Bayesian modelling of brain network data via latent space models

Emanuele Aliverti,
University of Padova, Department of Statistical Sciences

emanuelealiverti.github.io
aliverti@stat.unipd.it

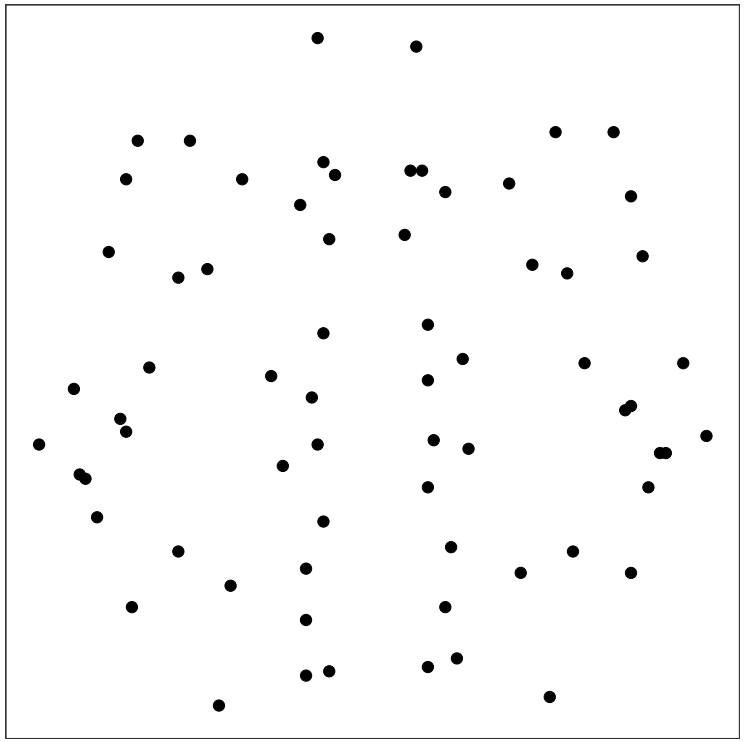
22th November 2019

Università degli Studi di Padova

Brain Networks

- Non-invasive imaging technologies provide **accurate** data on brain activity and structure at increasing resolution for multiple subjects

- Neuro–imaging study comprising data for $m = 21$ individuals (Landman et al., 2011).
- $n = 68$ brain regions (nodes), spatially located



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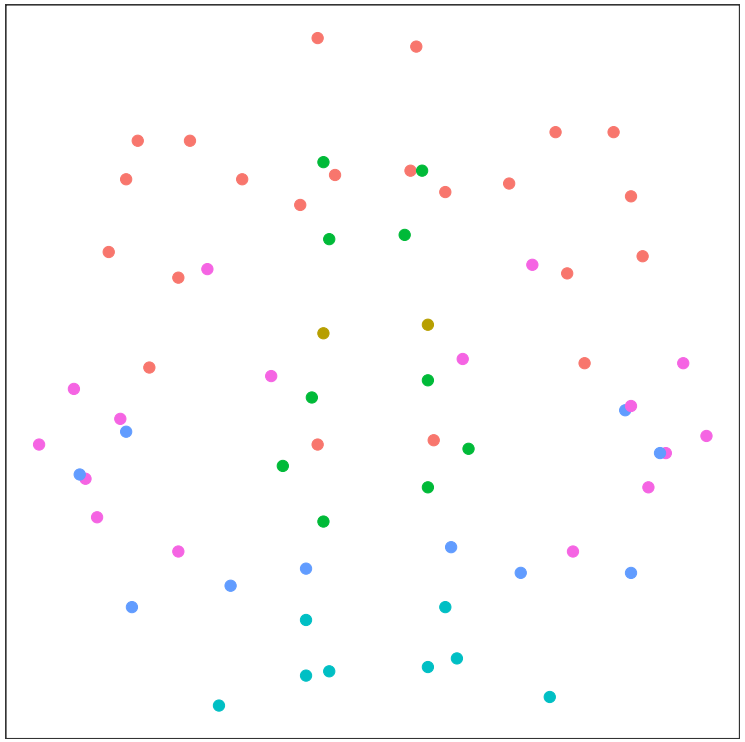

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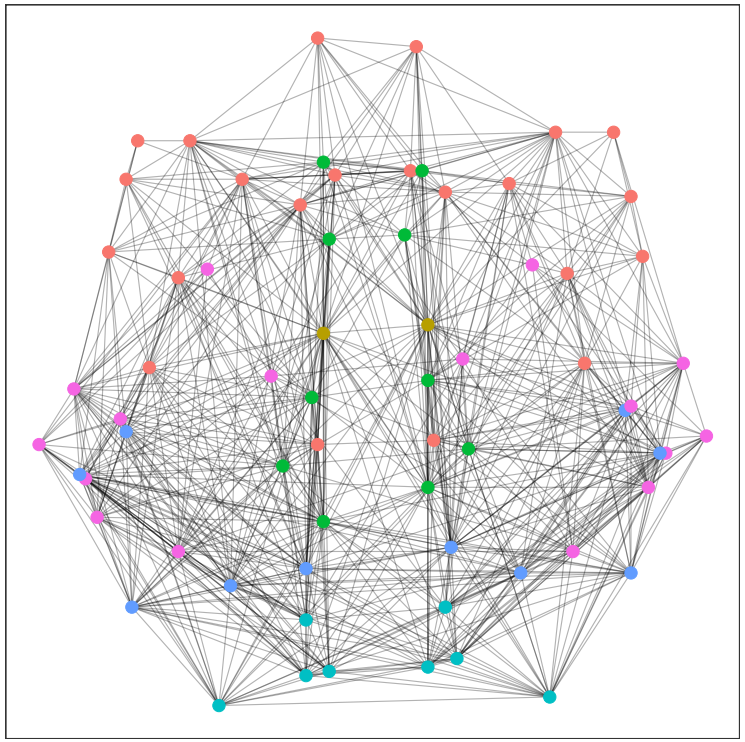

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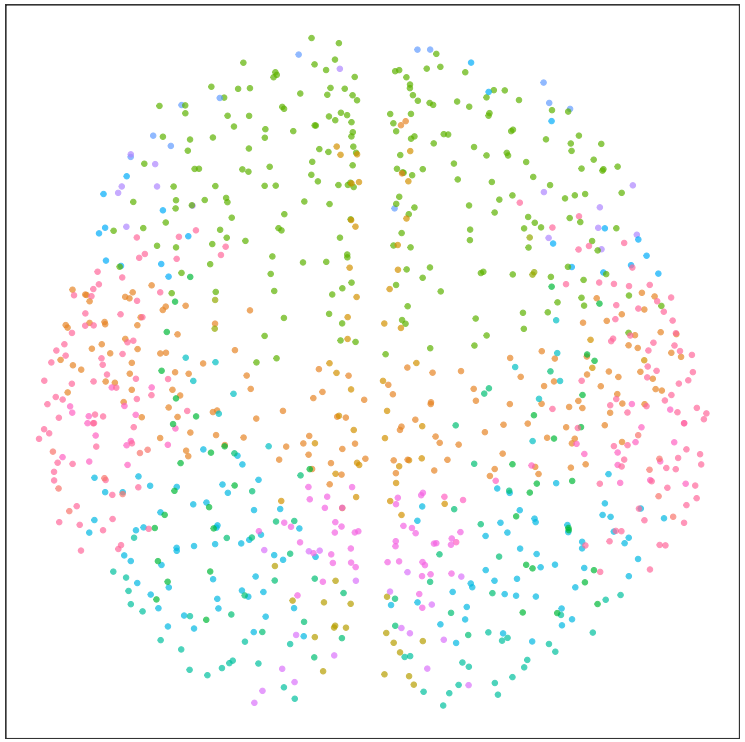

