Spatial Bayesian Models for Task fMRI

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StatMIND
Statistical Methods for Individualized Neuro-Discovery

Outline

1. Bayesian statistics primer
2. Spatial priors
3. Spatial Bayesian GLM for task fMRI
4. Demo of BayesfMRI R package

Bayesian Statistics Primer

Frequentist vs. Bayesian Statistics

Frequentist Statistics

- Use only the observed data to estimate parameters, typically by maximizing the *likelihood*
- Usually fast & easy to compute 👍 (e.g., sample mean)
- Noise in the data is reflected in the estimates 👎
- Need to collect more data to reduce noise

Bayesian Statistics

- Take into account *prior beliefs* about parameter via a *prior distribution*
- Estimation done by maximizing the *posterior distribution*, which reflects updated beliefs based on data
- Results in better (more efficient) estimates 👍
- Estimation can be difficult and/or slow 👎

What do we believe about task activation?

1. **Patterns of task activation should be fairly similar across subjects**
    - Encode this belief via a prior on the activation amplitude that reflects variability observed in the population
    - *Hierarchical Bayesian models* use this kind of prior

2. **Patterns of task activation should be similar for “proximal” locations**
    - Encode this belief via a multivariate prior across locations with covariance structure that represents the expected spatial dependence among “neighbors”
    - *Spatial Bayesian models* use this kind of prior (a *spatial prior*)

Likelihood, Prior and Posterior

- The **likelihood** $f(\mathbf{y} \mid \mu)$ is the probability of observing the data $\mathbf{y}$, given a particular value of the parameter μ

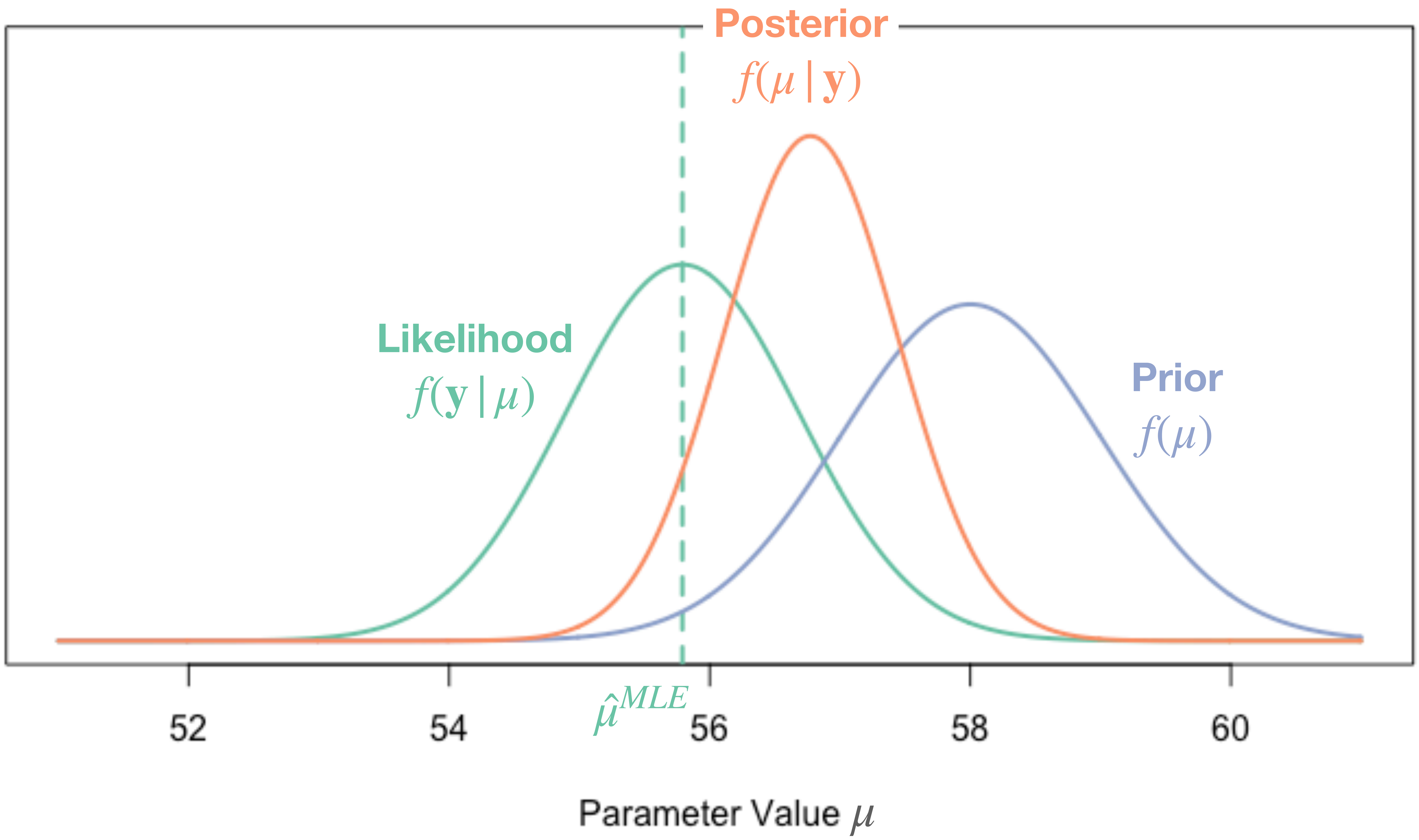
- The **prior distribution** $f(\mu)$ reflects our <u>original or prior</u> beliefs, absent data, about a parameter μ

