# A Bayesian Model for Brain Network Functional Connectivity using PyMC3

Rui Wang
M.S. Defense Presentation

Department of Biostatistics

# 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

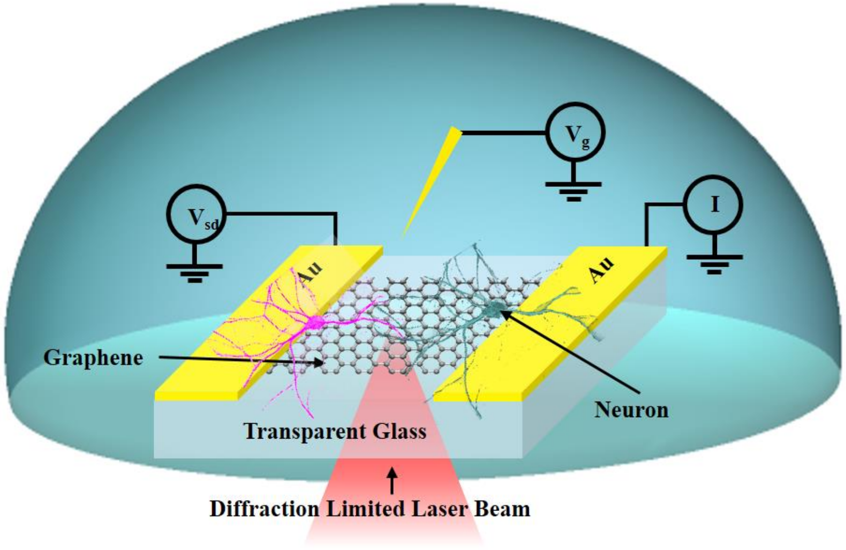
Precise Timing

High Electrical Sensitivity

High Throughput

High Spatial Accuracy

Long-term Duration

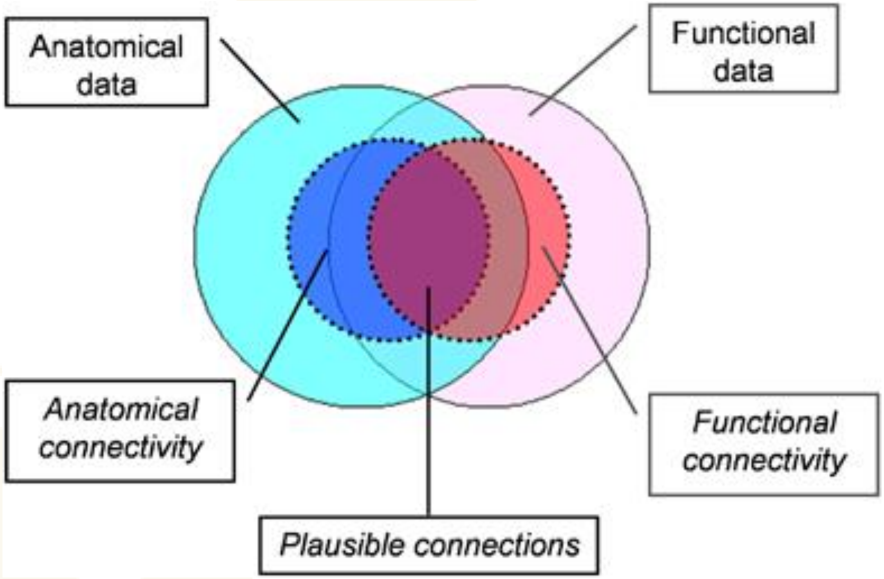



Wang, R et. al, ***Nano Letter*** (in review)

