A Bayesian Model for Brain Network Functional Connectivity using PyMC3

Rui Wang Ph.D.
M.S. Thesis Presentation

Department of Biostatistics

VANDERBILT UNIVERSITY
MEDICAL CENTER

Outline

- Introduction

- Methods
  - Spatiotemporal Structure
  - Hierarchical Structure
  - Double Fusion
  - Prior Distribution
  - PyMC3 and NUTS
  - Optimization and Decomposition

- Simulation and Case Study

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Previous Study

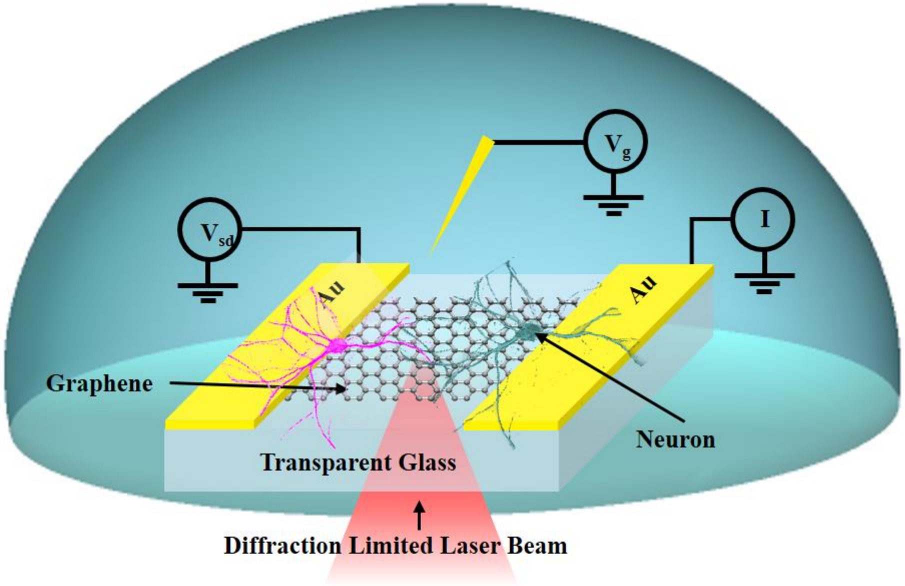
Precise Timing

High Electrical Sensitivity

High Throughput

High Spatial Accuracy

Long-term Duration

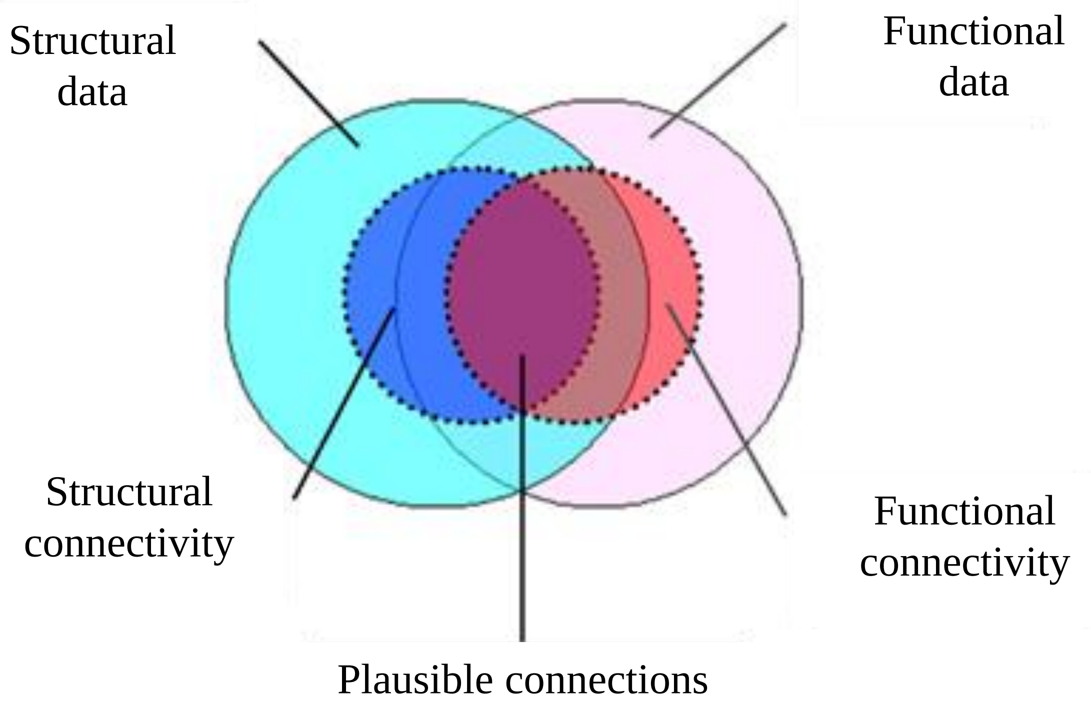


Wang, R et. al, ***Nano Letter*** (in review)

Brain Imaging

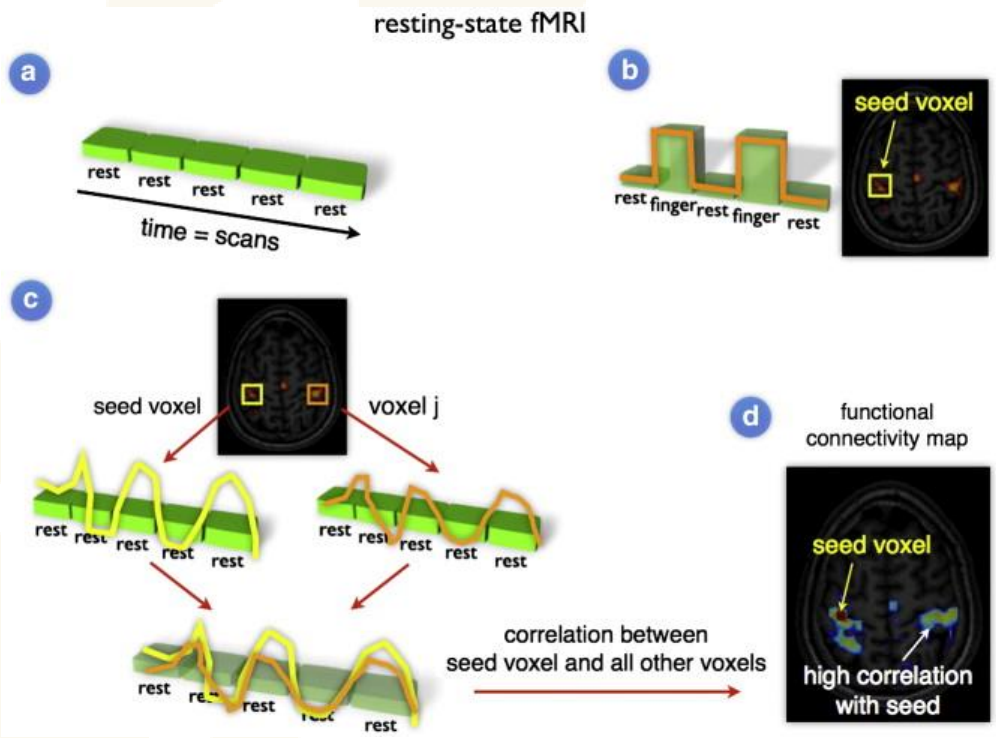
https://www.sciencedaily.com/releases/2016/11/161103141437.htm