- The **posterior distribution** $f(\mu \mid \mathbf{y})$ reflects our <u>updated</u> beliefs about μ based on the data $\mathbf{y}$

$$\overbrace{f(\mu \mid \mathbf{y})}^{\text{Posterior}} \underset{\text{Bayes Rule}}{=} \frac{\overbrace{f(\mathbf{y} \mid \mu)}^{\text{Likelihood}}\;\overbrace{f(\mu)}^{\text{Prior}}}{\underbrace{f(\mathbf{y})}_{\text{Marginal Likelihood}}} \overset{\mu}{\propto} \overbrace{f(\mathbf{y} \mid \mu)}^{\text{Likelihood}}\;\overbrace{f(\mu)}^{\text{Prior}}$$

Likelihood, Prior and Posterior

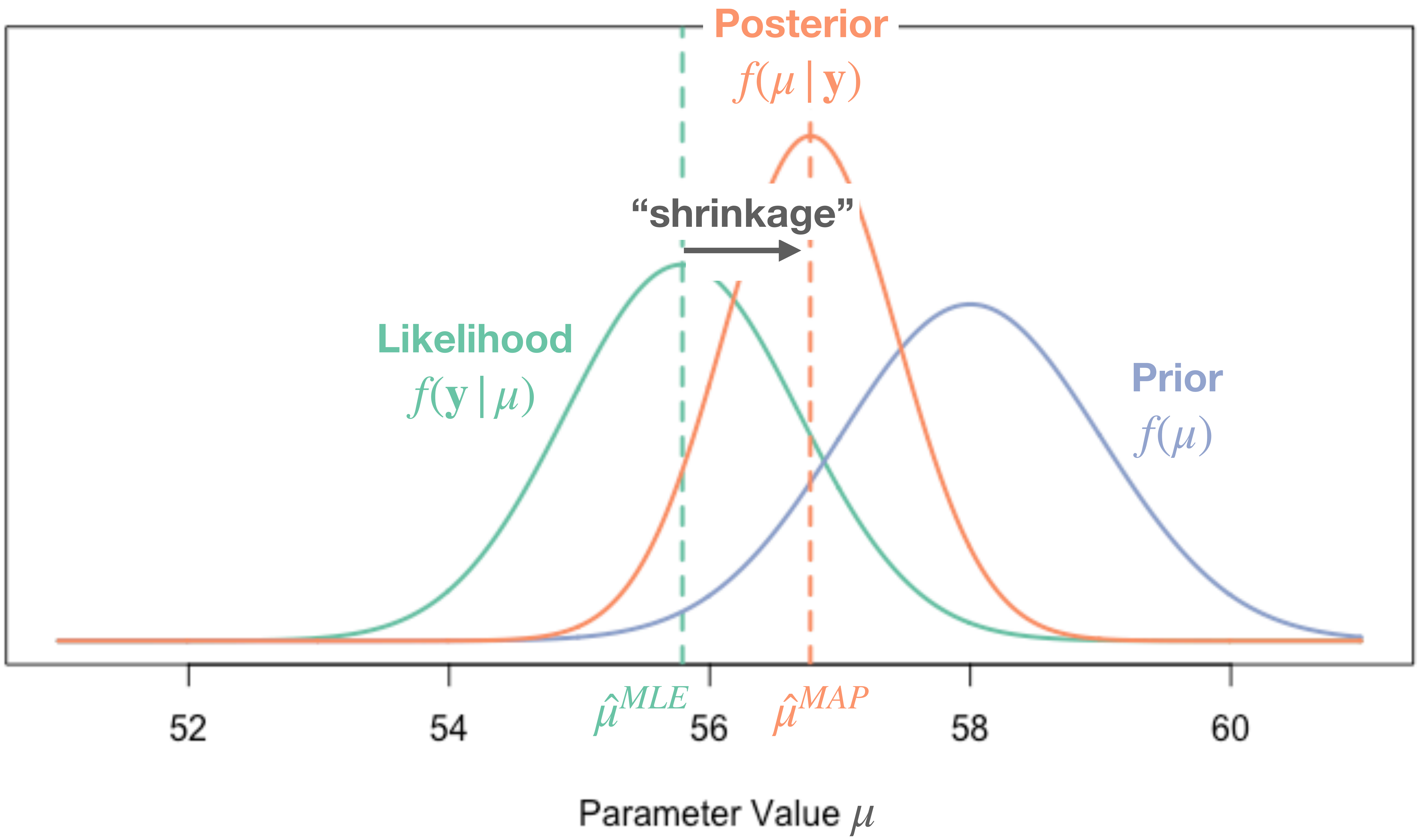
MLE = the value of μ that maximizes the *likelihood*