# Brain Imaging

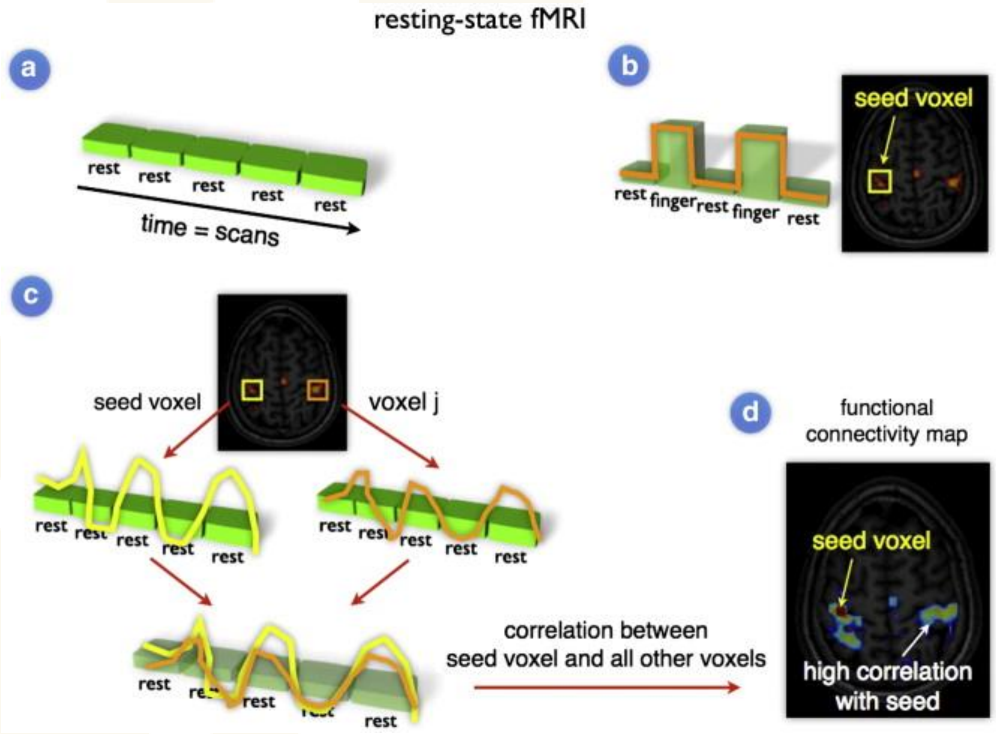
https://www.sciencedaily.com/releases/2016/11/161103141437.htm

# Brain Imaging



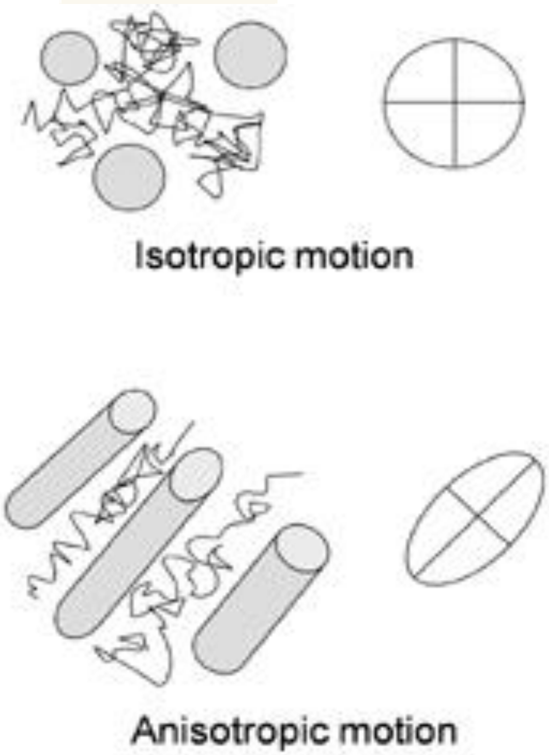

Rykhlevskaia et. al, ***Psychophysiology*** 45, 2 (2008)

# Functional Connectivity




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

# Structural Connectivity




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

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# Spatiotemporal Structure

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

- $\beta_c$: 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 (2008)

# 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 | $K(x,x') = \exp(-\frac{\|x-x'\|^2}{2l^2})$ |
| Exponential | $K(x,x') = \exp(-\frac{\|x-x'\|}{l})$ |
| Matérn | $K(x,x') = \frac{2^{1-v}}{\Gamma(v)}\left(\frac{\sqrt{2v}\|x-x'\|}{l}\right)^v B_v(\frac{\sqrt{2v}\|x-x'\|}{l})$ |
| Periodic | $K(x,x') = \exp(-\frac{2sin^2(\frac{x-x'}{2})}{l^2})$ |
| Rational quadratic | $K(x,x') = (1+\ \|x-x'\|^2)^{-\alpha}, \alpha \geq 0$ |