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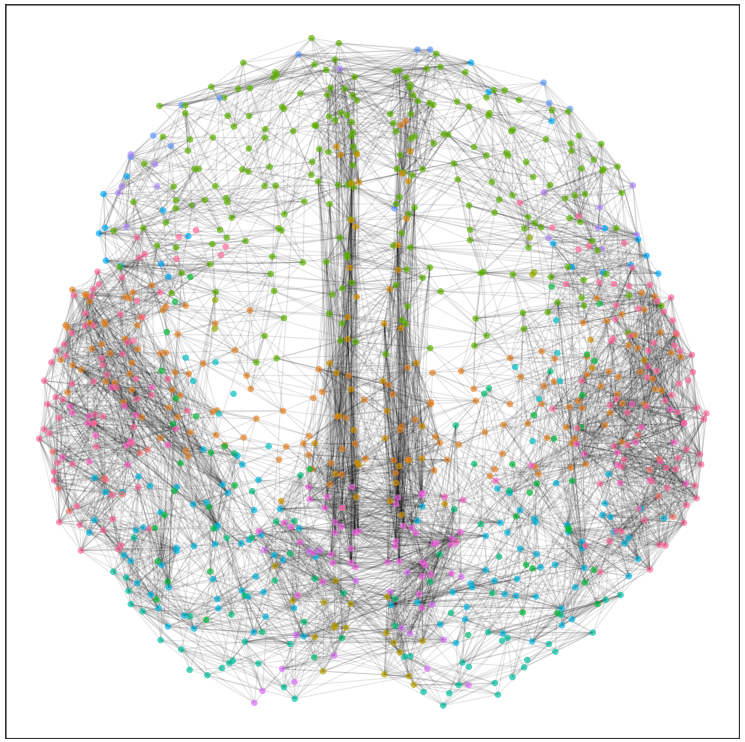

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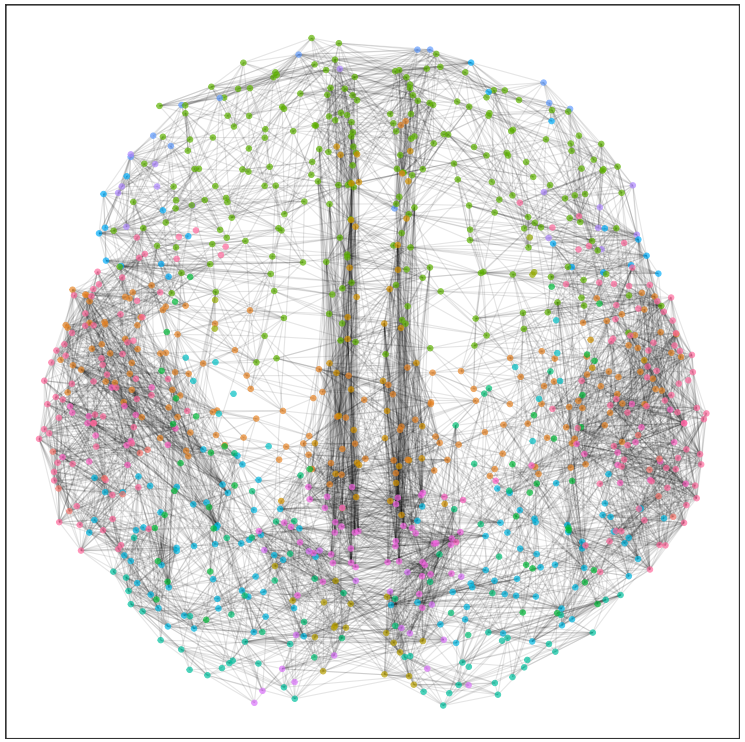
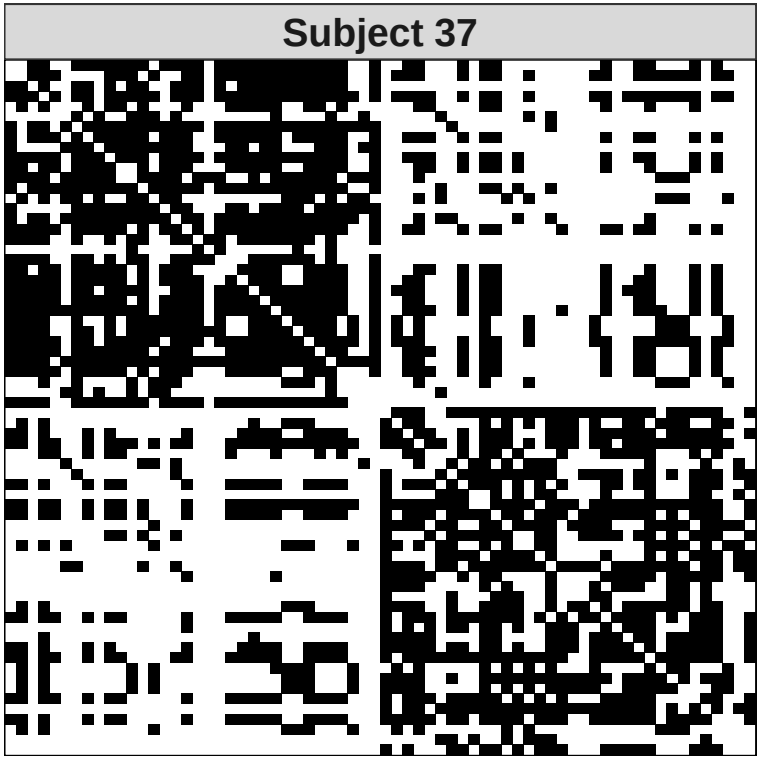


- **Goal:** investigate network connectivity patterns, accounting for anatomical constraints and unobservable patters (e.g. shapes, functionalities)

Brain Network Data

- For each subject, data can be represented as an $(n \times n)$ symmetric adjacency matrix $A^{(k)}$, $k = 1, \ldots, m$