Maximum-a-posteriori (MAP) estimators

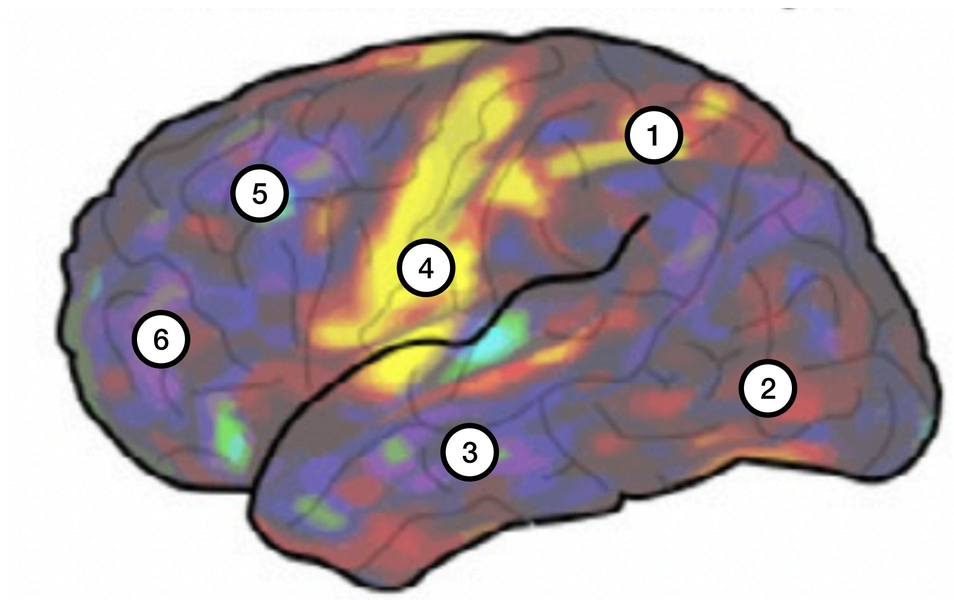
MAP = the value of μ that maximizes the *posterior*

MLE = the value of μ that maximizes the *likelihood*



Spatial Priors

What is a spatial prior?



latent spatial map $\boldsymbol{\beta}$

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \\ \beta_6 \end{pmatrix} \sim (\underset{(6x1)}{\boldsymbol{\mu}_0}, \underset{(6x6)}{\boldsymbol{\Sigma}_0})$$

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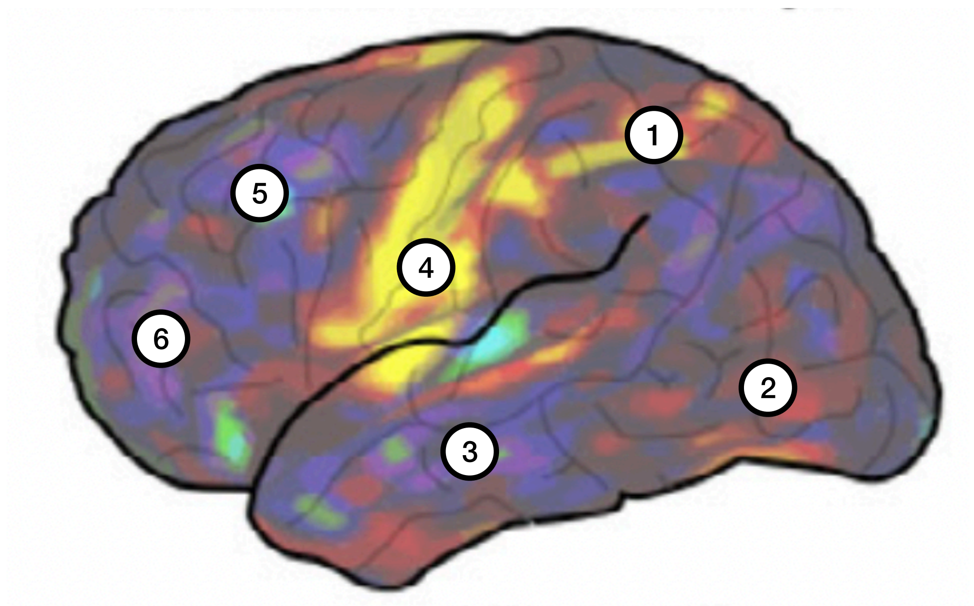