# Kernel Covariance Function

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

Exponential (Matérn1/2):

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

Gaussian or square exponential (Matérn∞):

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

Matérn5/2:

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

Matérn3/2:

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

# Temporal Correlation

AR (1) structure:

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

- $\delta_c$: the constant shift
- $\phi_{cv}$: 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

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

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

# 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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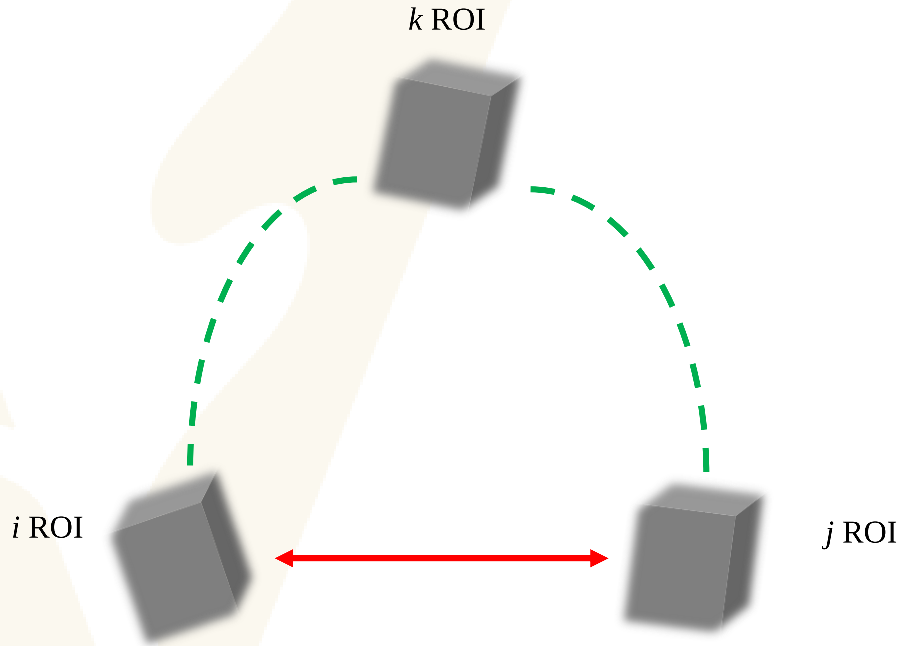
# Double Fusion



# Double Fusion

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

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

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

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

# Double Fusion

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

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

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# Prior Information

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

- $\beta_c \sim \mathrm{N}(0, 0.01^2)$

# Prior Information

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

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

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

# Prior Information

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

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

# Prior Information

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

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

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

# Prior Information

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

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

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# PyMC3 and NUTS

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

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

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

# PyMC3 and 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:

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

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# Optimization and Decomposition

