\mathbf{S} + \epsilon \mathbf{I}_p)^{-1}),$$
 (5)

where  ${\bf S}$  is the sums of squares matrix  ${\bf Y'Y}$  and  $\epsilon$  is a constant.

When using the conjugate Wishart prior,  $\mathcal{W}(k, \mathbf{I}_p)$ , with k degrees of freedom and identity matrix  $\mathbf{I}_p$ , the posterior distribution also has a Wishart distribution—i.e.,

$$\Theta|\mathbf{Y} \sim \mathcal{W}(k+n, (\mathbf{S} + \epsilon \mathbf{I}_p)^{-1}),$$
 (5)

where **S** is the sums of squares matrix  $\mathbf{Y}'\mathbf{Y}$  and  $\epsilon$  is a constant.

The posterior mode then has a closed form

$$\operatorname{argmax}_{\boldsymbol{\Theta}} p(\boldsymbol{\Theta}|\mathbf{Y}) = (k + n - p - 1)(\mathbf{S} + \epsilon \mathbf{I}_p)^{-1}. \tag{6}$$

The posterior variance also has a closed form-i.e.,

$$Var(\boldsymbol{\Theta}|\mathbf{Y}) = (k+n)((\mathbf{S} + \epsilon \mathbf{I}_p)^{-1^2} + \boldsymbol{dd}'), \tag{7}$$

where  $\boldsymbol{d} = \operatorname{diag}(\boldsymbol{S} + \epsilon \boldsymbol{I}_p)$ .

The posterior variance also has a closed form-i.e.,

$$Var(\boldsymbol{\Theta}|\mathbf{Y}) = (k+n)((\boldsymbol{S} + \epsilon \mathbf{I}_p)^{-1^2} + \boldsymbol{d}\boldsymbol{d}'), \tag{7}$$

where  $\boldsymbol{d} = \operatorname{diag}(\boldsymbol{S} + \epsilon \boldsymbol{I}_p)$ .

By setting k=p+1, and  $\epsilon$  to a small value, say,  $1.0\times 10^{-10}$ , results (approximately) in the maximum likelihood estimate  $n(\mathbf{S}^{-1})$ .

The posterior variance also has a closed form-i.e.,

$$Var(\boldsymbol{\Theta}|\mathbf{Y}) = (k+n)((\mathbf{S} + \epsilon \mathbf{I}_p)^{-1^2} + \boldsymbol{d}\boldsymbol{d}'), \tag{7}$$

where  $\boldsymbol{d} = \operatorname{diag}(\boldsymbol{S} + \epsilon \boldsymbol{I}_p)$ .

By setting k=p+1, and  $\epsilon$  to a small value, say,  $1.0\times 10^{-10}$ , results (approximately) in the maximum likelihood estimate  $n(\mathbf{S}^{-1})$ .

Consequently, assuming that  $p(\theta_{ij}|\mathbf{Y})$  is normally distributed, allows for constructing credible intervals and computing posterior probabilities.

The posterior variance also has a closed form-i.e.,

$$Var(\boldsymbol{\Theta}|\mathbf{Y}) = (k+n)((\mathbf{S} + \epsilon \mathbf{I}_p)^{-1^2} + d\mathbf{d}'), \tag{7}$$

where  $\boldsymbol{d} = \operatorname{diag}(\boldsymbol{S} + \epsilon \boldsymbol{I}_p)$ .

By setting k=p+1, and  $\epsilon$  to a small value, say,  $1.0\times 10^{-10}$ , results (approximately) in the maximum likelihood estimate  $n(\mathbf{S}^{-1})$ .

Consequently, assuming that  $p(\theta_{ij}|\mathbf{Y})$  is normally distributed, allows for constructing credible intervals and computing posterior probabilities. The former can be computed as

$$\int_{I}^{u} p(\theta_{ij}|\mathbf{Y}) d\theta_{ij} = 1 - \alpha, \tag{8}$$

where I and u denote the lower and upper bounds of the interval.