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One example of a spatial prior:

Multivariate Gaussian prior with mean zero and sparse inverse covariance

$$\boldsymbol{\beta} \sim N(\mathbf{0}, \mathbf{Q}^{-1})$$

$\mathbf{Q}$ contains zeros everywhere except along diagonal & in cells corresponding to “neighbors”

Toy fMRI example

Consider a single task, and for simplicity let the design column $\mathbf{x}$ be all 1's

- Likelihood: $\underset{(T \times 1)}{\mathbf{y}(v)} = \beta(v)\underset{(T \times 1)}{\mathbf{x}} + \underset{(T \times 1)}{\mathbf{e}(v)}, \quad \mathbf{e}(v) \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_T)$
- Likelihood in full vector form: $\underset{(TV \times 1)}{\mathbf{y}} = \mathbf{X}\underset{(V \times 1)}{\boldsymbol{\beta}} + \mathbf{e}, \quad \mathbf{e} \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_{TV})$
- Prior on $\boldsymbol{\beta}$: $\underset{(V \times 1)}{\boldsymbol{\beta}} \sim N(\underset{(V \times 1)}{\mathbf{0}}, \underset{(V \times V)}{\mathbf{Q}^{-1}})$

$$\underset{(TV \times V)}{\mathbf{X} = \begin{pmatrix} \mathbf{x} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{x} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{x} \end{pmatrix}}$$

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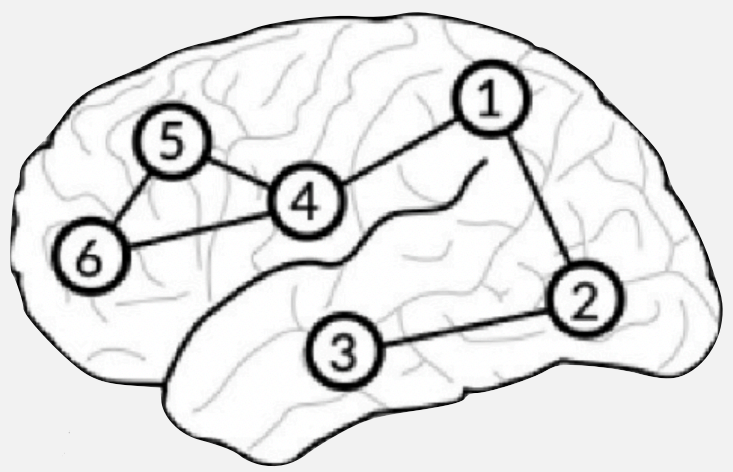
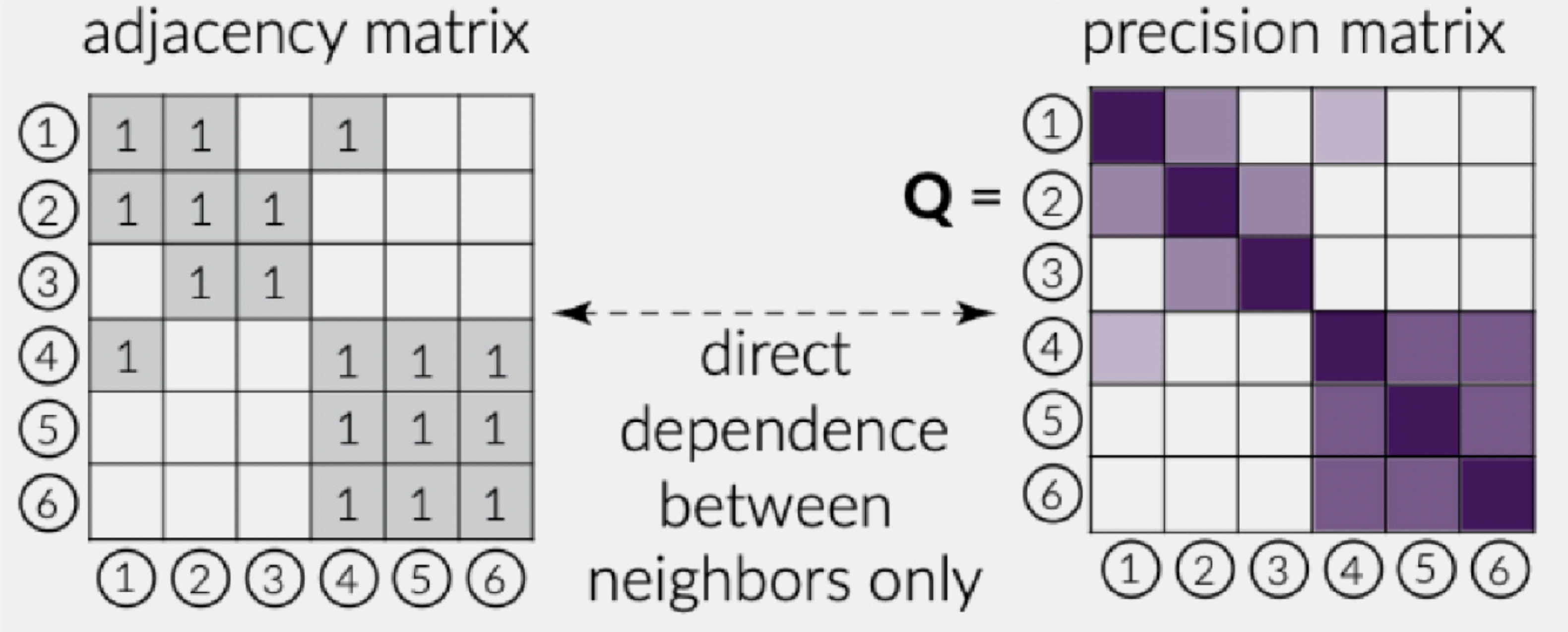
$\mathbf{Q}$ represents our beliefs about the spatial dependence of task activation amplitudes in $\boldsymbol{\beta}$.