Brain Imaging



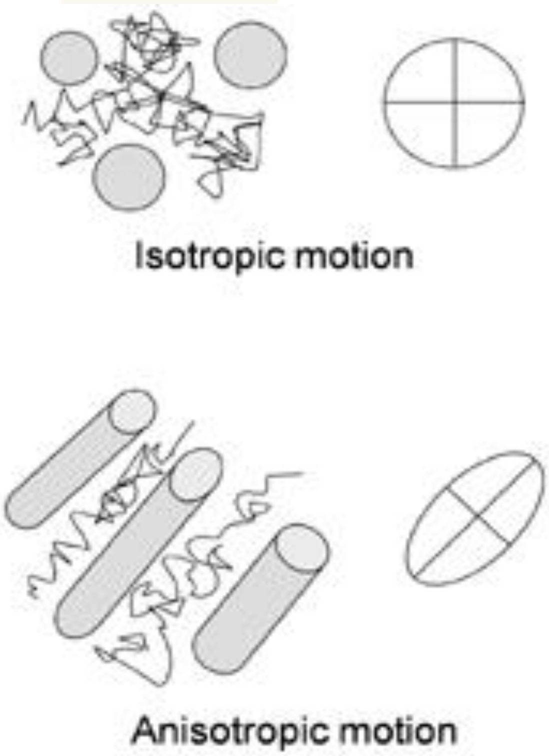
Rykhlevskaia et. al, ***Psychophysiology*** 45(2) (2008)

Functional Connectivity



van den Heuvel et. al, ***European Neuropsychopharmacology*** 20(8) (2008)

Structural Connectivity



Rykhlevskaia et. al, ***Psychophysiology*** 45(2) (2008)

Goal

- A Bayesian hierarchical spatiotemporal model
  - Combine resting-state fMRI and DTI data
  - Apply various kernel covariance functions
  - **Improve precision of estimation of functional connectivity**

- PyMC3 for simulation and case study

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Spatiotemporal Structure

$$Y_{cv}(t) = \beta_c + b_c(v) + d_c + \epsilon_{cv}(t)$$

- β_c: the grand mean
- $b_c(v)$: the zero-mean voxel-specific random effect
    - Local spatial dependency:

$$Cov\big(b_c(v), b_c(v')\big) = K_c(\|v - v'\|)$$

- d_c: the zero-mean ROI-specific random effect
- $\epsilon_{cv}(t)$: the noise
    - AR (1) temporal structure

Kang, H et. al, ***Brain Connectivity*** 7(4) (2017)

Kernel Covariance Function

Constant	$K(x,x') = c$
Linear	$K(x,x') = x^T x'$
Gaussian noise	$K(x,x') = \sigma^2 \delta_{x,x'}$
Squared exponential	$K(x,x') = \exp(-\frac{\lVert x-x'\rVert^2}{2l^2})$
Exponential	$K(x,x') = \exp(-\frac{\lVert x-x'\rVert}{l})$
Matérn	$K(x,x') = \frac{2^{1-v}}{\Gamma(v)}\left(\frac{\sqrt{2v}\lVert x-x'\rVert}{l}\right)^v B_v(\frac{\sqrt{2v}\lVert x-x'\rVert}{l})$
Periodic	$K(x,x') = \exp(-\frac{2sin^2(\frac{x-x'}{2})}{l^2})$
Rational quadratic	$K(x,x') = (1+ \lVert x-x'\rVert^2)^{-\alpha}, \alpha \geq 0$

Kernel Covariance Function

$$r = \|v - v'\| \varphi_c$$

Exponential (Matérn 1/2):

$${\sigma_{b_c}}^2 \exp(-r)$$

Gaussian or square exponential (Matérn ∞):

$${\sigma_{b_c}}^2 \exp(-\frac{1}{2} r^2)$$

Matérn 5/2:

$${\sigma_{b_c}}^2 (1 + \sqrt{5}\mathrm{r} + \frac{5}{3} r^2) \exp(-\sqrt{5} r)$$

Matérn 3/2:

$${\sigma_{b_c}}^2 (1 + \sqrt{3} r) \exp(-\sqrt{3} r)$$

Temporal Correlation

AR (1) structure:

$$\epsilon_{cv}(t) = \delta_c + \phi_{cv}\, \epsilon_{cv}(t-1) + w(t)$$

- δ_c: the constant shift
- ϕ_{cv}: the coefficient with $|\phi_{cv}| < 1$
- $w(t)$: the Gaussian random noise

$$\mathrm{E}[\epsilon_{cv}(t)] = \frac{\delta_c}{1-\phi_{cv}}$$

$$\mathrm{Var}[\epsilon_{cv}(t)] = \frac{{\sigma_{cv}}^2}{1-{\phi_{cv}}^2}$$

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Hierarchical Structure

$$\boldsymbol{Y}_c(t) = \boldsymbol{\beta}_c + \boldsymbol{b}_c + \boldsymbol{d}_c + \boldsymbol{\epsilon}_c(t)$$

- $\boldsymbol{Y}_c(t) = [Y_{c1}(t), Y_{c2}(t), \ldots, Y_{cV}(t)]^T$
- $\boldsymbol{\beta}_c = \beta_c \boldsymbol{J}_{(1\times V)}$
- $\boldsymbol{b}_c = [b_{c1}, b_{c2}, \ldots, b_{cV}]^T$
- $\boldsymbol{d}_c = d_c \boldsymbol{J}_{(1\times V)}$
- $\boldsymbol{\epsilon}_c(t) = [\epsilon_{c1}(t), \epsilon_{c2}(t), \ldots, \epsilon_{cV}(t)]^T$

Hierarchical Structure

$$\boldsymbol{Y}_c(t) = \boldsymbol{\beta}_c + \boldsymbol{b}_c + \boldsymbol{d}_c + \boldsymbol{\epsilon}_c(t)$$