- Vectorization
- Cholesky decomposition

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

$$\Sigma = U^T U$$

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

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# Simulation Study

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

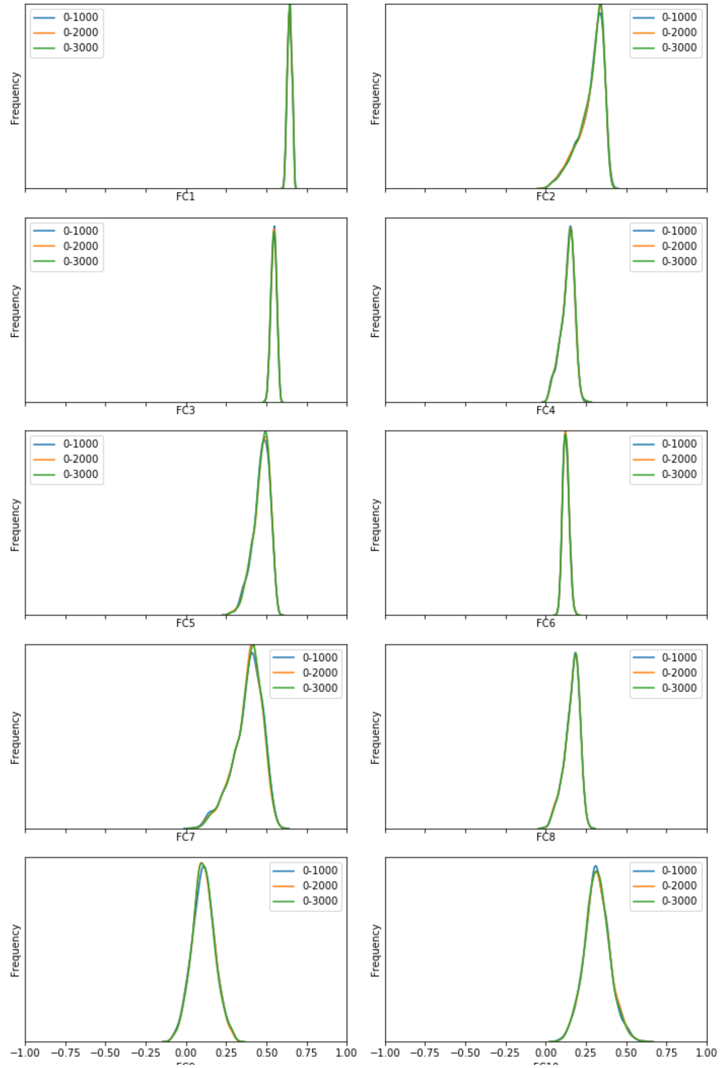
$$\rho_{\mathrm{d}} = \begin{pmatrix} 1 & 0.6 & 0 & 0.5 & 0 \\ & 1 & 0.2 & 0.1 & 0 \\ & & 1 & 0 & 0.1 \\ & & & 1 & 0.2 \\ & & & & 1 \end{pmatrix}$$