some example numbers

$$\mathbf{Q} = \begin{pmatrix} 5 & -1 & 0 & -1 & 0 & 0 \\ -1 & 5 & -1 & 0 & 0 & 0 \\ 0 & -1 & 5 & 0 & 0 & 0 \\ -1 & 0 & 0 & 5 & -2 & -2 \\ 0 & 0 & 0 & -2 & 5 & -2 \\ 0 & 0 & 0 & -2 & -2 & 5 \end{pmatrix}$$

(Inverse covariance)

$$\mathbf{Q}^{-1} = \begin{pmatrix} 0.23 & 0.05 & 0.01 & 0.10 & 0.07 & 0.07 \\ 0.05 & 0.22 & 0.04 & 0.02 & 0.01 & 0.01 \\ 0.01 & 0.04 & 0.21 & 0.00 & 0.00 & 0.00 \\ 0.10 & 0.02 & 0.00 & 0.47 & 0.31 & 0.31 \\ 0.07 & 0.01 & 0.00 & 0.31 & 0.45 & 0.30 \\ 0.07 & 0.01 & 0.00 & 0.31 & 0.30 & 0.45 \end{pmatrix}$$

(covariance matrix)

Toy example

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}, \quad \mathbf{e} \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_{TV})$$

<u>Frequentist estimate of $\boldsymbol{\beta}$</u>

(MLE equivalent to OLS)

$$\hat{\boldsymbol{\beta}}^{MLE} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = (\bar{y}_1, \cdots \bar{y}_V)'$$

$$\mathbf{x} = (1,1,\ldots,1)'$$

$$\mathbf{X} = \begin{pmatrix} \mathbf{x} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{x} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{x} \end{pmatrix} \quad \mathbf{X}'\mathbf{X} = \begin{pmatrix} T & & \\ & \ddots & \\ & & T \end{pmatrix} \quad \mathbf{X}'\mathbf{y} = \begin{pmatrix} \sum_t y_{t,1} \\ \vdots \\ \sum_t y_{t,V} \end{pmatrix}$$

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<u>Bayesian estimate of $\boldsymbol{\beta}$:</u> $\hat{\boldsymbol{\beta}}^{MAP} = \left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{X} + \mathbf{Q}\right)^{-1}\left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{y}\right)$

Toy example

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What if $\mathbf{Q}$ → a matrix of zero's?