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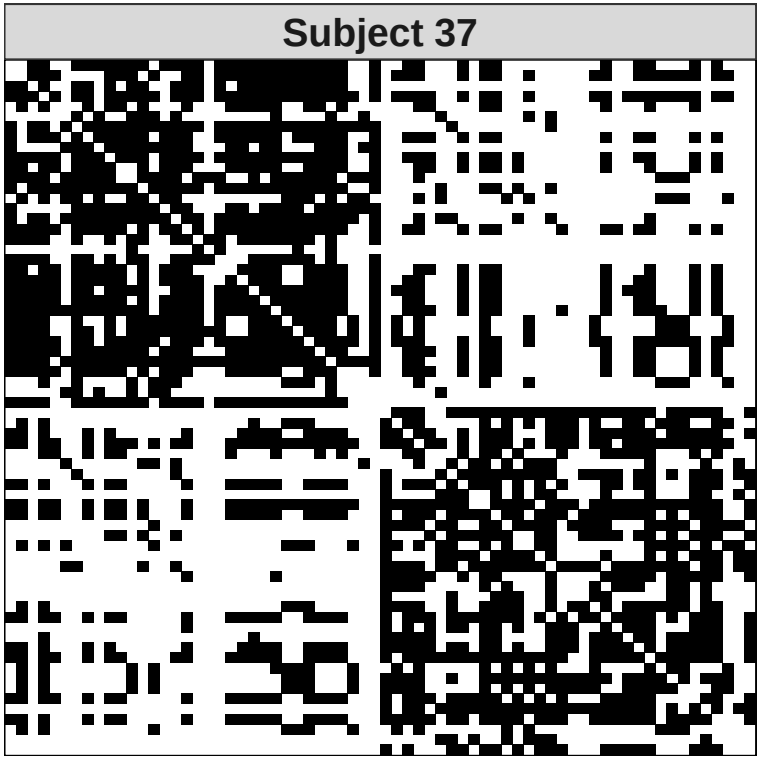

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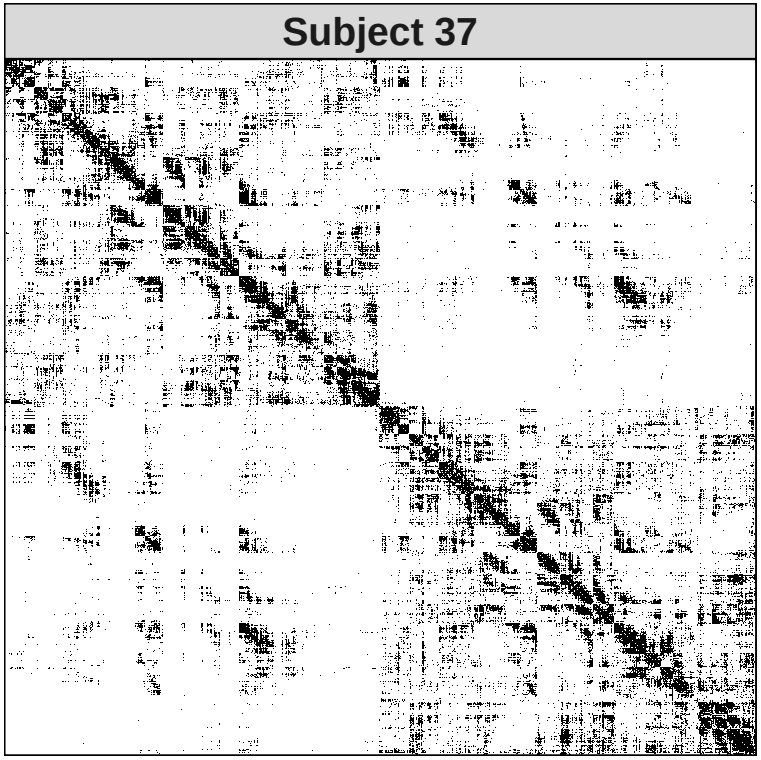
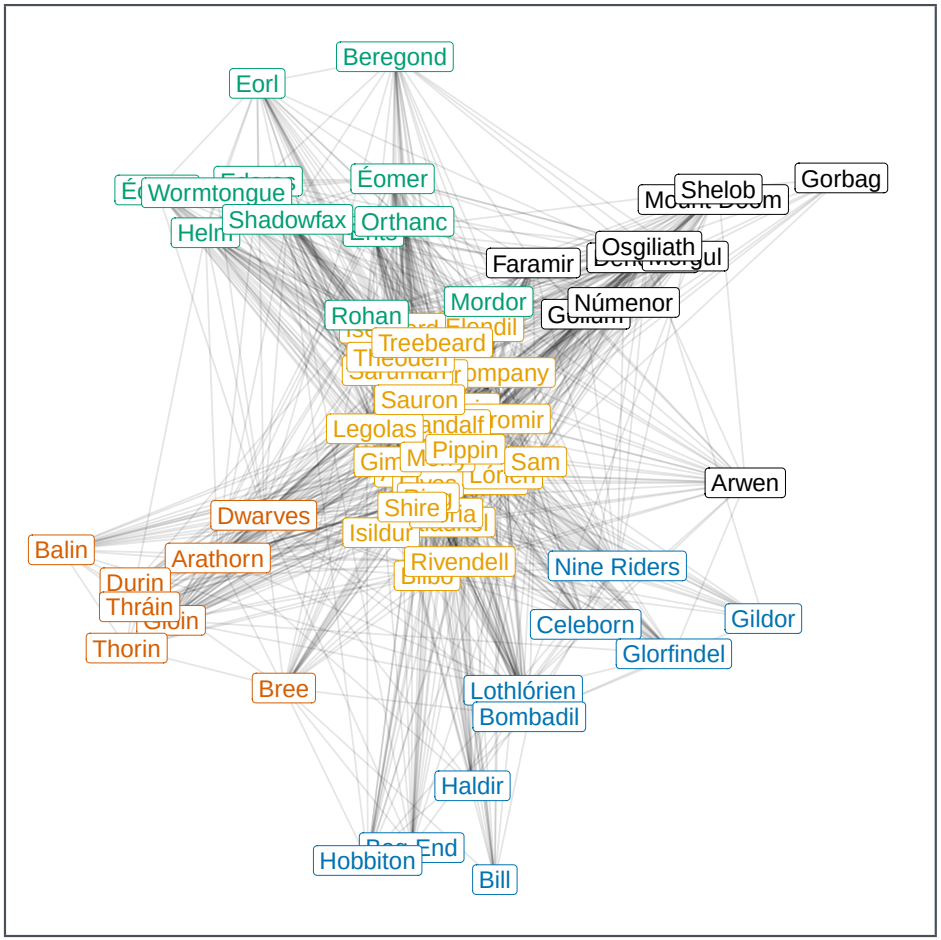
Anatomical information

- Spatial coordinates for the i-th region (x_i, y_i, z_i)
- Lobes and hemisphere membership
  - $\rightarrow$ $\texttt{lobe}_{ij} = 1$ region i and region j are in the same lobe
  - $\rightarrow$ $\texttt{hemi}_{ij} = 1$ region i and region j are in the same hemisphere



Latent Space Models - intuition

- Developed in social sciences (e.g. Hoff et al., 2002; Hoff, 2008)