- $\beta_c \sim \mathrm{N}\left(0, {\sigma_{\beta_c}}^2\right)$
- $\boldsymbol{b}_c \sim \mathrm{N}\left(0, \Sigma_{b_c}\right)$
- $d_c \sim \mathrm{N}(0, \Sigma_d)$
- $\epsilon_{cv}(t) \sim \mathrm{N}(\frac{\delta_c}{1-\phi_{cv}}, \frac{{\sigma_{cv}}^2}{1-{\phi_{cv}}^2})$

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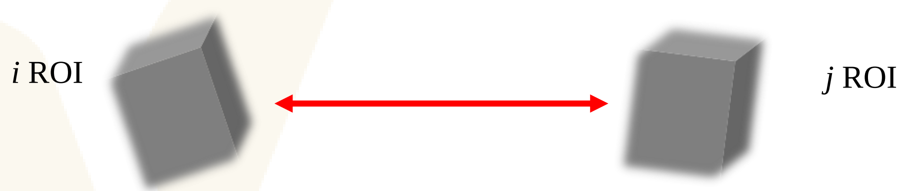
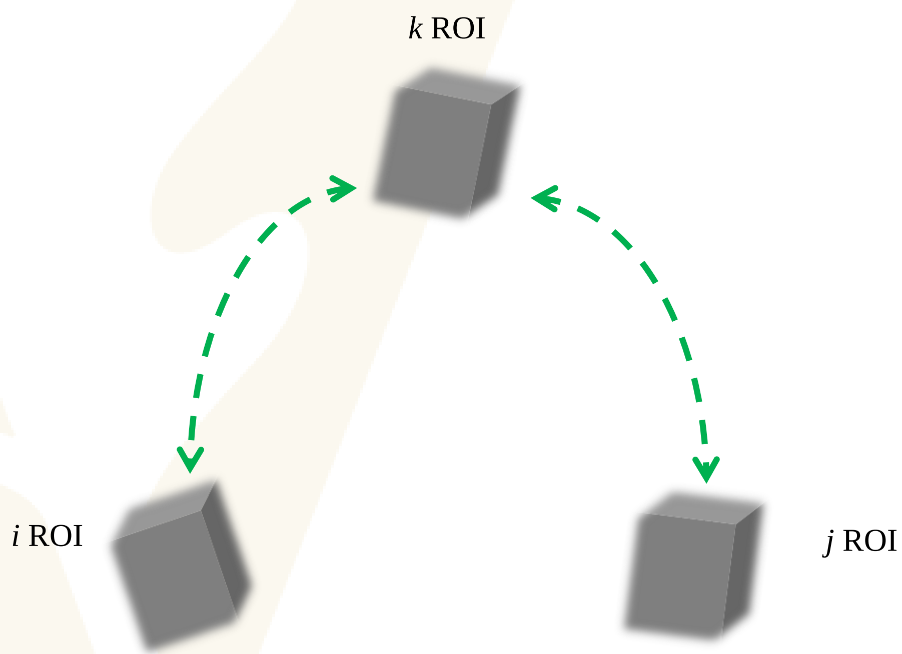
Double Fusion



Double Fusion

Double Fusion



Cholesky Decomposition

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \cdots & \Sigma_{1n} \\ & \Sigma_{22} & \ddots & \vdots \\ & & \ddots & \Sigma_{(n-1)n} \\ & & & \Sigma_{\mathrm{nn}} \end{pmatrix}_{n\times n}$$

$$[\Sigma_{11}, \Sigma_{12}, \dots, \Sigma_{1n}, \Sigma_{22}, \dots, \Sigma_{2n}, \dots, \Sigma_{\mathrm{nn}}]$$

Double Fusion

$$L_d(direct) = \lambda L_{sc} + (1 - \lambda)L_{nfc}$$
$$L_d(indirect) = M_{sc}\lambda L_{sc} + (1 - M_{sc}\lambda)L_{nfc}$$

$$L_d = \omega L_d(direct) + (1 - \omega)L_d(indirect)$$

$$\Sigma_d = L_d \times {L_d}^T$$

Double Fusion

$$\rho_d = \begin{pmatrix} 1 & \rho_{12} & \cdots & \rho_{1n} \\ & 1 & \ddots & \vdots \\ & & 1 & \rho_{(n-1)n} \\ & & & 1 \end{pmatrix}_{n \times n}$$

$$\left[\rho_{12}, \dots, \rho_{1n}, \rho_{23}, \dots, \rho_{2n}, \dots, \rho_{(n-1)n}\right]$$

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Prior Information

$$Y_{cv}(t) = \beta_c + b_c(v) + d_c + \epsilon_{cv}(t)$$

- $\beta_c \sim \mathrm{N}(0, 100^2)$

Prior Information

$$Y_{cv}(t) = \beta_c + b_c(v) + d_c + \epsilon_{cv}(t)$$

$$Cov\big(b_c(v), b_c(v')\big) = \sigma_{b_c}{}^2 \exp(-\|v - v'\|\varphi_c)$$

- $\varphi_c \sim \text{Unif}(0, 20)$
- $\sigma_{b_c} \sim \text{Unif}\,(0, 100)$

Prior Information

$$Y_{cv}(t) = \beta_c + b_c(v) + d_c + \epsilon_{cv}(t)$$

- $\lambda \sim \text{Beta}(1,1)$
- $\omega \sim \text{Beta}(1,1)$
- $\log \sigma_{d_c} \sim \text{Unif}(-8,8)$

Prior Information

$$Y_{cv}(t) = \beta_c + b_c(v) + d_c + \epsilon_{cv}(t)$$

$$\epsilon_{cv}(t) = \delta_c + \phi_{cv}\,\epsilon_{cv}(t-1) + w(t)$$

- $\phi_{cv} \sim \mathrm{Unif}(0,1)$
- $\sigma_{cv} \sim \mathrm{Unif}(0,100)$

Prior Information

$$\boldsymbol{Y}_{obs} \sim \mathrm{N}(\boldsymbol{Y}_{cv}, \sigma^2)$$

- $\sigma \sim \mathrm{Unif}(0, 100)$

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PyMC3 Example

$$Y \sim \mathrm{N}(\mu, \sigma^2)$$

$$\mu = \alpha + \beta_1 X_1 + \beta_2 X_2$$

- $\alpha \sim \mathrm{N}(0, 100)$
- $\beta_1\ or\ \beta_2 \sim \mathrm{N}(0, 20)$
- $\sigma \sim \mathrm{HalfNormal}(0, 1)$

No-U-Turn Sampler (NUTS)

```
import pymc3 as pm
with pm.Model() as basic_model:

    # Priors for unknown model parameters
    alpha = pm.Normal('alpha', mu=0, sd=100)
    beta = pm.Normal('beta', mu=0, sd=20, shape=2)
    sigma = pm.HalfNormal('sigma', sd=1)

    # Expected value of outcome
    mu = alpha + beta[0]*X1 + beta[1]*X2

    # Likelihood (sampling distribution) of observations
     Y_obs = pm.Normal('Y_obs', mu=mu, sd=sigma, observed=Y)

with basic_model:

    # Instatiate sampler
    step = pm.NUTS()

    # Draw 1000 posterior samples and tune 500 as default
    trace = pm.sample(1000, step = step)
```