(Prior var → ∞)

$$\hat{\boldsymbol{\beta}}^{MAP} \rightarrow \left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{X}\right)^{-1}\left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{y}\right) = \hat{\boldsymbol{\beta}}^{MLE}$$

Toy example

Bayesian estimate of $\boldsymbol{\beta}$: $\hat{\beta}^{MAP} = \left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{X} + \mathbf{Q}\right)^{-1}\left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{y}\right)$

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What if $\mathbf{Q}$ equals a diagonal matrix, $\frac{1}{\sigma_0^2}\mathbf{I}_V$?

(no dependence information, prior var = σ_0^2)

Toy example

<u>Bayesian estimate of $\boldsymbol{\beta}$:</u> $\hat{\boldsymbol{\beta}}^{MAP} = \left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{X} + \mathbf{Q}\right)^{-1}\left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{y}\right)$

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(no dependence information, prior var = σ_0^2)

$$\left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{X} + \mathbf{Q}\right) = \left(\frac{T}{\sigma^2} + \frac{1}{\sigma_0^2}\right)\mathbf{I}_V$$

$$\frac{1}{\sigma^2}\mathbf{X}'\mathbf{y} = \frac{T}{\sigma^2}(\bar{y}_1, \cdots, \bar{y}_V)' = \frac{T}{\sigma^2}\hat{\boldsymbol{\beta}}^{MLE}$$

$$\Rightarrow \hat{\boldsymbol{\beta}}^{MAP} = \frac{\sigma_0^2}{\sigma_0^2 + \sigma^2/T}\hat{\boldsymbol{\beta}}^{MLE} = \lambda\hat{\boldsymbol{\beta}}^{MLE}$$

If $T = 100, \sigma^2 = 1, \sigma_0^2 = 1/5$, then $\lambda = 0.988$

Toy example

<u>Bayesian estimate of $\boldsymbol{\beta}$:</u> $\hat{\beta}^{MAP} = \left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{X} + \mathbf{Q}\right)^{-1}\left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{y}\right)$

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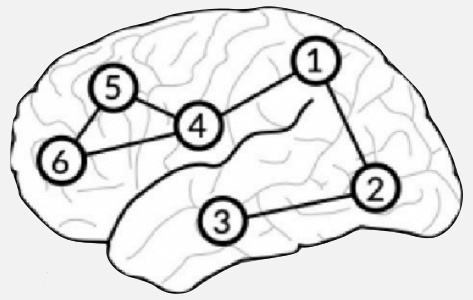

Toy example

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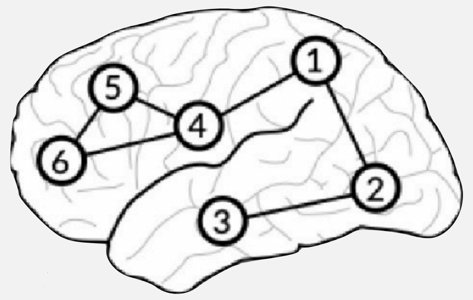

We just showed that

$$\hat{\boldsymbol{\beta}}^{MAP} = \frac{T}{\sigma^2}\left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{X} + \mathbf{Q}\right)^{-1}\hat{\boldsymbol{\beta}}^{MLE} = \boldsymbol{\Lambda}\hat{\boldsymbol{\beta}}^{MLE}.$$

If $T = 100$ and $\sigma^2 = 1$, $\boldsymbol{\Lambda} = \begin{pmatrix} 0.95 & 0.01 & 0 & 0.01 & 0 & 0 \\ 0.01 & 0.95 & 0.01 & 0 & 0 & 0 \\ 0 & 0.01 & 0.95 & 0 & 0 & 0 \\ 0.01 & 0 & 0 & 0.95 & 0.02 & 0.02 \\ 0 & 0 & 0 & 0.02 & 0.95 & 0.02 \\ 0 & 0 & 0 & 0.02 & 0.02 & 0.95 \end{pmatrix}$

Toy example

<u>Bayesian estimate of $\boldsymbol{\beta}$:</u> $\hat{\boldsymbol{\beta}}^{MAP} = \left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{X} + \mathbf{Q}\right)^{-1}\left(\frac{1}{\sigma^2}\mathbf{X}'\mathbf{y}\right)$