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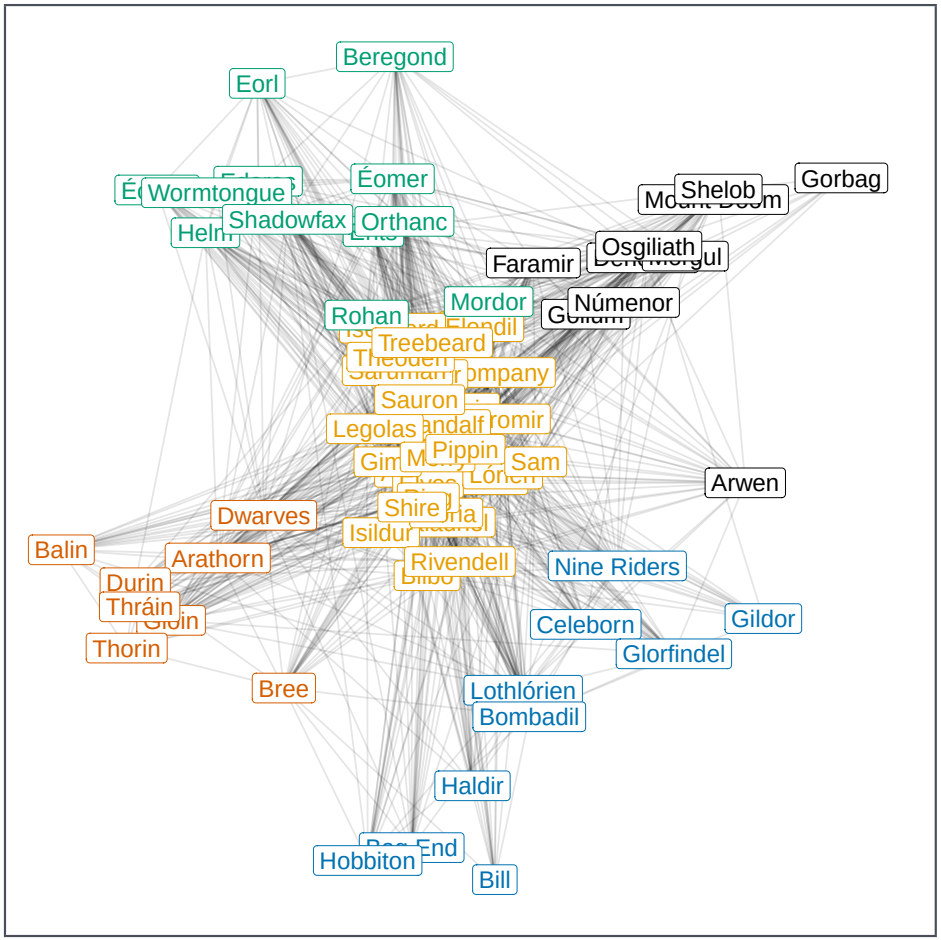

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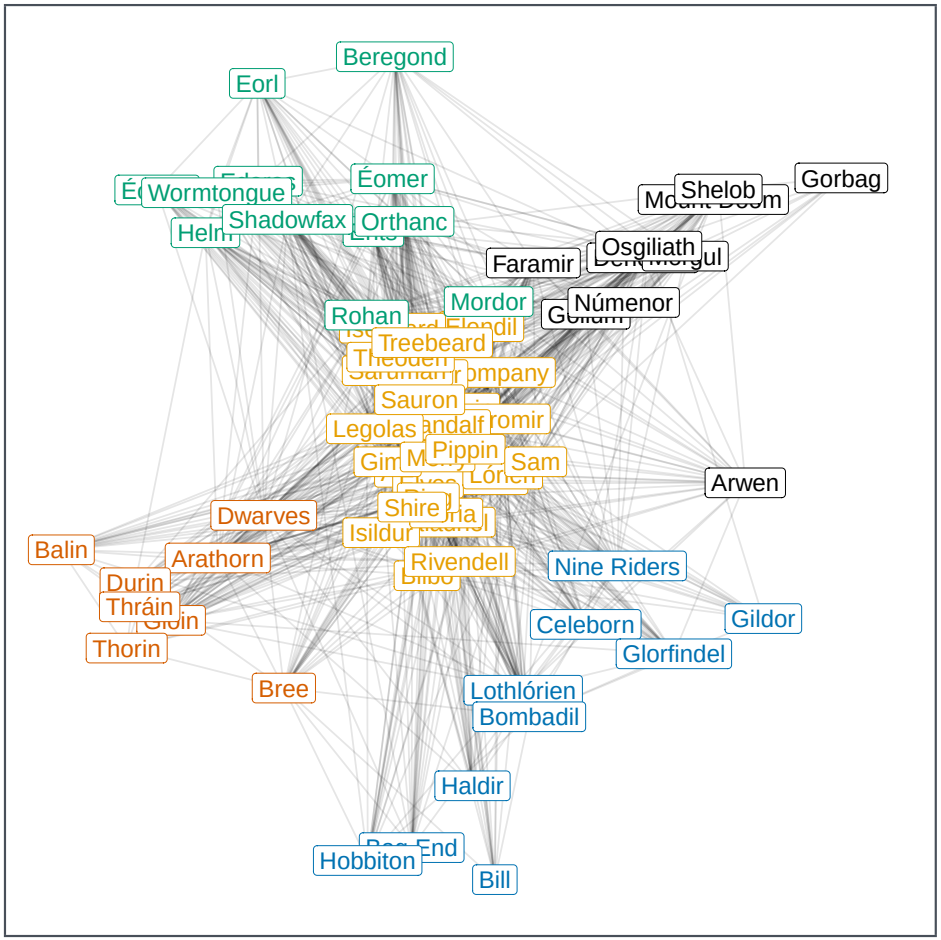

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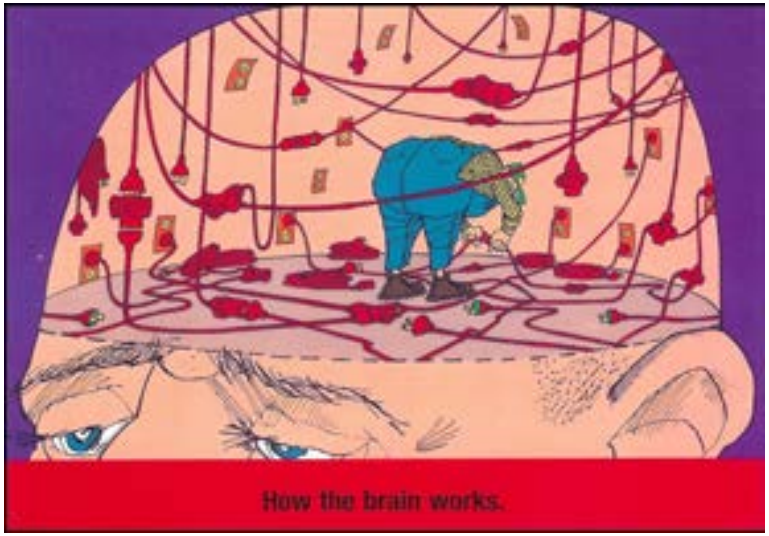
Benefits

- Reduce dimensionality from $n \times (n-1)/2$ to $n \times H$
- Takes into account network properties (e.g. transitivity, homophily)

Latent spaces and beyond

- Each latent coordinate may be interpreted as measure of its "propensity" for different functions / metabolic processes
- Regions with similar propensities are more likely to be connected