A posterior probability can also be computed, for example with

$$\int_0^\infty p(\theta_{ij}|\mathbf{Y})d\theta_{ij},\tag{9}$$

which corresponds to the posterior probability of a positive effect. Both can be computed analytically with the point estimate in (Equation 6) and variance in (Equation 7).

A posterior probability can also be computed, for example with

$$\int_0^\infty p(\theta_{ij}|\mathbf{Y})d\theta_{ij},\tag{9}$$

which corresponds to the posterior probability of a positive effect. Both can be computed analytically with the point estimate in (Equation 6) and variance in (Equation 7).

In  $\mathbf{BGGM}$ , this simple solution can be used for determining E and analytically deriving "network" predictability

A posterior probability can also be computed, for example with

$$\int_0^\infty p(\theta_{ij}|\mathbf{Y})d\theta_{ij},\tag{9}$$

which corresponds to the posterior probability of a positive effect. Both can be computed analytically with the point estimate in (Equation 6) and variance in (Equation 7).

In  $\mathbf{BGGM}$ , this simple solution can be used for determining E and analytically deriving "network" predictability

There is one drawback of this analytic form. Namely, because there are no posterior samples, this limits its applicability to some of the functions in **BGGM** 

#### \_\_\_\_\_\_

**BGGM** include an additional approach for conveniently drawing samples from the posterior distribution.

**BGGM** include an additional approach for conveniently drawing samples from the posterior distribution.

Assuming the Jeffrey's prior,  $p(\Theta^{-1}) \propto |\Theta^{-1}|^{-(p+1)/2}$ , allows for sampling directly from the a Wishart distribution–i.e.,

$$\boldsymbol{\Theta} \sim \mathcal{W}(n-1, \boldsymbol{S}^{-1}). \tag{10}$$

**BGGM** include an additional approach for conveniently drawing samples from the posterior distribution.

Assuming the Jeffrey's prior,  $p(\Theta^{-1}) \propto |\Theta^{-1}|^{-(p+1)/2}$ , allows for sampling directly from the a Wishart distribution–i.e.,

$$\boldsymbol{\Theta} \sim \mathcal{W}(n-1, \boldsymbol{S}^{-1}). \tag{10}$$

These samples, s=1,...,S, are used to compute the posterior distribution for the  $p\times p$  partial correlation matrix, with  $\rho_{ij}\in \mathcal{P}$ -i.e.,

$$\mathcal{P}^{(s)} = -([\operatorname{diag}(\boldsymbol{\sigma})^{(s)}]^{-1}\boldsymbol{\Theta}^{(s)}[\operatorname{diag}(\boldsymbol{\sigma})^{(s)}]^{-1}), \tag{11}$$

where  $\sigma$  are the square roots of diag( $\Theta$ ) and multiplying by -1 reverses the direction ( $\pm$ ).

Because  $\rho$  is a standardized effect, and thus each  $\rho_{ij}$  is on the same scale, **BGGM** allows for defining a *region of practical equivalence*.

Because  $\rho$  is a standardized effect, and thus each  $\rho_{ij}$  is on the same scale, **BGGM** allows for defining a *region of practical equivalence*.

Rather than determining E in reference to 0, a neighborhood around zero is defined (a null area).

Because  $\rho$  is a standardized effect, and thus each  $\rho_{ij}$  is on the same scale, **BGGM** allows for defining a *region of practical equivalence*.

Rather than determining E in reference to 0, a neighborhood around zero is defined (a null area).

Consequently, given some region,  $|\rho_{ij}| \leq \vartheta_0$ , there is support for null values when the posterior probability is above a pre-determined threshold,

$$\int_{-\vartheta_0}^{\vartheta_0} p(\rho_{ij}|\mathbf{Y}) d\rho_{ij} > 1 - \alpha, \tag{12}$$

where  $p(\rho_{ij}|\mathbf{Y})$  is the posterior distribution.