Model Diagnostics

- Gelman Rubin statistics:

$$\hat{R} = \frac{\hat{V}}{W}$$

- Effective sample size:

$$\hat{n}_{\text{eff}} = \frac{mn}{1 + 2\sum_{t=1}^{T} \hat{\rho}_t}$$

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Optimization and Decomposition

- Vectorization
- Cholesky decomposition

$$X \sim \mathrm{N}(\mu, \Sigma)$$

$$\Sigma = U^T U$$

$$X = \mu + U^T Z, Z \sim \mathrm{N}(0, 1)$$

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Simulation Study

- Generate time-series data with a length of $T = 128$ scans using AR (1) (coefficient: 0.6) at 5 ROIs and each ROI contains 100 voxels
- Imposed correlation using a multivariate normal distribution

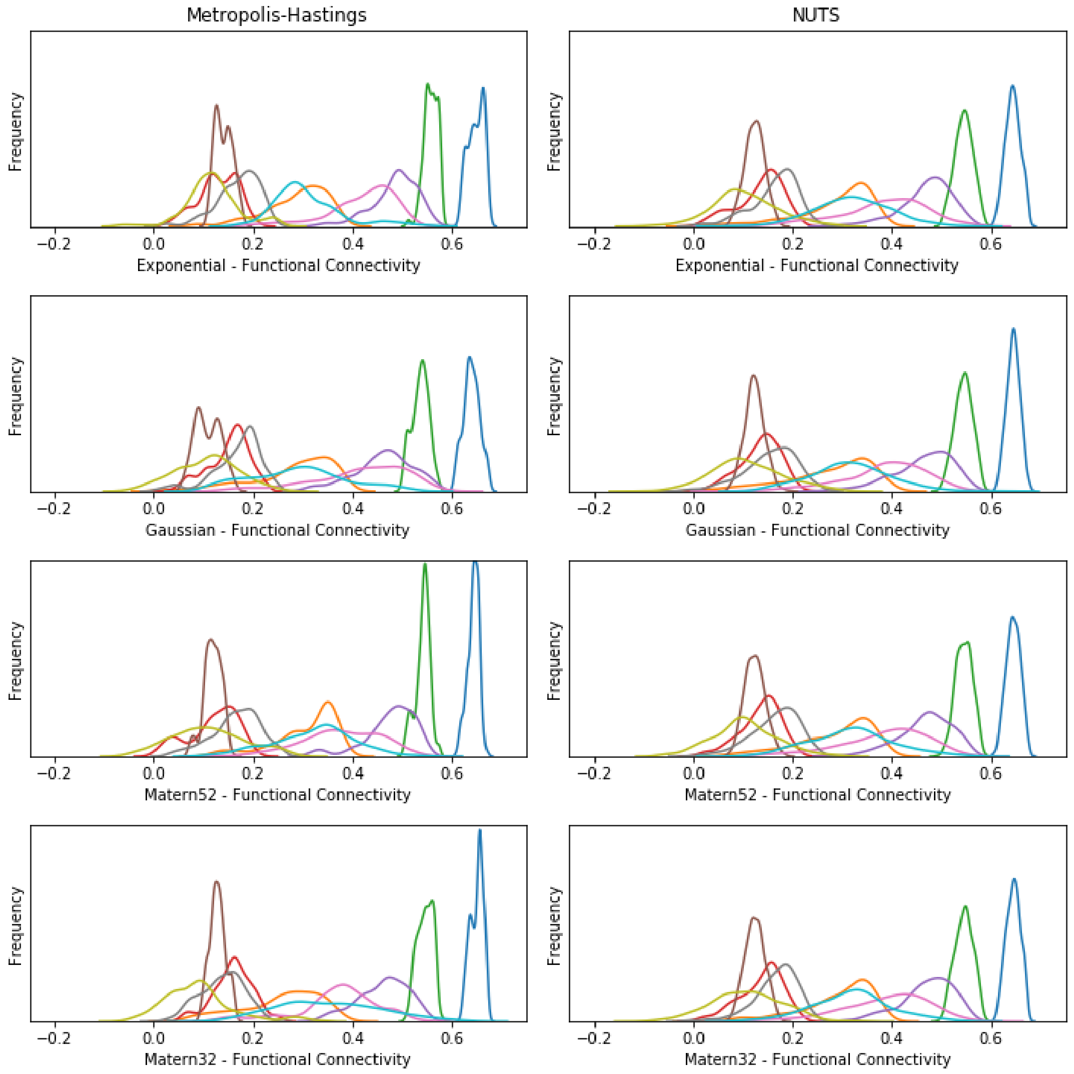
$$\rho_d = \begin{pmatrix} 1 & 0.6 & 0 & 0.5 & 0 \\ & 1 & 0.2 & 0.1 & 0 \\ & & 1 & 0 & 0.1 \\ & & & 1 & 0.2 \\ & & & & 1 \end{pmatrix}$$

- $\mathrm{SC} \sim \mathrm{Wishart}_p(6, \rho_d)$

Simulation Study

		Bayesian correct SC				Bayesian independence			
FC	*Correct*	*Median (SD)*	*[2.5% 97.5%]*	$\hat{R}$	$\hat{n}_{eff}$	*Median (SD)*	*[2.5% 97.5%]*	$\hat{R}$	$\hat{n}_{eff}$
ρ_1	0.6	0.645 (0.014)	[0.617 0.669]	0.999	1675.438	0.531 (0.125)	[0.170 0.652]	1.002	979.951
ρ_2	0.0	0.310 (0.080)	[0.074 0.378]	0.999	1110.936	0.305 (0.078)	[0.091 0.379]	0.999	1303.385
ρ_3	0.5	0.546 (0.017)	[0.513 0.576]	0.999	1877.821	0.463 (0.108)	[0.151 0.572]	0.999	1033.009
ρ_4	0.0	0.145 (0.042)	[0.039 0.204]	0.999	1341.864	0.146 (0.042)	[0.040 0.204]	0.999	1034.929
ρ_5	0.2	0.478 (0.053)	[0.340 0.547]	0.999	1152.252	0.432 (0.090)	[0.197 0.537]	1.001	1285.429
ρ_6	0.1	0.123 (0.020)	[0.088 0.165]	1.000	1721.880	0.017 (0.106)	[-0.194 0.216]	1.000	1218.262
ρ_7	0.0	0.399 (0.083)	[0.180 0.522]	0.999	1102.607	0.419 (0.098)	[0.174 0.558]	0.999	1381.804
ρ_8	0.0	0.173 (0.049)	[0.047 0.235]	0.999	1293.770	0.158 (0.068)	[0.016 0.283]	1.000	1251.840
ρ_9	0.1	0.105 (0.070)	[-0.026 0.254]	0.999	1417.283	0.057 (0.063)	[-0.066 0.177]	1.000	1458.304
ρ_{10}	0.2	0.316 (0.077)	[0.165 0.484]	1.000	1524.805	0.348 (0.118)	[0.054 0.532]	0.999	1095.445