- $SC \sim W_p(6, \rho_d)$

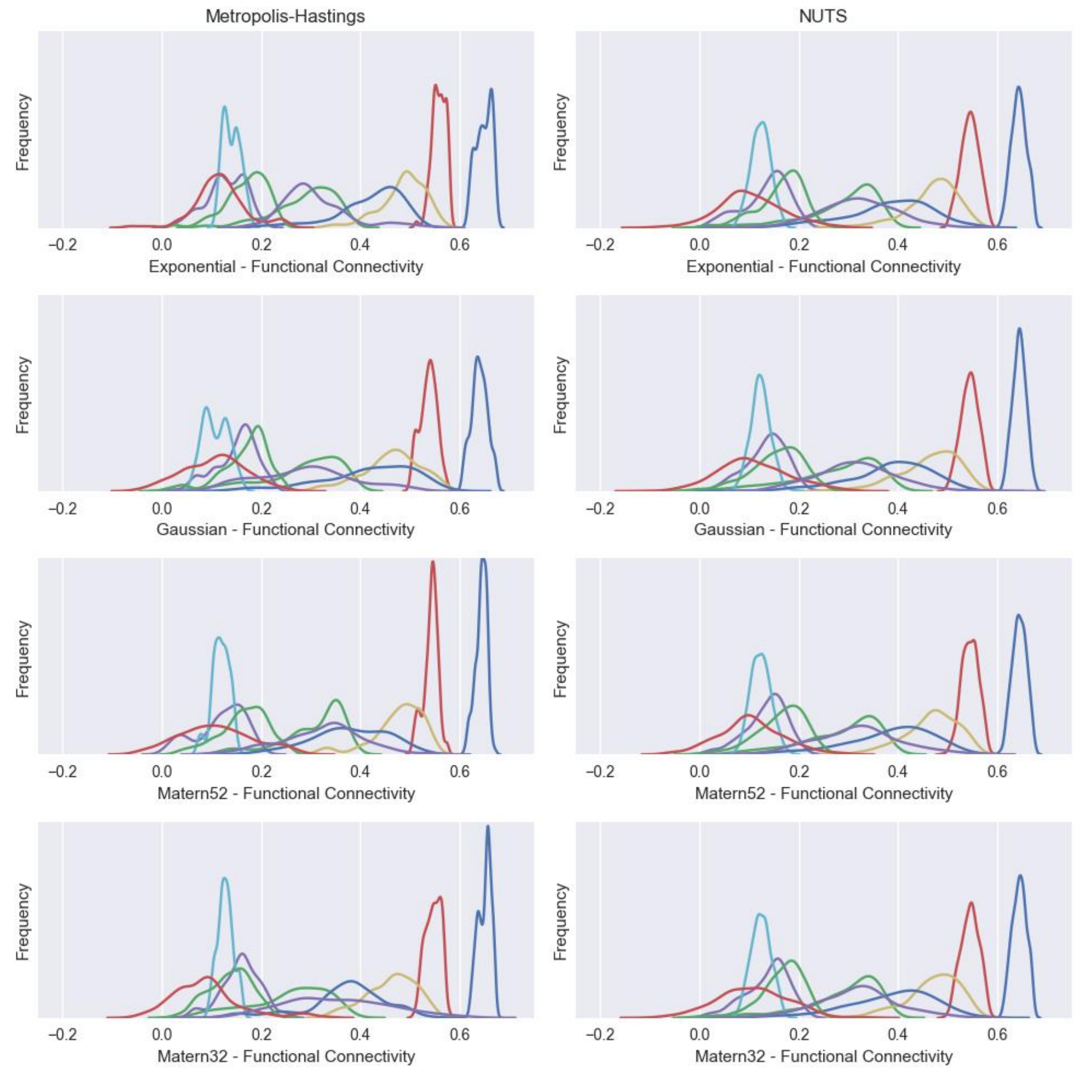
# Simulation Study

| | ***Bayesian correct SC*** | | | | ***Bayesian independence*** | | | |
|---|---|---|---|---|---|---|---|---|
| ***FC*** | ***Median (SD)*** | ***[2.5% 97.5%]*** | $\hat{R}$ | $\hat{n}_{eff}$ | ***Median (SD)*** | ***[2.5% 97.5%]*** | $\hat{R}$ | $\hat{n}_{eff}$ |
| $\rho_1$ | 0.645 (0.014) | [0.617 0.669] | 0.999 | 1675.438 | 0.531 (0.125) | [0.170 0.652] | 1.002 | 979.951 |
| $\rho_2$ | 0.310 (0.080) | [0.074 0.378] | 0.999 | 1110.936 | 0.305 (0.078) | [0.091 0.379] | 0.999 | 1303.385 |
| $\rho_3$ | 0.546 (0.017) | [0.513 0.576] | 0.999 | 1877.821 | 0.463 (0.108) | [0.151 0.572] | 0.999 | 1033.009 |
| $\rho_4$ | 0.145 (0.042) | [0.039 0.204] | 0.999 | 1341.864 | 0.146 (0.042) | [0.040 0.204] | 0.999 | 1034.929 |
| $\rho_5$ | 0.478 (0.053) | [0.340 0.547] | 0.999 | 1152.252 | 0.432 (0.090) | [0.197 0.537] | 1.001 | 1285.429 |
| $\rho_6$ | 0.123 (0.020) | [0.088 0.165] | 1.000 | 1721.880 | 0.017 (0.106) | [-0.194 0.216] | 1.000 | 1218.262 |
| $\rho_7$ | 0.399 (0.083) | [0.180 0.522] | 0.999 | 1102.607 | 0.419 (0.098) | [0.174 0.558] | 0.999 | 1381.804 |
| $\rho_8$ | 0.173 (0.049) | [0.047 0.235] | 0.999 | 1293.770 | 0.158 (0.068) | [0.016 0.283] | 1.000 | 1251.840 |
| $\rho_9$ | 0.105 (0.070) | [-0.026 0.254] | 0.999 | 1417.283 | 0.057 (0.063) | [-0.066 0.177] | 1.000 | 1458.304 |
| $\rho_{10}$ | 0.316 (0.077) | [0.165 0.484] | 1.000 | 1524.805 | 0.348 (0.118) | [0.054 0.532] | 0.999 | 1095.445 |