Conversely, determining practically meaningful edges, and thus belonging to E, are determined with

$$\int_{-\infty}^{-\vartheta_0} p(\rho_{ij}|\mathbf{Y}) d\rho_{ij} + \int_{\vartheta_0}^{\infty} p(\rho_{ij}|\mathbf{Y}) d\rho_{ij} > 1 - \alpha.$$
 (13)

Conversely, determining practically meaningful edges, and thus belonging to E, are determined with

$$\int_{-\infty}^{-\vartheta_0} p(\rho_{ij}|\mathbf{Y}) d\rho_{ij} + \int_{\vartheta_0}^{\infty} p(\rho_{ij}|\mathbf{Y}) d\rho_{ij} > 1 - \alpha.$$
 (13)

This is implemented in **BGGM** for both determining conditional dependent and practically independent relations, as well as comparing two edges (e.g.,  $\rho_{1,2}-\rho_{1,3}$ ).

Conversely, determining practically meaningful edges, and thus belonging to E, are determined with

$$\int_{-\infty}^{-\vartheta_0} p(\rho_{ij}|\mathbf{Y}) d\rho_{ij} + \int_{\vartheta_0}^{\infty} p(\rho_{ij}|\mathbf{Y}) d\rho_{ij} > 1 - \alpha.$$
 (13)

This is implemented in **BGGM** for both determining conditional dependent and practically independent relations, as well as comparing two edges (e.g.,  $\rho_{1,2}-\rho_{1,3}$ ).

These posterior samples are also used to compute Bayesian  $\mathbb{R}^2$  and Bayesian leave-one-out cross-validation.

### The analytic form is implemented with:

```
library(BGGM)
# fit model
Y <- BGGM::bfi[,1:5]
# fit model (analytic = T)
fit_analytic <- estimate(Y, analytic = T)</pre>
```

### The analytic form is implemented with:

```
library(BGGM)
# fit model
Y <- BGGM::bfi[,1:5]
# fit model (analytic = T)
fit_analytic <- estimate(Y, analytic = T)

# print
print(fit_analytic)</pre>
```

```
## BGGM: Bayesian Gaussian Graphical Models
## ---
## Type: Estimation (Analytic Solution)
## Posterior Samples:
## Observations (n): 2709
## Variables (p): 5
## Edges: 10
## ---
## Call:
## estimate.default(x = Y, analytic = T)
## ---
## ---
## Date: Thu May 23 11:36:07 2019
```

#### The edge set *E* is selected with:

```
# select E
E <- select(fit analytic, ci width = 0.95)
summary(E)
## BGGM: Bayesian Gaussian Graphical Models
## Type: Selected Graph (Analytic Solution)
## Credible Interval: 95 %
## Connectivity: 80 %
## ---
## Call:
## select.estimate(x = fit_analytic, ci_width = 0.95)
## ---
## Selected:
##
## Partial correlations
##
     0.00 -0.24 -0.11 0.00 0.00
## 2 -0.24 0.00 0.29 0.16 0.16
## 3 -0.11 0.29 0.00 0.18 0.36
     0.00 0.16 0.18 0.00 0.12
## 5 0.00 0.16 0.36 0.12 0.00
## ---
## Adjacency
     1 2 3 4 5
## 1 0 1 1 0 0
```

## 2 1 0 1 1 1

The analytic solution estimates  $\Theta$ , and thus, further information (e.g., credible intervals) is not provided.

The analytic solution estimates  $\Theta$ , and thus, further information (e.g., credible intervals) is not provided.

This is because the non-standardized off-diagonal elements are in the opposite direction of the partial correlations, which in our experience, can lead to confusion.

The analytic solution estimates  $\Theta$ , and thus, further information (e.g., credible intervals) is not provided.

This is because the non-standardized off-diagonal elements are in the opposite direction of the partial correlations, which in our experience, can lead to confusion.

The sampling based method can be used to summarize the partial correlations—i.e.,

The analytic solution estimates  $\Theta$ , and thus, further information (e.g., credible intervals) is not provided.

This is because the non-standardized off-diagonal elements are in the opposite direction of the partial correlations, which in our experience, can lead to confusion.