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- Allow modelling of *replicated* networks, multiple subjects
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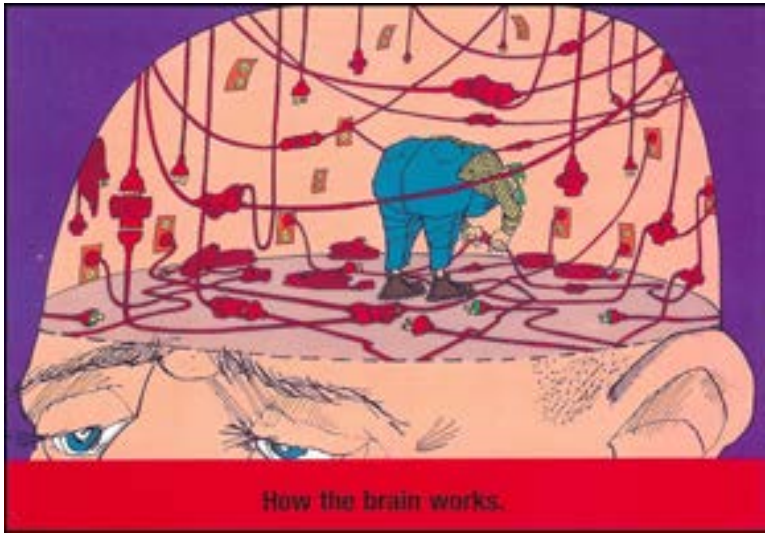

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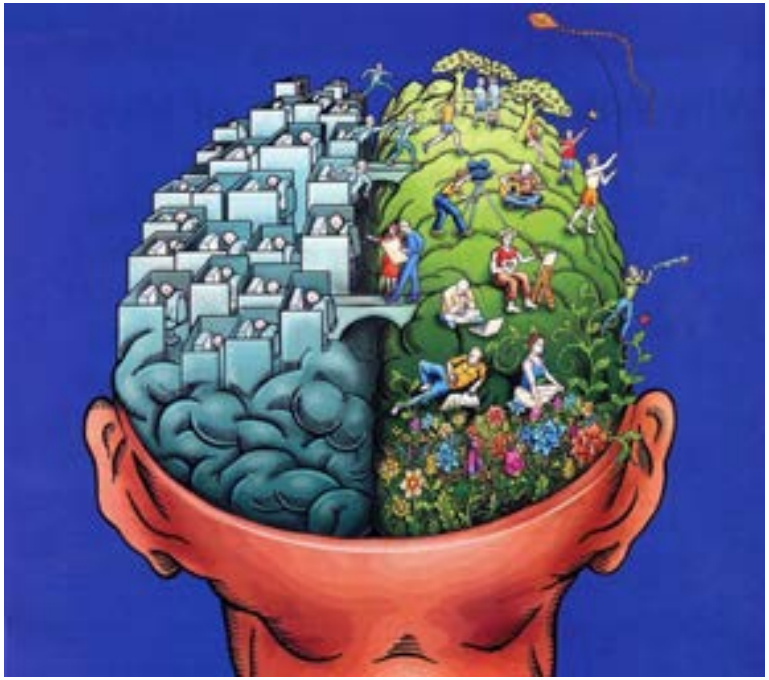

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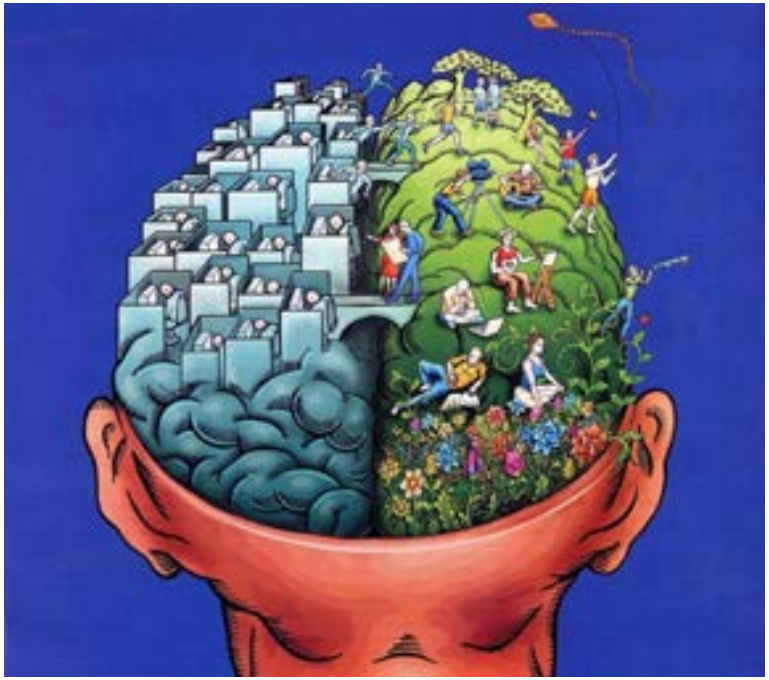
- Include covariates
  - → Connectivity as a function of anatomical constraints (distance, lobes)
- Estimate *local* clusters of brain regions
  - → Some regions might be similar only wrt *subset* of latent features.



Specification

- Focus on modelling $\mathbf{A} = \sum_{k=1}^{m} A^{(k)}$

$$(a_{ij} \mid \pi_{ij}) \sim \text{Binom}(m, \pi_{ij})$$
$$\text{logit}(\pi_{ij}) = \beta_0 + \beta_1 \texttt{hem}_{ij} + \beta_2 \texttt{lobe}_{ij} + \beta_3 d_{ij} - \bar{d}_{ij}$$

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  $\rightarrow$ Euclidean distance between region i and j **in the original space**
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- $\bar{d}_{ij} = \sqrt{(\bar{x}_i - \bar{x}_j)^2 + (\bar{y}_i - \bar{y}_j)^2 + (\bar{z}_i - \bar{z}_j)^2}$
  $\rightarrow$ Euclidean distance between region i and j **in the latent space**
- $(\bar{x}_i, \bar{y}_i, \bar{z}_i) \in \mathbb{R}^3$ **latent coordinates** of region i

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- Estimate groups of brain regions similar to *subsets* of latent features