Bayesian Correct SC



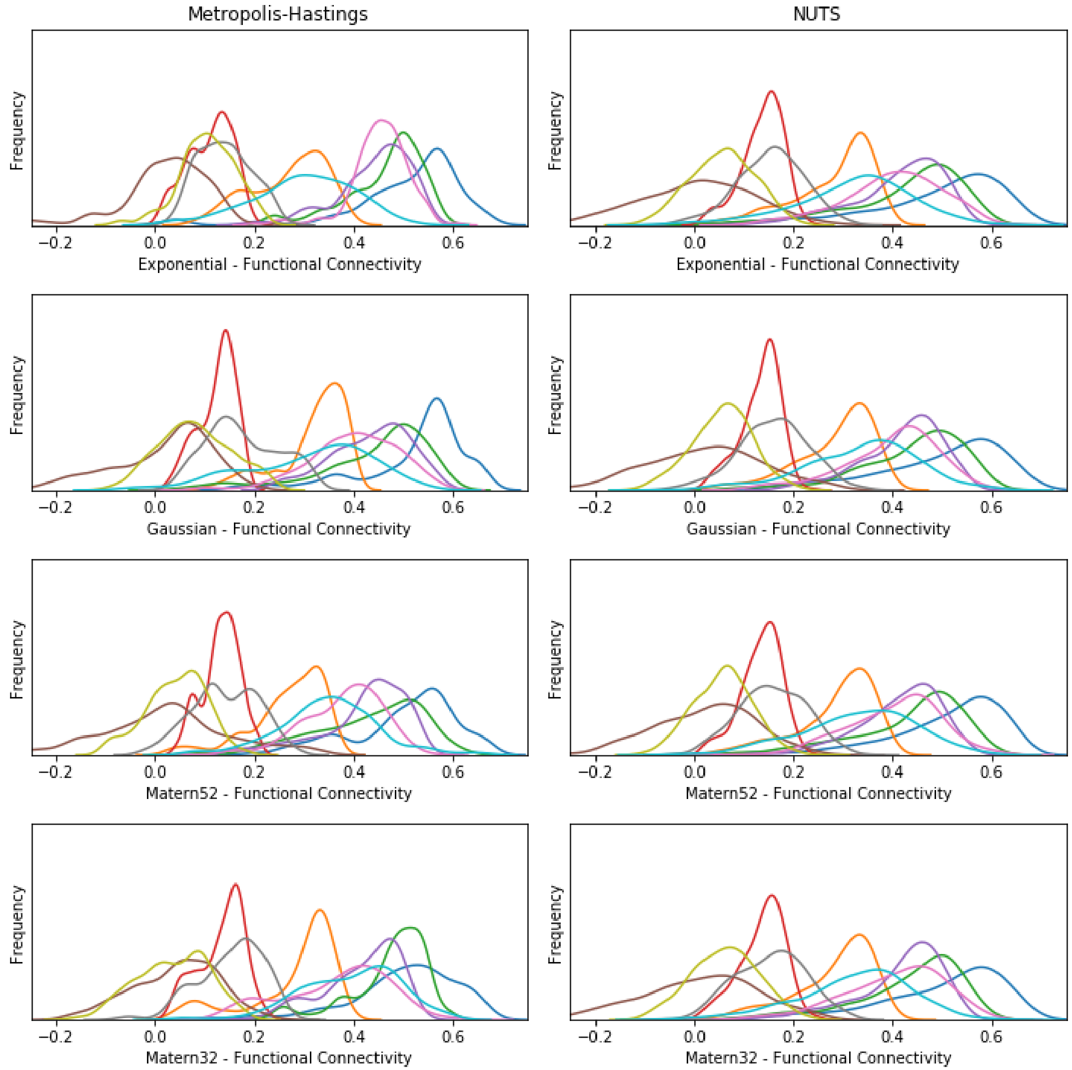
Bayesian Correct SC

		Metropolis-Hastings Median (SD)				NUTS Median (SD)			
FC	***Correct***	***Exponential***	***Gaussian***	***Matérn52***	***Matérn32***	***Exponential***	***Gaussian***	***Matérn52***	***Matérn32***
ρ_1	0.6	0.651(0.016)	0.640(0.016)	0.645(0.016)	0.654(0.016)	0.651(0.015)	0.640(0.015)	0.645(0.015)	0.654(0.015)
ρ_2	0.0	0.303(0.061)	0.305(0.061)	0.333(0.061)	0.273(0.061)	0.303(0.077)	0.305(0.077)	0.333(0.077)	0.273(0.077)
ρ_3	0.5	0.559(0.014)	0.540(0.014)	0.544(0.014)	0.548(0.014)	0.559(0.018)	0.540(0.018)	0.544(0.018)	0.548(0.018)
ρ_4	0.0	0.129(0.040)	0.160(0.040)	0.132(0.040)	0.162(0.040)	0.129(0.046)	0.160(0.046)	0.132(0.046)	0.162(0.046)
ρ_5	0.2	0.492(0.046)	0.469(0.046)	0.486(0.046)	0.470(0.046)	0.492(0.052)	0.469(0.052)	0.486(0.052)	0.470(0.052)
ρ_6	0.1	0.139(0.017)	0.107(0.017)	0.119(0.017)	0.128(0.017)	0.139(0.019)	0.107(0.019)	0.119(0.019)	0.128(0.019)
ρ_7	0.0	0.438(0.068)	0.430(0.068)	0.378(0.068)	0.379(0.068)	0.438(0.088)	0.430(0.088)	0.378(0.088)	0.379(0.088)
ρ_8	0.0	0.179(0.043)	0.182(0.043)	0.170(0.043)	0.142(0.043)	0.179(0.047)	0.182(0.047)	0.170(0.047)	0.142(0.047)
ρ_9	0.1	0.116(0.053)	0.111(0.053)	0.108(0.053)	0.086(0.053)	0.116(0.066)	0.111(0.066)	0.108(0.066)	0.086(0.066)
ρ_{10}	0.2	0.293(0.069)	0.293(0.069)	0.336(0.069)	0.350(0.069)	0.293(0.077)	0.293(0.077)	0.336(0.077)	0.350(0.077)