The sampling based method can be used to summarize the partial correlations—i.e.,

### This object is then summarized with:

summary(E, summarize = T, digits = 2)

```
## BGGM: Bayesian Gaussian Graphical Models
## Type: Selected Graph (Sampling)
## Credible Interval: 95 %
## Connectivity: 80 %
## ---
## Call:
## select.estimate(x = fit sampling, ci width = 0.95, rope = NULL.
      prob = NULL)
## ---
## Estimates:
   egde post_mean post_sd 2.5% 97.5%
## 1--2 -0.2400 0.018 -0.275 -0.205
## 1--3 -0.1075 0.019 -0.145 -0.069
   2--3 0.2869 0.017 0.253 0.320
## 1--4 -0.0071 0.019 -0.045 0.030
## 2--4 0.1648 0.019 0.128 0.201
## 3--4 0.1774 0.018 0.141 0.214
## 1--5 -0.0095 0.019 -0.047 0.028
## 2--5 0.1558 0.019 0.119 0.192
## 3--5 0.3582 0.016 0.326 0.389
## 4--5
        0.1216
                   0.019 0.085 0.158
```

A key feature of GGMs is the tradition of visualizing the underlying structure.

A key feature of GGMs is the tradition of visualizing the underlying structure.

To this end, BGGM offers several plotting options.

A key feature of GGMs is the tradition of visualizing the underlying structure.

To this end, BGGM offers several plotting options.

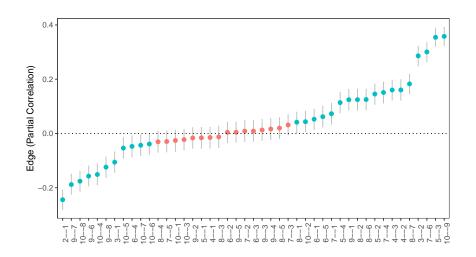
The partial correlations can be plotted with:

A key feature of GGMs is the tradition of visualizing the underlying structure.

To this end, BGGM offers several plotting options.

The partial correlations can be plotted with:

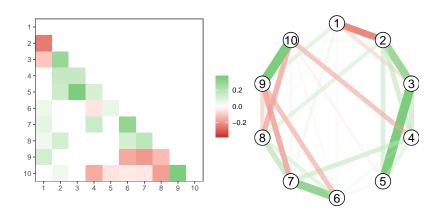
Note the plots can be further customized with ggplot2.



**BGGM** also includes two options for visualizing E.

A heatmap is plotted with:

On the other hand, a "network" plot follows:



**BGGM** extends inference beyond identifying non-zero partial correlations. The region of practical equivalence can be used for this purpose, as it allows for determining which relations are practically zero.

```
# p = 10
Y <- BGGM::bfi[,1:10]
# sample posterior
fit_sample <- estimate(Y, samples = 5000, analytic = F)
# E
E <- select(fit_sample, rope = 0.1, prob = 0.95)</pre>
```

```
head(E, nrow = 10, summarize = T, digits = 2)
## BGGM: Bayesian Gaussian Graphical Models
## ---
## Type: Selected Graph (Sampling)
## Probability: 0.95
## Region of Practical Equivalence: [-0.1, 0.1]
## Connectivity: 31.1 %
## ---
## Call:
## select.estimate(x = fit sample, rope = 0.1, prob = 0.95)
## pr_out: post prob outside of rope
## pr in: post prob inside of rope
## ---
## Estimates:
##
   egde post_mean post_sd pr_out pr_in
## 1--2
          -0.244 0.018 1.00 0.0000
         -0.105 0.020 0.61 0.3916
  1--3
   2--3
          0.286 0.018 1.00 0.0000
         -0.015 0.019 0.00 1.0000
  1--4
         0.161 0.019 1.00 0.0008
## 2--4
         0.160 0.019 1.00 0.0004
## 3--4
## 1--5
         -0.016
                   0.019 0.00 1.0000
## 2--5
          0.145
                   0.019 0.99 0.0080
## 3--5
          0.354
                   0.017 1.00 0.0000
```

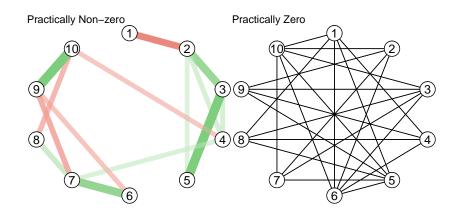
0.019 0.77 0.2286

0.114

## 4--5

## ---

In this case, the plot function returns two objects: (1) the selected, non-zero, edges; (2) those for which there is support for the null values.