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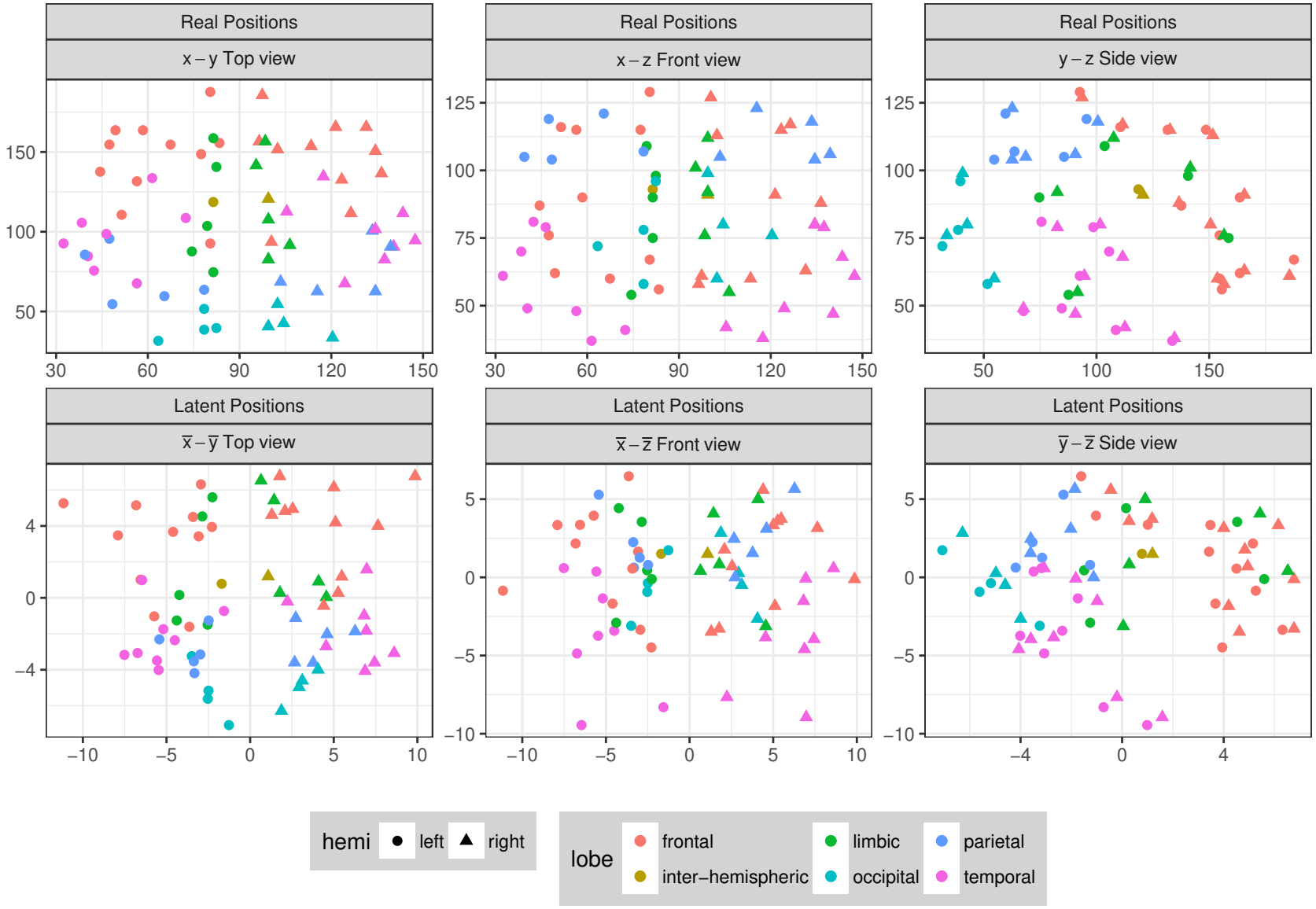
- Sparse Dirichlet on $\boldsymbol{\nu}_\mathsf{x}$, $\boldsymbol{\nu}_\mathsf{x}$ and $\boldsymbol{\nu}_\mathsf{y}$ to favour deletion of redundant components (Rousseau and Mengersen, 2011)
- Gaussian for $(\beta_0, \beta_1, \beta_2, \beta_3)$, conditionally conjugate trough the Pòlya-Gamma data augmentation (Polson et al., 2013).
- Metropolis step for updating the latent coordinates (Euclidean distance)

Results


Real Positions
x – y Top view
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x – z Front view
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y – z Side view
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right
lobe
frontal
inter–hemispheric
limbic
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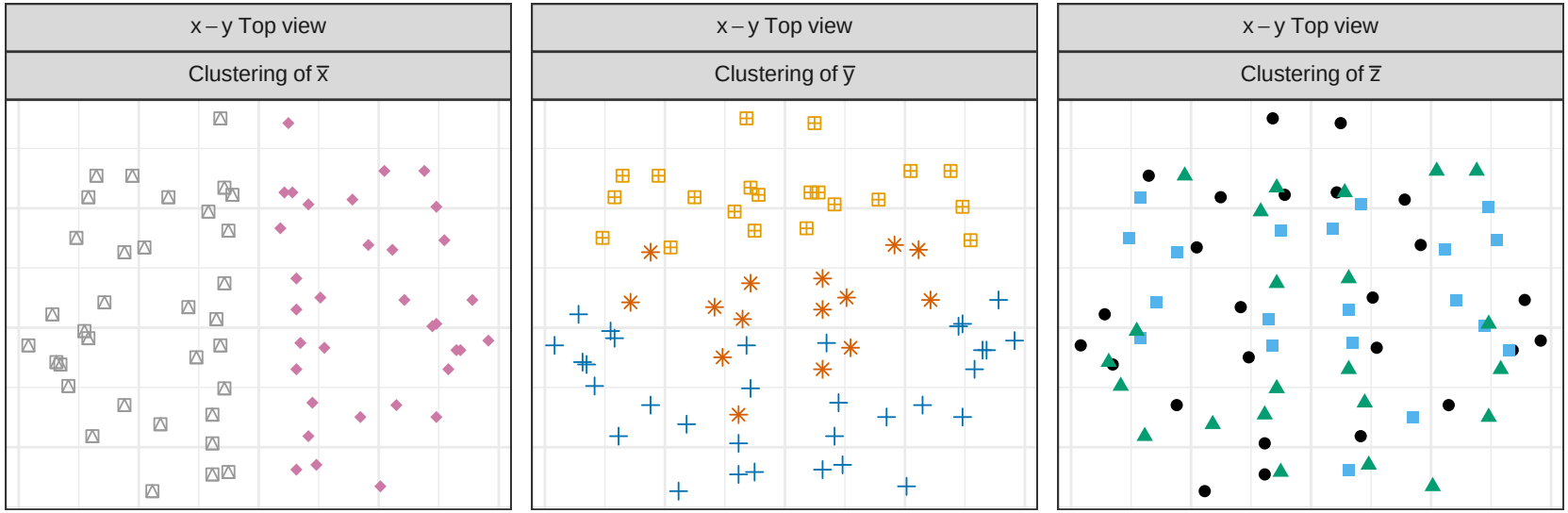
parietal
temporal

Results 2

- Inference on the separate partitions



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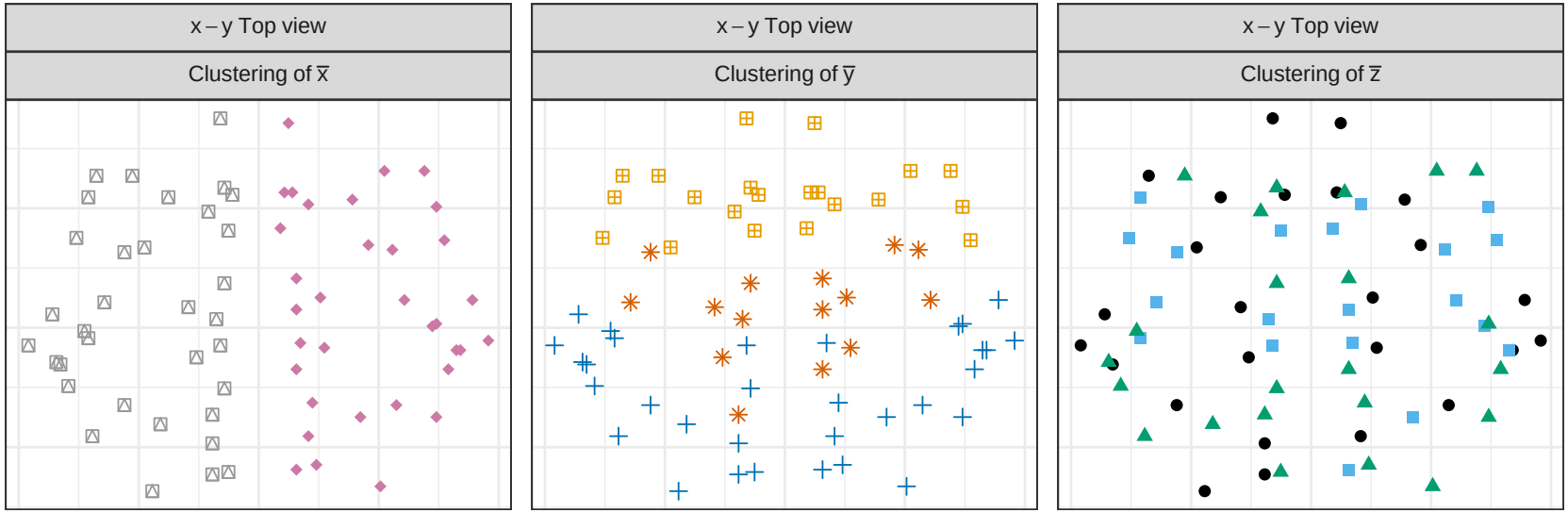