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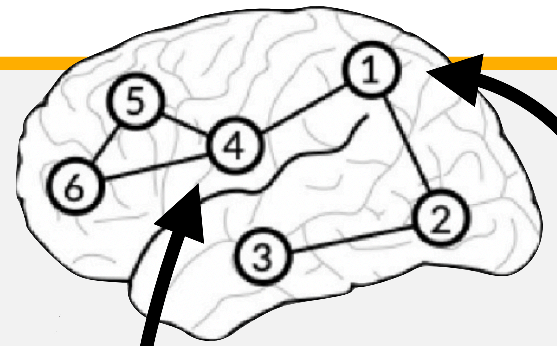
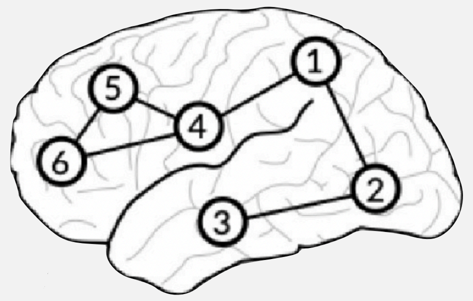


For example:

$$\hat{\beta}_1^{MAP} = 0.95\hat{\beta}_1^{MLE} + 0.01\hat{\beta}_2^{MLE} + 0.01\hat{\beta}_4^{MLE}$$

$$\hat{\beta}_4^{MAP} = 0.95\hat{\beta}_4^{MLE} + 0.01\hat{\beta}_1^{MLE} + 0.02\hat{\beta}_5^{MLE} + 0.02\hat{\beta}_6^{MLE}$$

What if $\mathbf{Q} = \begin{pmatrix} 5 & -1 & 0 & -1 & 0 & 0 \\ -1 & 5 & -1 & 0 & 0 & 0 \\ 0 & -1 & 5 & 0 & 0 & 0 \\ -1 & 0 & 0 & 5 & -2 & -2 \\ 0 & 0 & 0 & -2 & 5 & -2 \\ 0 & 0 & 0 & -2 & -2 & 5 \end{pmatrix}$ **?**



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Spatial Bayesian GLM

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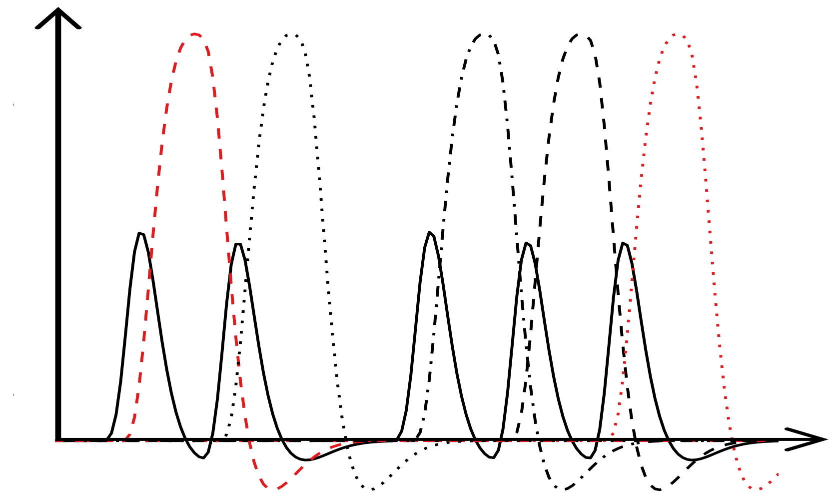
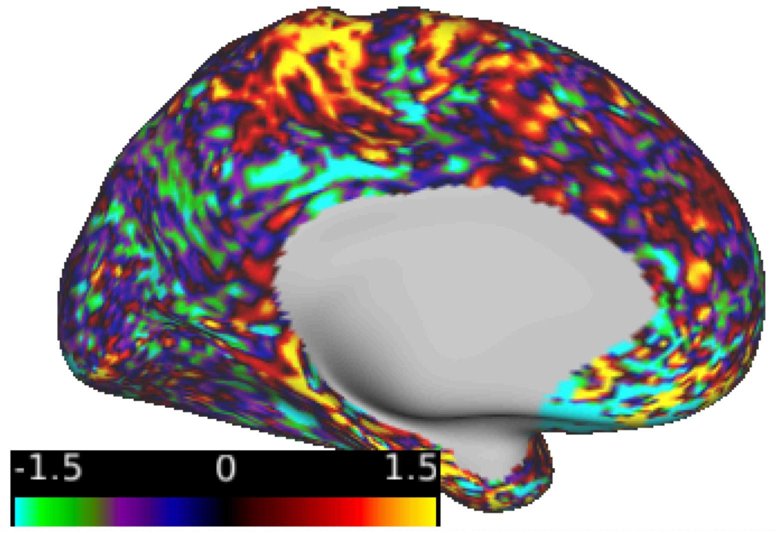
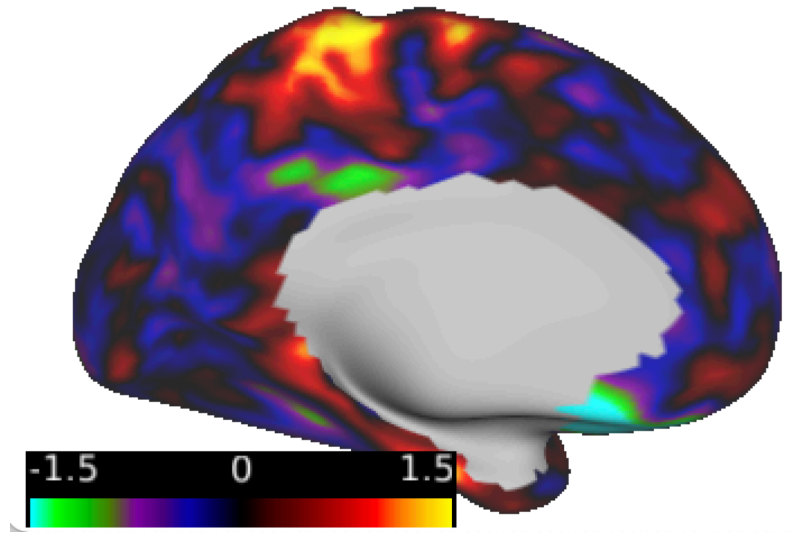