Bayesian Correct SC

	Metropolis-Hastings				NUTS			
MSE	***Exponential***	***Gaussian***	***Matérn52***	***Matérn32***	***Exponential***	***Gaussian***	***Matérn52***	***Matérn32***
Total FC	0.043	0.042	0.040	0.037	0.040	0.039	0.040	0.041
Zero FC	0.083	0.084	0.075	0.066	0.076	0.073	0.076	0.078
Low FC	0.024	0.020	0.025	0.024	0.023	0.022	0.023	0.024
High FC	0.003	0.002	0.002	0.003	0.002	0.002	0.002	0.002

Bayesian Independence



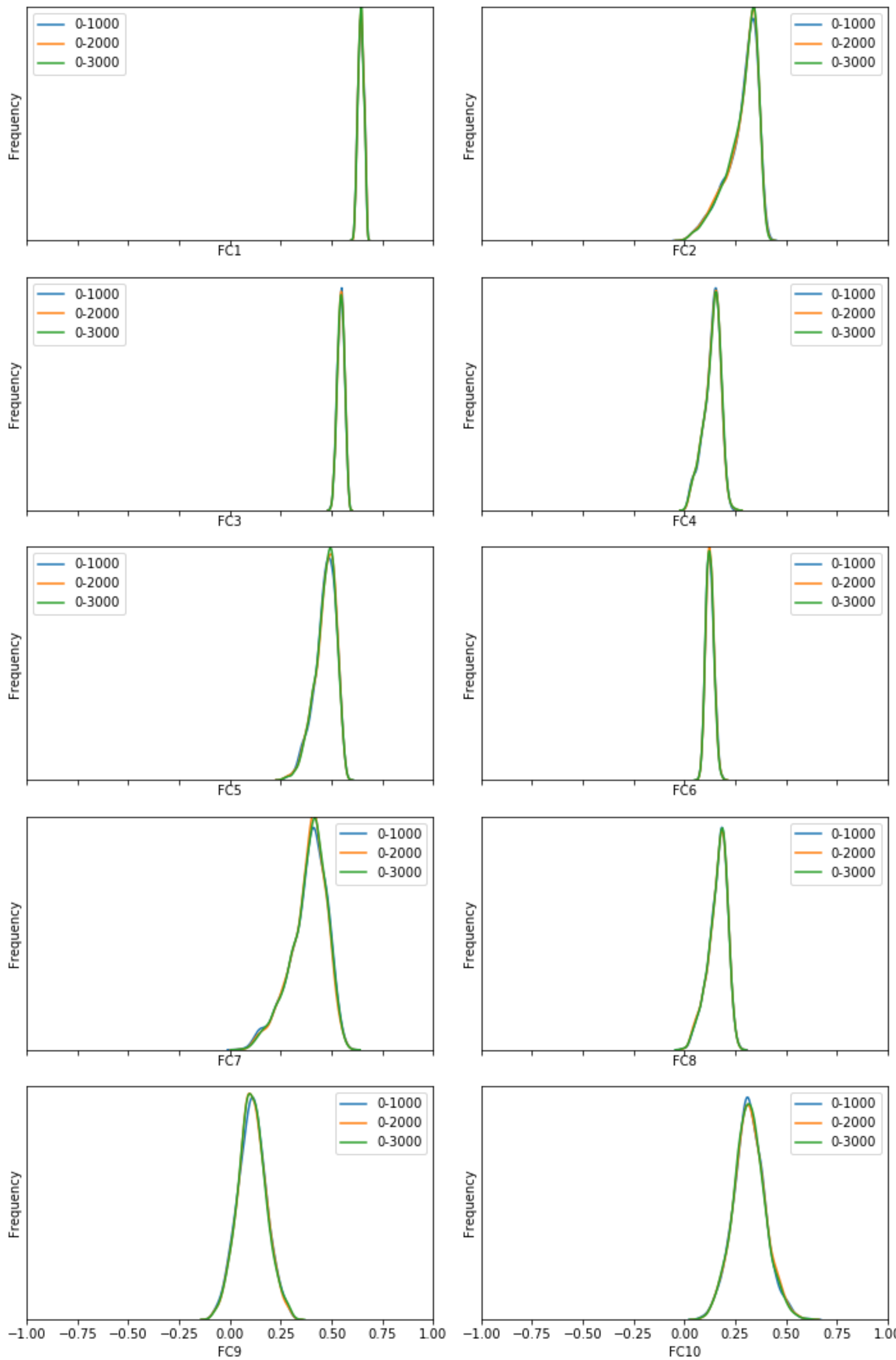
Bayesian Independence

		Metropolis-Hastings Median (SD)				NUTS Median (SD)			
FC	***Correct***	***Exponential***	***Gaussian***	***Matérn52***	***Matérn32***	***Exponential***	***Gaussian***	***Matérn52***	***Matérn32***
ρ_1	0.6	0.547(0.016)	0.56(0.016)	0.529(0.016)	0.517(0.016)	0.547(0.015)	0.560(0.015)	0.529(0.015)	0.517(0.015)
ρ_2	0.0	0.283(0.061)	0.339(0.061)	0.283(0.061)	0.317(0.061)	0.283(0.077)	0.339(0.077)	0.283(0.077)	0.317(0.077)
ρ_3	0.5	0.488(0.014)	0.481(0.014)	0.453(0.014)	0.493(0.014)	0.488(0.018)	0.481(0.018)	0.453(0.018)	0.493(0.018)
ρ_4	0.0	0.116(0.040)	0.134(0.040)	0.136(0.040)	0.145(0.040)	0.116(0.046)	0.134(0.046)	0.136(0.046)	0.145(0.046)
ρ_5	0.2	0.461(0.046)	0.449(0.046)	0.443(0.046)	0.434(0.046)	0.461(0.052)	0.449(0.052)	0.443(0.052)	0.434(0.052)
ρ_6	0.1	0.032(0.017)	0.047(0.017)	0.025(0.017)	0.053(0.017)	0.032(0.019)	0.047(0.019)	0.025(0.019)	0.053(0.019)
ρ_7	0.0	0.456(0.068)	0.407(0.068)	0.391(0.068)	0.391(0.068)	0.456(0.088)	0.407(0.088)	0.391(0.088)	0.391(0.088)
ρ_8	0.0	0.136(0.043)	0.162(0.043)	0.139(0.043)	0.167(0.043)	0.136(0.047)	0.162(0.047)	0.139(0.047)	0.167(0.047)
ρ_9	0.1	0.108(0.053)	0.079(0.053)	0.048(0.053)	0.042(0.053)	0.108(0.066)	0.079(0.066)	0.048(0.066)	0.042(0.066)
ρ_{10}	0.2	0.307(0.069)	0.339(0.069)	0.356(0.069)	0.411(0.069)	0.307(0.077)	0.339(0.077)	0.356(0.077)	0.411(0.077)