- ...and on the coefficients

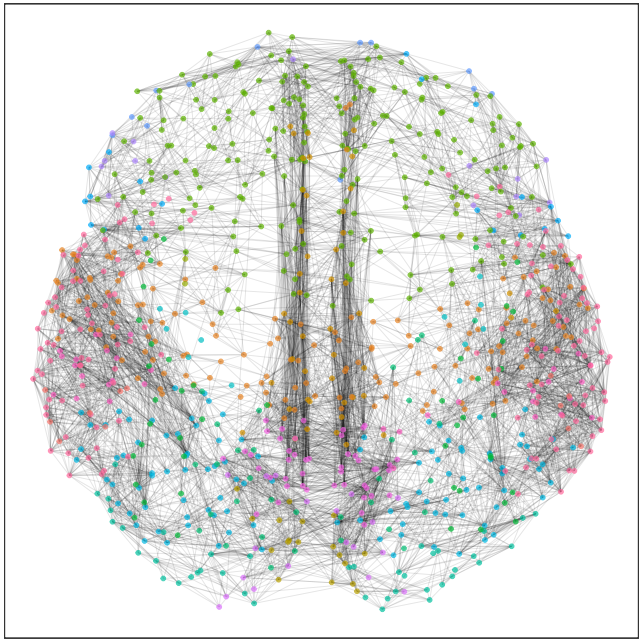
	Mean	Median	Std. Dev.	Cred. Int.$_{95\%}$
`Intercept`	7.27	7.27	0.18	(6.94, 7.60)
`hemisphere`	0.60	0.61	0.18	(0.29, 0.92)
`lobes`	0.24	0.24	0.06	(0.13,0.35)
`distance`	-0.35	-0.35	0.06	(-0.47,-0.23)

Goodness of fit

Computational Drawbacks

- **Issue:** Inference relying on Markov Chain Monte Carlo scales poorly

- CPU time
  - $\rightarrow$ $n = 68$, 2 min $\times 1000$ it.
  - $\rightarrow$ $n = 998$, **7 hours** $\times 1000$ it.



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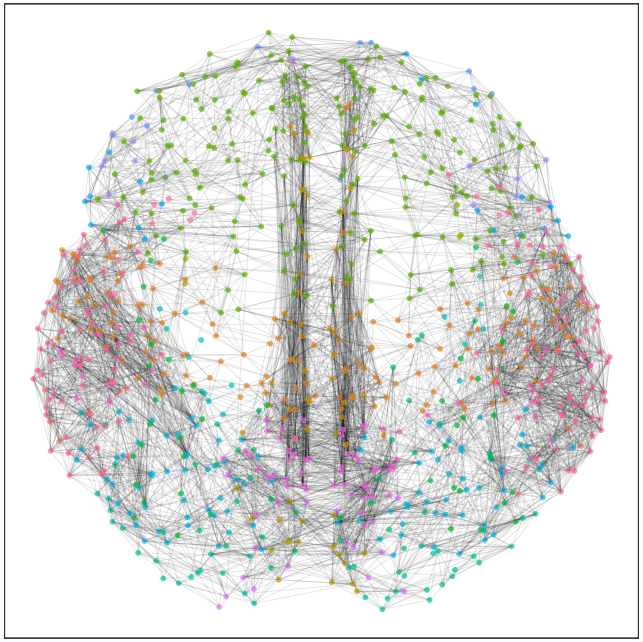

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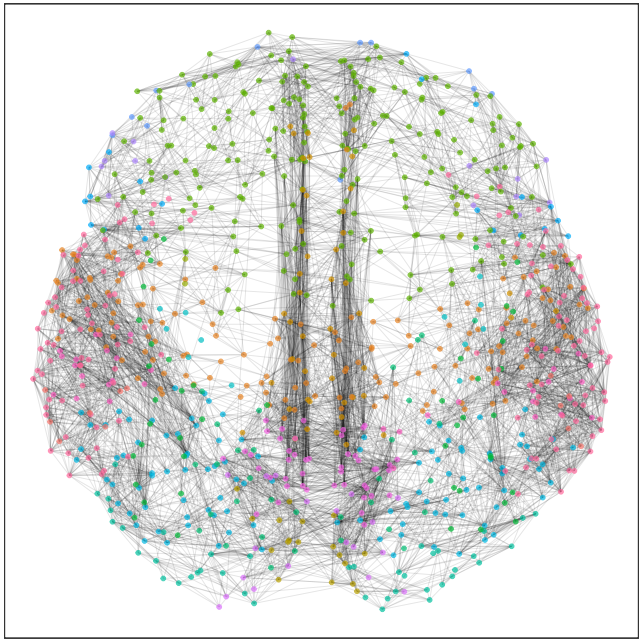

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- Variational inference is widely popular in the network-science literature (Gollini and Murphy, 2016; Salter-Townshend and Murphy, 2013)
- The Euclidean distance requires several Taylor expansions of the complete data log-likelihood

A different specification

- Latent Factor Model (Hoff, 2008)

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- $\mathbf{w}_i = (\tilde{x}_i, \tilde{y}_i, \tilde{z}_i) \in \mathbb{R}^3$ **latent positions** of region i
- $\boldsymbol{\psi} = (\psi_x, \psi_y, \psi_z) \in \mathbb{R}^3$ **importance** of latent coordinates

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- Gaussian priors

$$\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2, \beta_3)^\intercal \sim \text{N}_4(0, \boldsymbol{\Sigma}_0), \qquad \boldsymbol{\Sigma}_0 = \text{diag}(\sigma_0, \ldots, \sigma_3),$$
$$\tilde{x}_i \sim \text{N}(0,1), \quad \tilde{y}_i \sim \text{N}(0,1), \quad \tilde{z}_i \sim \text{N}(0,1) \quad i = 1, \ldots, n,$$
$$(\psi_x, \psi_y, \psi_x) \sim \text{N}_3(0, \gamma_{\psi_0} I_3)$$

- **Conditional conjugancy** introducing $(\omega_{ij} \mid -) \sim \text{PG}\left(m, \text{logit}(\pi_{ij})\right)$