## **Estimation: Edge Differences**

Differences between partial correlations are often tested in GGMs. In **BGGM**, it is possible to use posterior probabilities to determine which edges are practically equivalent.

## **Estimation: Edge Differences**

Differences between partial correlations are often tested in GGMs. In **BGGM**, it is possible to use posterior probabilities to determine which edges are practically equivalent.

This is implemented with:

## **Estimation: Edge Differences**

```
summary(edge_difference)
```

```
## BGGM: Bayesian Gaussian Graphical Models
## Type: Edge comparison(s)
## Region of Practical Equivalence: [-0.1, 0.1]
## ---
## Call:
## edge compare.estimate(x = fit sample, contrast = list("1--5 - 1--3".
      "1--2 - 1--6", "1--4 - 1--7", "1--5 - 1--10", "1--2 - 1--9"),
      ci_width = 0.95, rope = 0.1)
## ---
## Posterior Estimates:
##
##
       contrast post mean post sd pr out pr in
   1--5 - 1--3 0.0911 0.0318 0.392 0.608
##
## 1--2 - 1--6 -0.2972 0.0263
## 1--4 - 1--7 -0.0871 0.0295 0.3316 0.6684
## 1--5 - 1--10 0.0106 0.0271 6e-04 0.9994
## 1--2 - 1--9 -0.3684 0.0265 1
```

ullet Direct Correspondence between the elements of ullet and regression (coefficients and error variance)

- ullet Direct Correspondence between the elements of ullet and regression (coefficients and error variance)
- Recall:

- ullet Direct Correspondence between the elements of ullet and regression (coefficients and error variance)
- Recall:
  - $\bullet \ \mathbf{Y}'\mathbf{Y} \ (\mathbf{\Sigma}_{\mathsf{MLE}} = \mathit{n}^{-1}\mathbf{Y}'\mathbf{Y})$

- ullet Direct Correspondence between the elements of ullet and regression (coefficients and error variance)
- Recall:
  - $\mathbf{Y}'\mathbf{Y} (\mathbf{\Sigma}_{\mathsf{MLE}} = n^{-1}\mathbf{Y}'\mathbf{Y})$
  - (Y'Y)' (non-normalized precision matrix)

- ullet Direct Correspondence between the elements of ullet and regression (coefficients and error variance)
- Recall:
  - $\mathbf{Y}'\mathbf{Y} (\mathbf{\Sigma}_{\mathsf{MLE}} = n^{-1}\mathbf{Y}'\mathbf{Y})$
  - (Y'Y)' (non-normalized precision matrix)
- $\bullet \ \beta = (X'X)'X'y$

For j=1,...,p, let  $\mathbf{y}=V_j$  and  $\mathbf{X}=V_{\backslash \{j\}}$ . Then fit the pth regression model—i.e.,

For j=1,...,p, let  $\mathbf{y}=V_j$  and  $\mathbf{X}=V_{\backslash\{j\}}$ . Then fit the pth regression model—i.e.,

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}^{(j)} + \boldsymbol{\varepsilon},\tag{14}$$

where  $\varepsilon$  is an *n*-dimensional vector, with the mean as a vector of zeroes, and the covariance matrix as  $\sigma^2 \mathbf{I}_n$ .

For j=1,...,p, let  $\mathbf{y}=V_j$  and  $\mathbf{X}=V_{\backslash\{j\}}$ . Then fit the pth regression model—i.e.,

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}^{(j)} + \boldsymbol{\varepsilon},\tag{14}$$

where  $\varepsilon$  is an *n*-dimensional vector, with the mean as a vector of zeroes, and the covariance matrix as  $\sigma^2 \mathbf{I}_n$ .