Bayesian Independence

	Metropolis-Hastings				NUTS			
MSE	***Exponential***	***Gaussian***	***Matérn52***	***Matérn32***	***Exponential***	***Gaussian***	***Matérn52***	***Matérn32***
Total FC	0.118	0.119	0.108	0.118	0.111	0.113	0.113	0.113
Zero FC	0.080	0.081	0.068	0.076	0.078	0.079	0.079	0.080
Low FC	0.080	0.081	0.081	0.090	0.077	0.080	0.077	0.078
High FC	0.268	0.272	0.242	0.255	0.247	0.251	0.255	0.250

Convergence



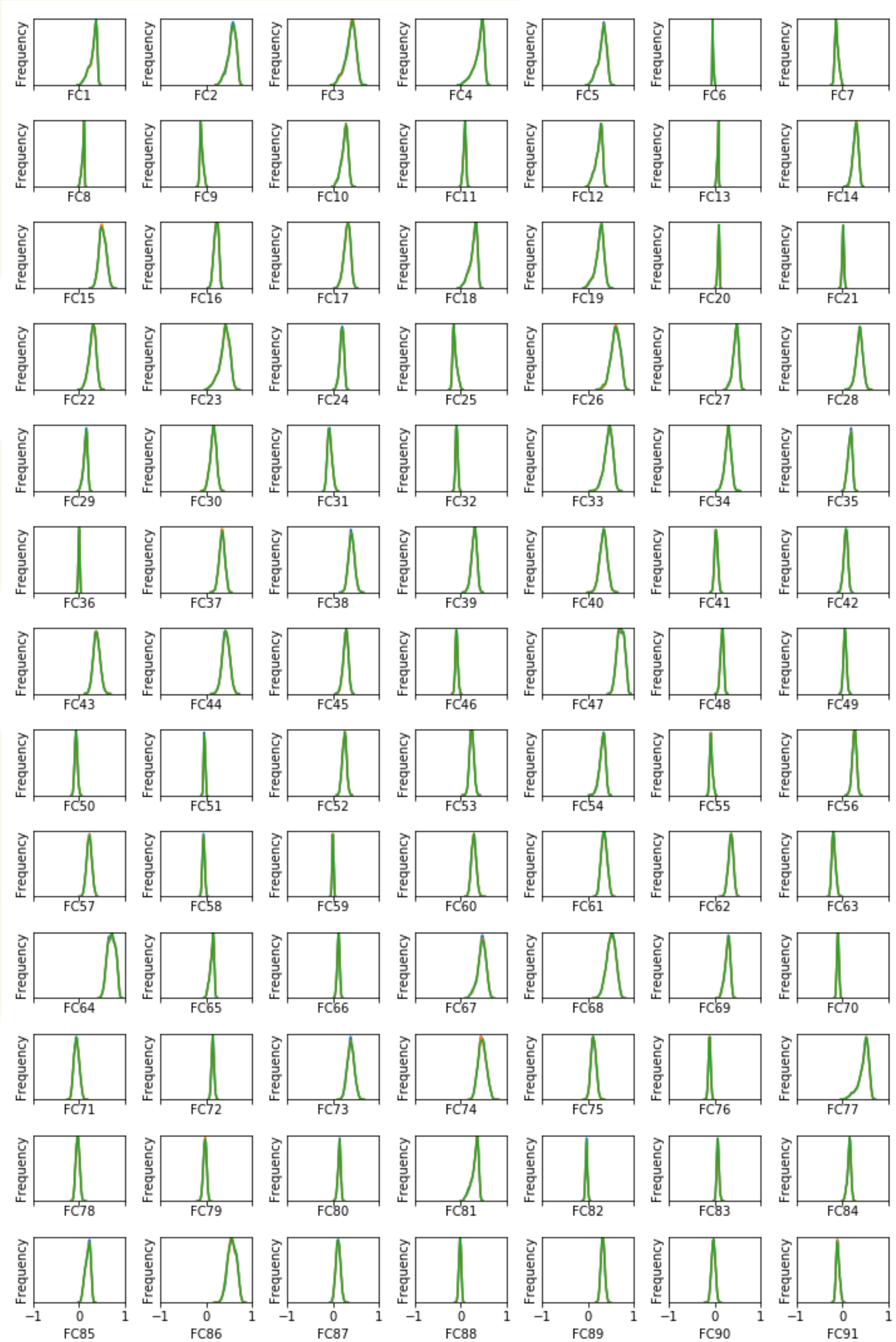
Major Depressive Disorder

	Control (n=23) *Mean (SD)*	*MDD (n=18)* *Mean (SD)*	*Wilcoxon Rank Sum Tests*
Age(years)	31.78 (10.16)	32.06 (8.55)	t = -0.512, p = 0.608
Sex (% female)	65%	50%	t = 0.828, p = 0.408
Education (years)	15.78 (1.73)	16.28 (1.90)	t = -0.512, p = 0.608
Beck Depression Inventory (BDI)	1.90 (2.62)	22.11 (9.38)	t = -4.085, p <0.001
Montgomery–Asberg Depression Rating Scale (MADRS)	0.70 (1.06)	25.29 (3.20)	t = -5.438, p < 0.001
Processing Speed Domain	0.36 (0.67)	0.20 (0.61)	t = 0.841, p = 0.401
Working Memory Domain	0.10 (0.88)	0.02 (0.81)	t = 0.158, p = 0.875
Episodic Memory Domain	0.23 (0.55)	0.07 (0.75)	t = 0.578, p = 0.563
Executive Function Domain	0.20 (0.55)	0.23 (0.59)	t = -0.053, p = 0.958