# Convergence



# Bayesian Correct SC



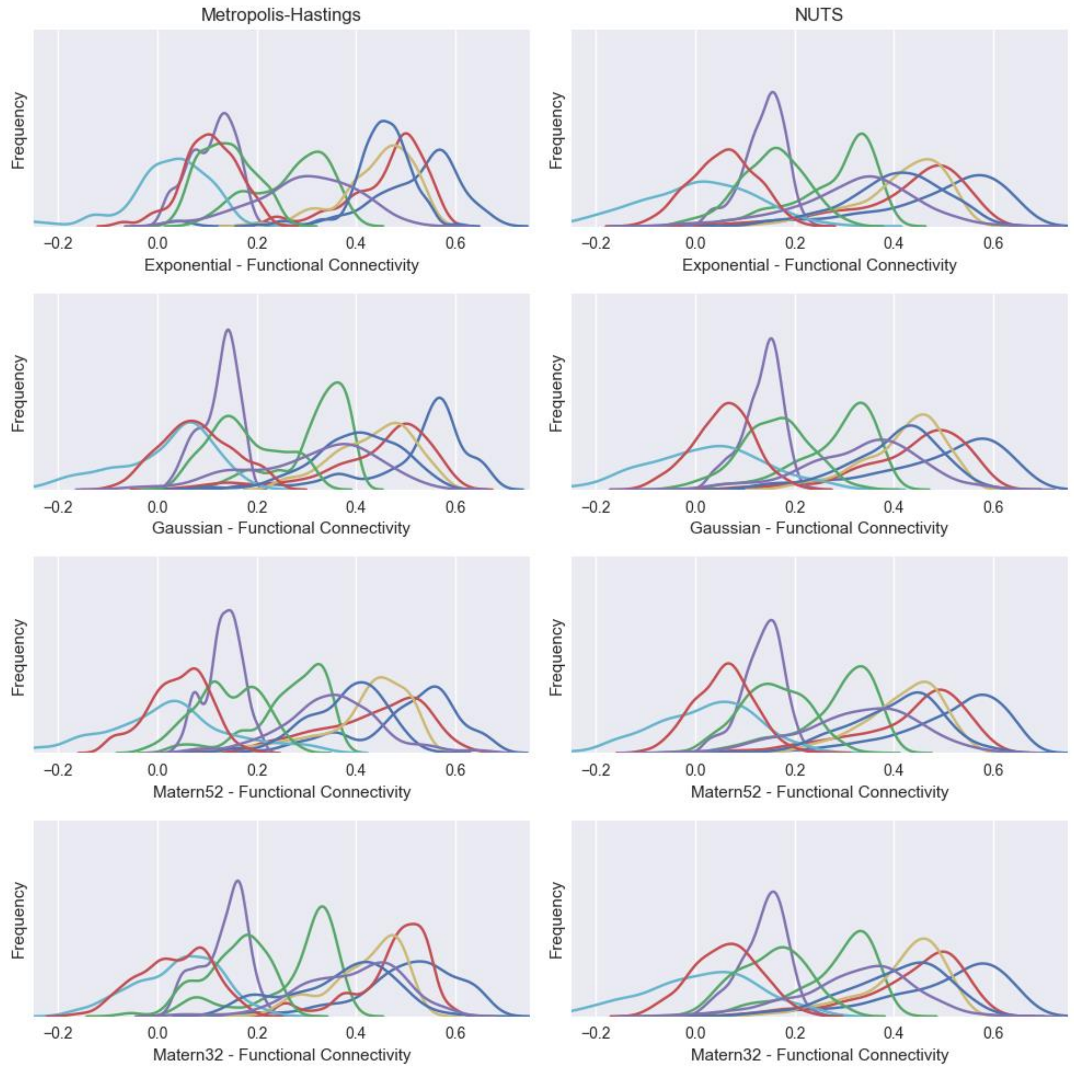
# Bayesian Correct SC

| | Metropolis-Hastings Median (SD) | | | | NUTS Median (SD) | | | |
|---|---|---|---|---|---|---|---|---|
| *FC* | *Exponential* | *Gaussian* | *Matérn52* | *Matérn32* | *Exponential* | *Gaussian* | *Matérn52* | *Matérn32* |
| $\rho_1$ | 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) |
| $\rho_2$ | 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) |
| $\rho_3$ | 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) |
| $\rho_4$ | 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) |
| $\rho_5$ | 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) |
| $\rho_6$ | 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) |
| $\rho_7$ | 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) |
| $\rho_8$ | 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) |
| $\rho_9$ | 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) |
| $\rho_{10}$ | 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*** | ***Exponential*** | ***Gaussian*** | ***Matérn52*** | ***Matérn32*** | ***Exponential*** | ***Gaussian*** | ***Matérn52*** | ***Matérn32*** |
| $\rho_1$ | 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) |
| $\rho_2$ | 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) |
| $\rho_3$ | 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) |
| $\rho_4$ | 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) |
| $\rho_5$ | 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) |
| $\rho_6$ | 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) |
| $\rho_7$ | 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) |
| $\rho_8$ | 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) |
| $\rho_9$ | 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) |
| $\rho_{10}$ | 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) |