 $eta^{(j)}$  denotes the (p-1) dimensional vector of coefficients for the jth regression model.

The regression coefficients and error variances then correspond to the off-diagonal and diagonal elements of  $\Theta$ -i.e.,

The regression coefficients and error variances then correspond to the off-diagonal and diagonal elements of  $\Theta$ -i.e.,

$$\theta_{ij} = \frac{-\beta_{ij}}{\sigma_j^2} \text{ and } \theta_{jj} = \frac{1}{\sigma_j^2},$$
 (15)

where  $\theta_{ij}$  denotes the covariance corresponding to *i*th row and *j*th column of  $\Theta$ .

The regression coefficients and error variances then correspond to the off-diagonal and diagonal elements of  $\Theta$ -i.e.,

$$\theta_{ij} = \frac{-\beta_{ij}}{\sigma_j^2} \text{ and } \theta_{jj} = \frac{1}{\sigma_j^2},$$
 (15)

where  $\theta_{ij}$  denotes the covariance corresponding to ith row and jth column of  $\Theta$ .

Consequently, for all posterior samples, s = 1, ..., S,

$$\beta_{ij}^{(s)} = \frac{-\theta_{ij}^{(s)}}{\theta_{ij}^{(s)}} \text{ and } \sigma_j^{2^{(s)}} = \frac{1}{\theta_{ij}^{(s)}}$$

$$\tag{16}$$

results in the posterior distribution for each regression coefficient and residual variance.

It follows that **BGGM** can also be used for the purpose of Bayesian multiple regression—i.e.,

It follows that **BGGM** can also be used for the purpose of Bayesian multiple regression—i.e.,

```
fit <- estimate(Y, samples = 5000)
coefficients(fit, node = 1, ci width = 0.95)
## BGGM: Bayesian Gaussian Graphical Models
## Type: Inverse to Regression
## ---
## Call:
## BGGM:::beta summary(x = fit, node = node, ci width = ci width,
      samples = samples)
## ---
## Estimates:
##
   node post_mean post_sd 2.5% 97.5%
         -0.277 0.021 -0.318 -0.238
##
      3 -0.124 0.022 -0.166 -0.081
##
      4 -0.015 0.021 -0.055 0.026
        -0.018 0.021 -0.059 0.024
        0.056 0.021 0.017 0.096
##
      7 0.081 0.021 0.038 0.122
      8 0.044
                   0.020 0.004 0.085
          0.141
                   0.021 0.100 0.184
     10
           -0.028
                   0.021 -0.069 0.012
```

In-sample prediction error:

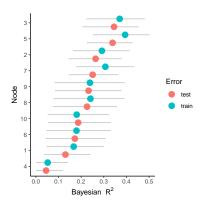
#### In-sample prediction error:

```
## BGGM: Bayesian Gaussian Graphical Models
## ---
## Type: In-sample predictive accuracy
## Measure: Variance Explained (R2)
## ---
## Call:
## predict.estimate(fit = fit_train, ci_width = 0.9, samples = 1000,
      measure = "R2")
## ---
## Estimates:
##
   node post_mean post_sd 2.5%
##
                                            97.5%
      1 0.1670357 0.06560828 0.04998099 0.2973988
##
      2 0.2917582 0.06505191 0.16503668 0.4128562
##
## ---
```

#### Out-of-sample prediction error:

The work flow is completed by visualizing Bayesian  $R^2$  for each node-i.e.,

```
# prior training and test error in the same plot
plt_6 <- plot(x1 = train_R2, x2 = test_R2, order = "test")</pre>
```