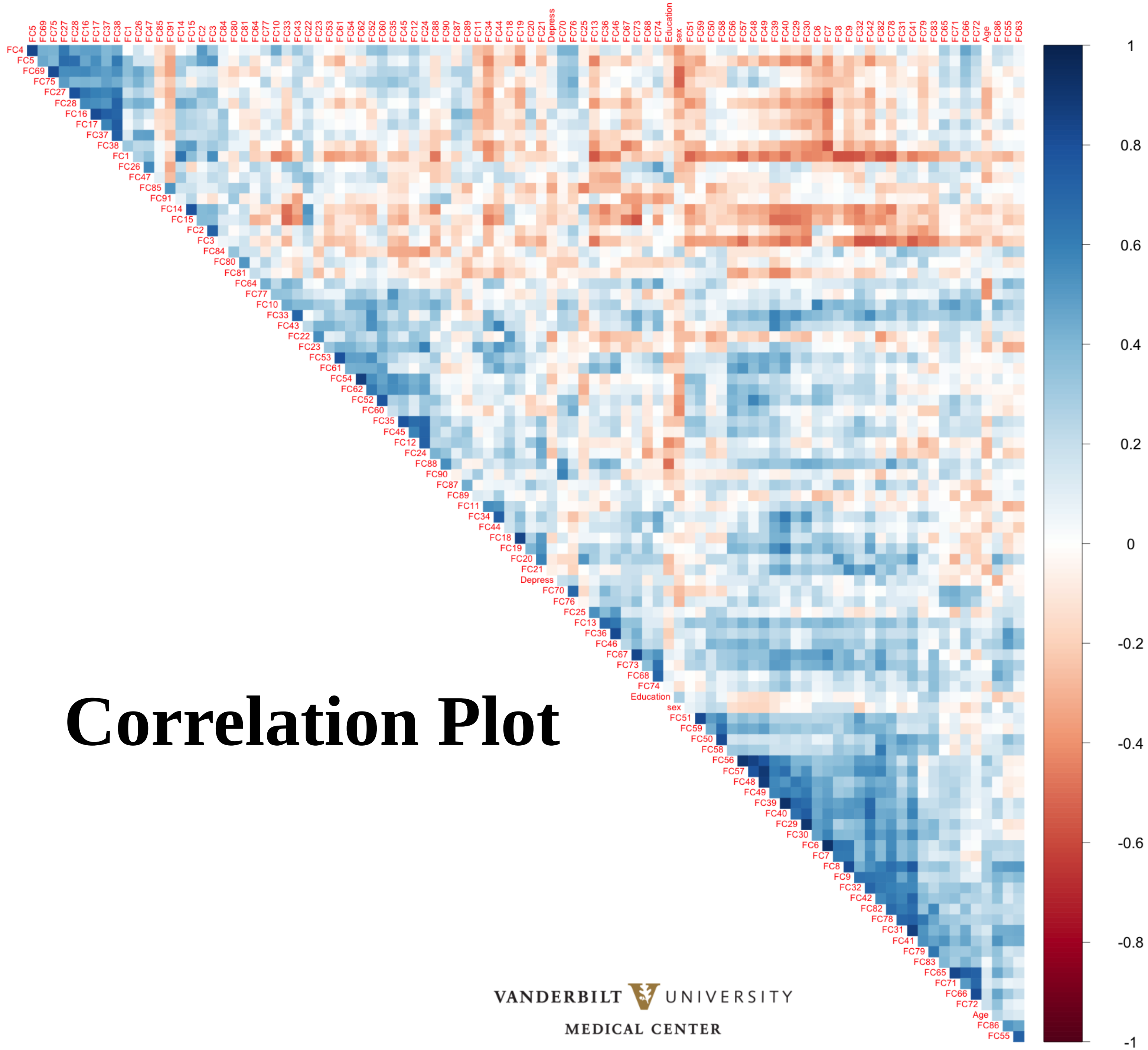
Convergence

$T = 150$ time-series scans
n = 14 ROIs
$m = 300$ voxels

For each subject:
$\sim$30 times computational cost



Correlation Plot



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Case Study

- Cognitive domain
  - processing speed domain
  - working memory domain
  - episodic memory domain
  - executive function domain

- Correlation test under FDR at 0.1:
  - For executive function domain, "FC80" in control group

- Cognitive domain $\sim$ Age $+$ Sex $+$ Education $+$ FC_i $+$ Depress $+$ $\mathrm{FC}_i * \mathrm{Depress}$
  - Interaction term $\mathrm{FC}_i * \mathrm{Depress}$: "FC80" in executive function domain

"FC80": the correlation between ROI 9 and ROI 13

Variable Selection

	Processing Speed Domain	*Working Memory Domain*	*Episodic Memory Domain*	*Executive Function Domain*
Exhaustive	FC4, FC27, FC28, FC48, FC57, FC69	FC26, FC29, FC62, FC64, FC69, FC71	FC6, FC9, FC42, FC57, FC78, FC79	FC6, FC7, FC26, FC27, FC50. FC79
Forward	FC10, FC20, FC29, FC44, FC51, FC58	FC20, FC26, FC33, FC62, FC69, FC85	FC6, FC9, FC11, FC26, FC35, FC65	FC18, FC20, FC26, FC43, FC50, FC77
Backward	FC2, FC4, FC6, FC12, FC20, FC24	FC7, FC18, FC19, FC25, FC26, FC33	FC7, FC9, FC11, FC22, FC29, FC30	FC3, FC6, FC8, FC11, FC13, FC26
Sequential	FC10, FC11, FC17, FC28, FC29, FC78	FC26, FC29, FC62, FC64, FC69, FC71	FC1, FC5, FC6, FC9, FC11, FC35	FC18, FC20, FC26, FC43, FC50, FC77
Lasso	FC10, FC11, FC26, FC29, FC70, FC85	FC20, FC26, FC62, FC64, FC69, FC84	FC6, FC25, FC34, FC57, FC77, FC86	FC11, FC26, FC58, FC70, FC77, FC85

Documentation

wangruinju minor change — Latest commit 304fe04 15 hours ago

accre	add examples	7 days ago
.Rhistory	add html	7 days ago
README.html	minor change	15 hours ago
README.md	minor change	15 hours ago
environment.yml	revise	7 days ago
model.py	update	21 hours ago
slides.pdf	kernel function	21 hours ago

README.md

Double-Fusion

This repository documentation is used to explain the model in the papar by Kang, Hakmook, et al. "A bayesian double fusion model for resting-state brain connectivity using joint functional and structural data." Brain connectivity 7.4 (2017): 219-227.

Since GitHub doest not render the equation in Markdown, you can read the Readme in HTML or slides.

Introduction

Our brain network, as a complex integrative system, consists of many different regions that have each own task and function and simultaneously share structural and functional information. With the developed imaging techniques such as functional magnetic resonance imaging (fMRI) and diffusion tensor imaging (DTI), researchers can investigate the underlying brain functions related to human behaviors and some diseases or disorders in the nervous system such as major depressive disorder (MDD).

We developed a Bayesian hierarchical spatiotemporal model that combined fMRI and DTI data jointly to enhance the estimation of resting-state functional connectivity. Structural connectivity from DTI data was utilized to construct an informative prior for functional connectivity based on resting-state fMRI data through the Cholesky decomposition in a mixture model. The analysis took the advantages of probabilistic programming package as PyMC3 and next-generation Markov Chain Monte Carlo (MCMC) sampling algorithm as No-U-Turn Sampler (NUTS). PyMC3 is new, open-source

Summary

- A Bayesian hierarchical model
  - Resting-state fMRI data
  - DTI data
- PyMC3 and NUTS
- Simulation with reduced MSE
- MDD case study
- Documentation

Future Work

- Other kernel covariance functions

- 200 ~ 300 subjects
  - Machine learning methods
  - MDD classification

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