Variational Inference

- **Variational Bayes**: find best approximation of the true posterior p in a restricted class $\mathcal{Q}$ of distributions

$$q^\star(\boldsymbol{\beta}, \mathbf{W}, \boldsymbol{\omega}, \boldsymbol{\psi}) = \underset{q \in \mathcal{Q}}{\arg\min}\, \mathrm{KL}\left\{ q(\boldsymbol{\beta}, \mathbf{W}, \boldsymbol{\omega}, \boldsymbol{\psi}) \,||\, p(\boldsymbol{\beta}, \mathbf{W}, \boldsymbol{\omega}, \boldsymbol{\psi} \mid \mathbf{A}) \right\}.$$

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- Analytical form for the optimal factors (same EF form than Full-Conditionals)

$$q^\star(\boldsymbol{\beta}) \propto \exp\left\{\mathbb{E}_{q(\mathbf{W}, \boldsymbol{\omega}, \boldsymbol{\psi})} \log p(\boldsymbol{\beta} \mid -)\right\} \qquad \text{(Gaussian)}$$

$$q_i^\star(\mathbf{w}_i) \propto \exp\left\{\mathbb{E}_{q(\boldsymbol{\beta}, \mathbf{W}_{-i}, \boldsymbol{\omega}, \boldsymbol{\psi})} \log p(\mathbf{w}_i \mid -)\right\}, \quad i = 1, \ldots, n \qquad \text{(Gaussian)}$$

$$q^\star(\boldsymbol{\psi}) \propto \exp\left\{\mathbb{E}_{q(\boldsymbol{\beta}, \mathbf{W}, \boldsymbol{\omega})} \log p(\boldsymbol{\psi} \mid -)\right\} \qquad \text{(Gaussian)}$$

$$q_{ij}^\star(\omega_{ij}) \propto \exp\left\{\mathbb{E}_{q(\boldsymbol{\beta}, \mathbf{w}_i, \mathbf{w}_j, \boldsymbol{\psi})} \log p(\omega_{ij} \mid -)\right\} \qquad \text{(Pòlya-Gamma)}$$

Variational Inference

- **Variational Bayes**: find best approximation of the true posterior p in a restricted class $\mathcal{Q}$ of distributions

$$q^\star(\boldsymbol{\beta}, \mathbf{W}, \boldsymbol{\omega}, \boldsymbol{\psi}) = \arg\min_{q \in \mathcal{Q}} \mathrm{KL}\left\{q(\boldsymbol{\beta}, \mathbf{W}, \boldsymbol{\omega}, \boldsymbol{\psi}) \,||\, p(\boldsymbol{\beta}, \mathbf{W}, \boldsymbol{\omega}, \boldsymbol{\psi} \mid \mathbf{A})\right\}.$$

- **Mean Field**: product restriction
  $\mathcal{Q} = \{q(\boldsymbol{\beta}, \mathbf{W}, \boldsymbol{\omega}, \boldsymbol{\psi}) : q(\boldsymbol{\beta}, \mathbf{W}, \boldsymbol{\omega}, \boldsymbol{\psi}) = q(\boldsymbol{\beta})q(\mathbf{W})q(\boldsymbol{\omega})q(\boldsymbol{\psi})\}$

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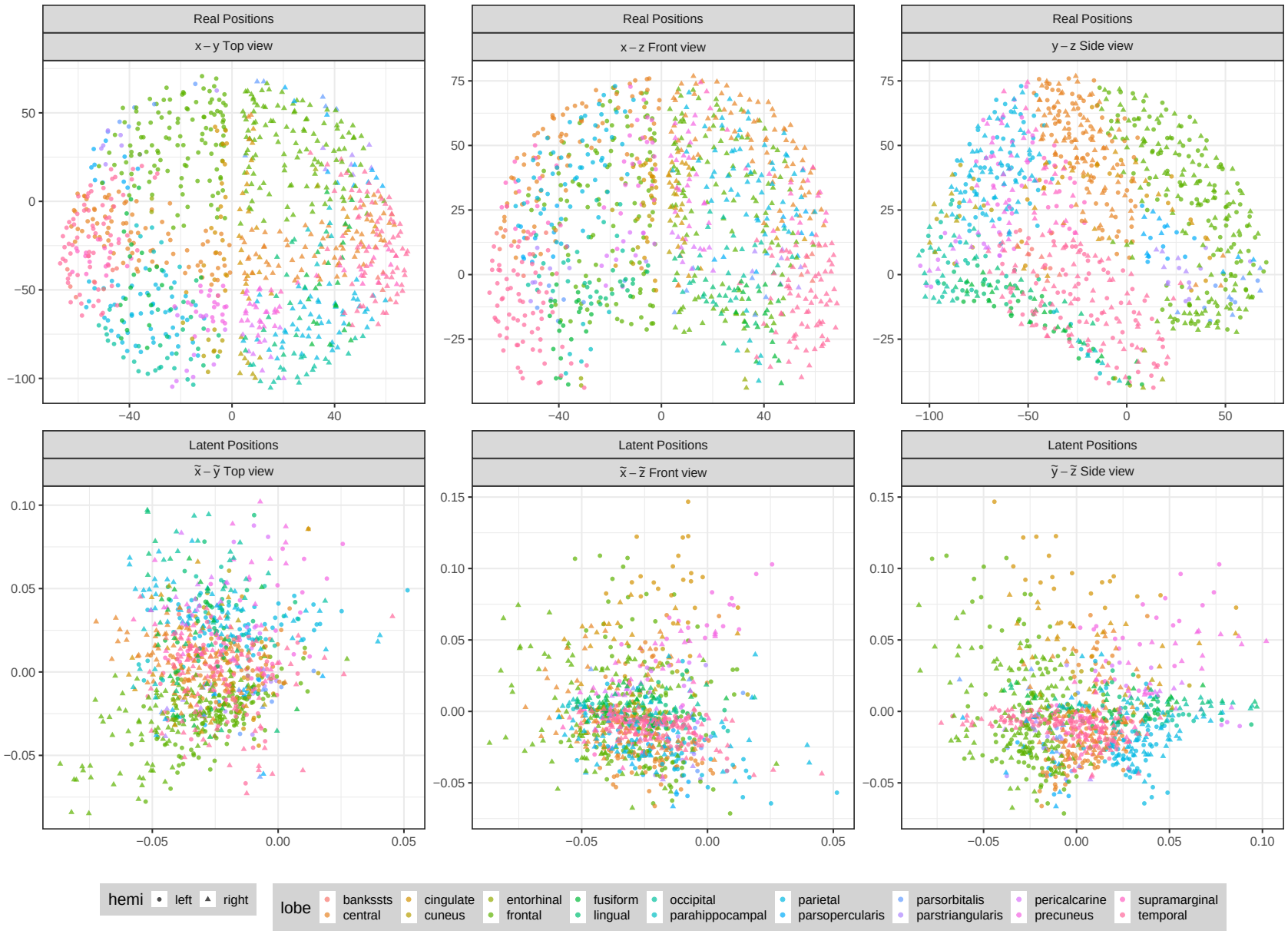
- **CAVI**: cycle over each variational factor until convergence

Results, part II



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Thank you! Questions, comments?