**BGGM** also includes Bayesian leave-one-out cross-validation.

**BGGM** also includes Bayesian leave-one-out cross-validation.

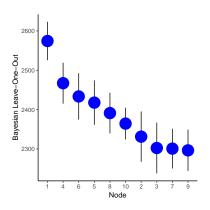
It is implemented with:

```
# p = 10
Y <- BGGM::bfi[1:1000,1:10]
# sample posterior
fit_sample <- estimate(Y, samples = 5000)
# Bayesian LOO
bayes_loo <- loocv(fit_sample)</pre>
```

```
# nodewise loo summary
summary(bayes_loo)
```

```
## BGGM: Bayesian Gaussian Graphical Models
## Type: Leave-One-Out Prediction Error (Bayesian)
## ---
## Call:
## loocv.default(x = fit_sample)
## Estimates:
               100
                     loo se
##
       1 2574 364 48 55682
       2 2331.292 63.81872
       3 2302 470 64 33004
       4 2467 128 51 75399
       5 2417.796 56.24886
       6 2433,493 58,62935
      7 2300.869 50.29901
      8 2391.216 51.31349
       9 2296.485 52.30362
      10 2364 485 40 15936
## ---
```

#### The results are plotted with:



**BGGM** includes a convenient, analytic form, for computing leave-one-out (*loo*) prediction error:

**BGGM** includes a convenient, analytic form, for computing leave-one-out (*loo*) prediction error:

$$- H = X^*(X^{*'}X^*)X^*$$

**BGGM** includes a convenient, analytic form, for computing leave-one-out (*loo*) prediction error:

$$- H = X^*(X^{*'}X^*)X^*$$

$$- H_d = diag(H)$$

**BGGM** includes a convenient, analytic form, for computing leave-one-out (*loo*) prediction error:

$$- H = X^*(X^{*'}X^*)X^*$$

$$- H_d = diag(H)$$

$$- \hat{\mathbf{y}} = \mathbf{X}^* \hat{\boldsymbol{\beta}}^*$$

**BGGM** includes a convenient, analytic form, for computing leave-one-out (*loo*) prediction error:

$$- H = X^*(X^{*'}X^*)X^*$$

$$- H_d = diag(H)$$

$$- \hat{\mathbf{y}} = \mathbf{X}^* \hat{\boldsymbol{\beta}}^*$$

$$- \varepsilon = y - \hat{y}$$

**BGGM** includes a convenient, analytic form, for computing leave-one-out (*loo*) prediction error:

 Let X\* ⊆ X denote the selected predictors for the pth regression model

$$- H = X^*(X^{*'}X^*)X^*$$

$$- \mathbf{H}_d = \operatorname{diag}(\mathbf{H})$$

$$- \hat{\mathbf{y}} = \mathbf{X}^* \hat{\boldsymbol{\beta}}^*$$

$$- \varepsilon = y - \hat{y}$$

$$loo = \sum_{i=1}^{n} \left(\frac{\varepsilon_i}{1 - H_d^i}\right)^2$$

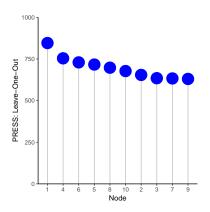
#### This method is implemented with

```
# p = 10
Y <= BGGM::bfi[1:1000,1:10]
# analytic solution
fit_analytic <- estimate(Y, analytic = T)
# analytic LOO (PRESS; based on point estimates)
press_loo <- loocv(fit_analytic)</pre>
```

```
summary(press loo)
## BGGM: Bayesian Gaussian Graphical Models
## Type: Leave-One-Out Prediction Error (Analytic)
## ---
## Call.
## loocv.default(x = fit_analytic)
## Estimates:
     node
               100
                        rss
       1 845 6207 838 6759
##
       2 654,2324 644,6005
       3 634.5554 629.3224
       4 753 9226 744 1923
       5 716.4956 710.4838
       6 729.5712 723.7107
      7 633 1005 626 5797
       8 697,7085 686,3148
       9 630.1037 621.9319
      10 677.4374 672.4343
```

## ---

#### The results are plotted with:



### **Conclusion**

Next DIPS presentation I will discuss the Bayesian hypothesis testing methods.

Then the following I will discuss the methods to compare any number of GGMs.

### **Conclusion**

Next DIPS presentation I will discuss the Bayesian hypothesis testing methods.

Then the following I will discuss the methods to compare any number of GGMs.

Thank You!