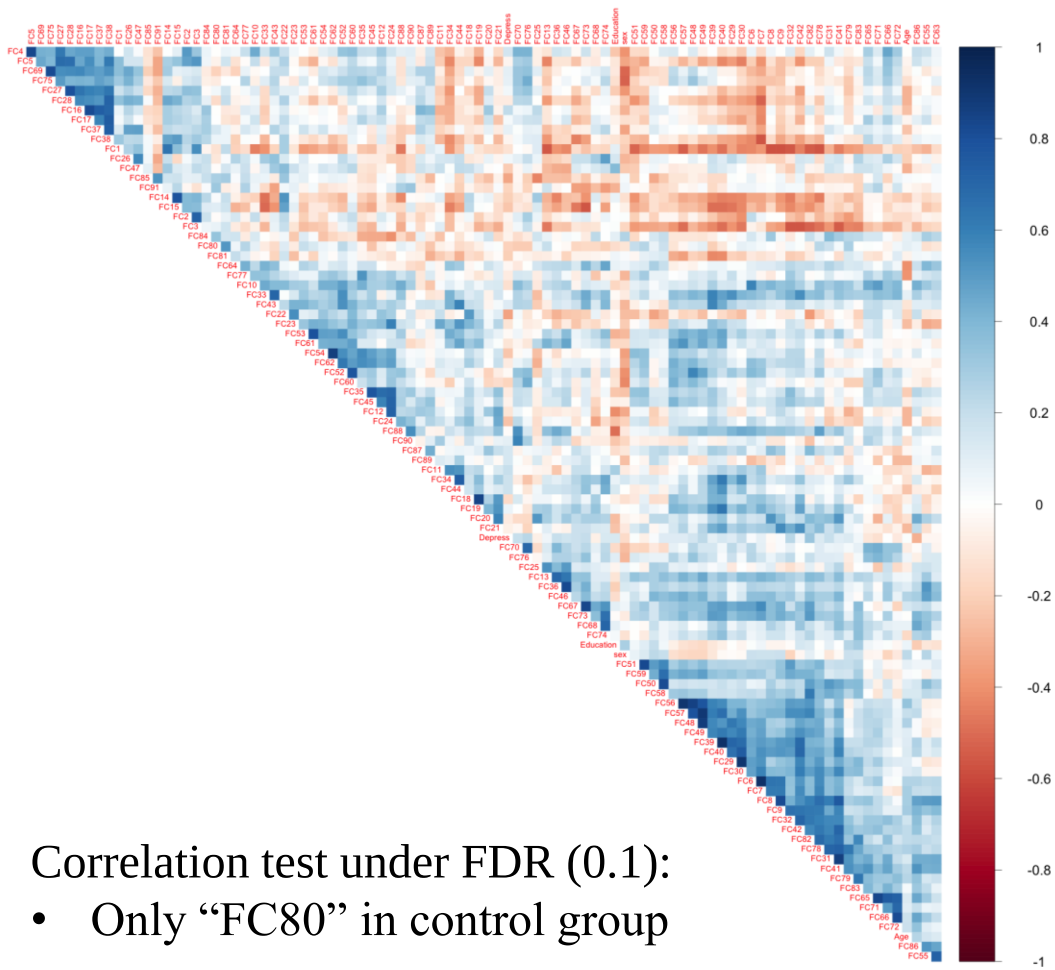
# Bayesian Independence

| | 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 |

# Case Study

| | *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 |

# Case Study




Correlation test under FDR (0.1):

- Only “FC80” in control group

# Case Study

$$\text{Cognitive domain} \sim \text{Age} + \text{Sex} + \text{Education} + \text{FC}_i + \text{Depress} + \text{FC}_i * \text{Depress}$$

- Cognitive domain:

Processing Speed Domain

Working Memory Domain

Episodic Memory Domain

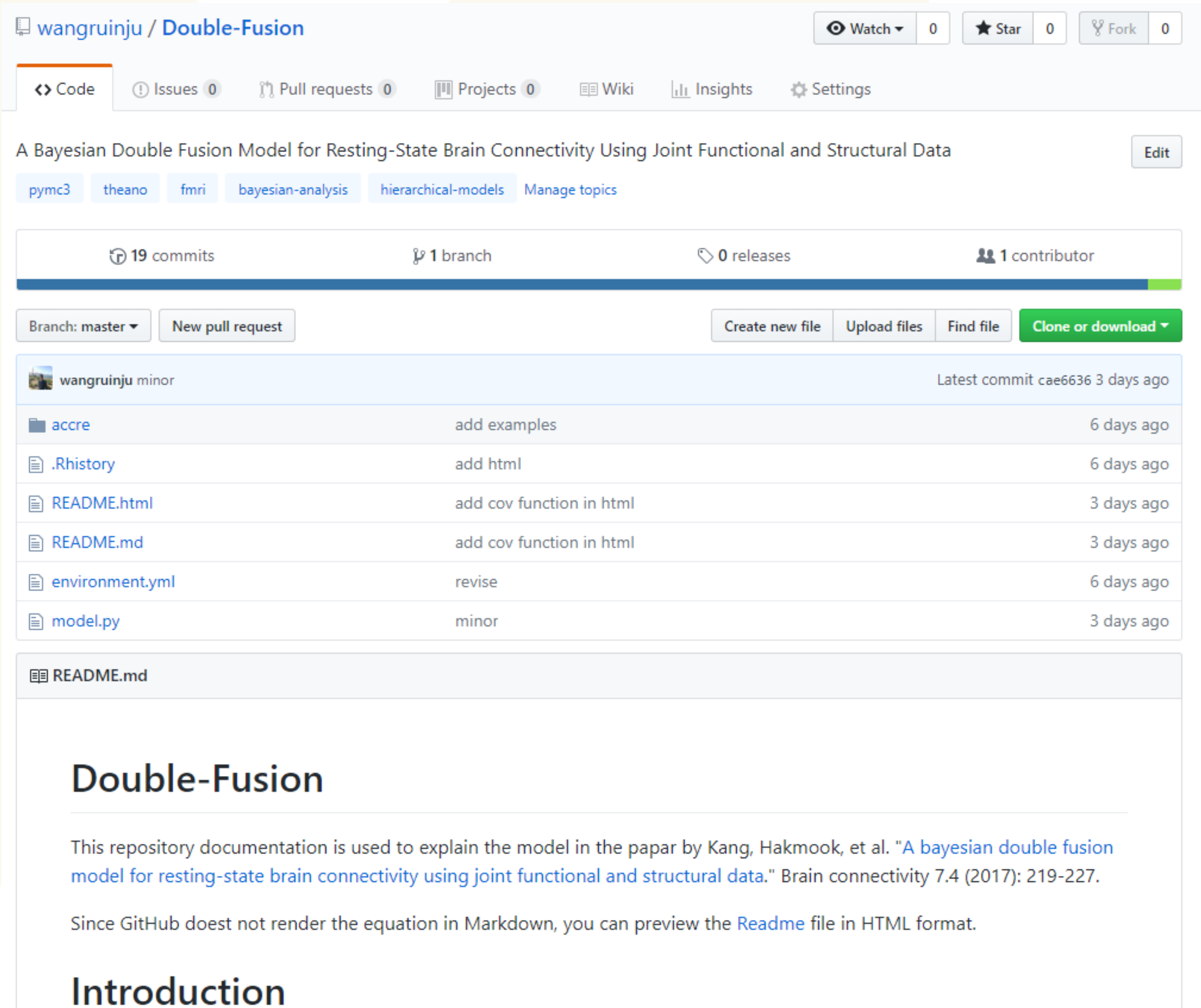
Executive Function Domain

- Interaction term $\text{FC}_i * \text{Depress}$: "FC80"

# 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



# Future Work

- Other kernel covariance functions
- 200-300 subjects
- Other machine learning methods of variable selection
- MDD classification

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