GLM (General Linear Model): Estimate amplitude and areas of activation during a task or stimulus



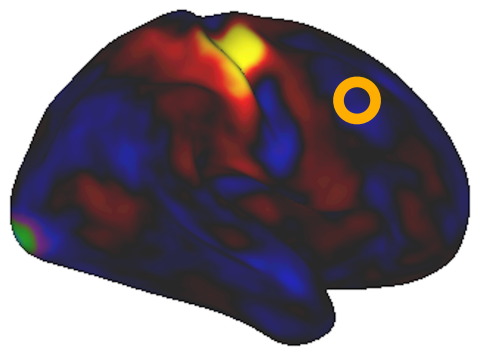
Classical GLM: Fit a separate linear model at every voxel or vertex (“massive univariate”) to estimate activation amplitude



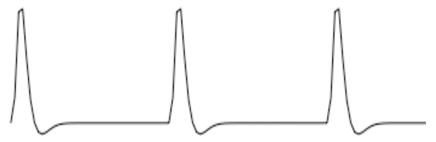
Spatial Bayesian GLM: Fit a single Bayesian model accounting for spatial dependence via spatial priors for greater accuracy & power

The Classical GLM

Observed BOLD signal at location v



Amplitude of activation for task k at location v

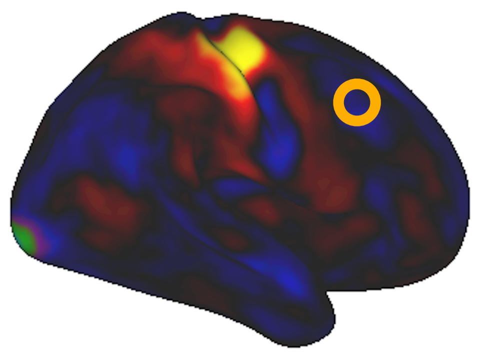


Expected BOLD response to task k

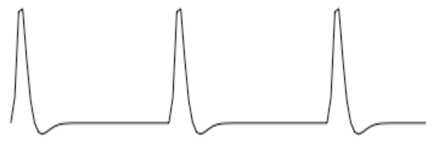
$$\underset{(T \times 1)}{\mathbf{y}(v)} = \sum_{k=1}^{K} \beta_k(v) \underset{(T \times 1)}{\mathbf{x}_k} + \underset{(T \times 1)}{\boldsymbol{\epsilon}(v)}, \ \boldsymbol{\epsilon}(v) \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$$

The Classical GLM

Observed BOLD signal at location v



Amplitude of activation for task k at location v



Expected BOLD response to task k

$$\underbrace{\mathbf{y}(v)}_{(T \times 1)} = \sum_{k=1}^{K} \beta_k(v)\underbrace{\mathbf{x}_k}_{(T \times 1)} + \underbrace{\epsilon(v)}_{(T \times 1)}, \ \epsilon(v) \sim N(\mathbf{0}, \sigma^2\mathbf{I})$$

No baseline field (data & design matrix have been centered)

No nuisance signals (Have been regressed from data & design)

Homoskedastic, uncorrelated residuals (data are prewhitened)

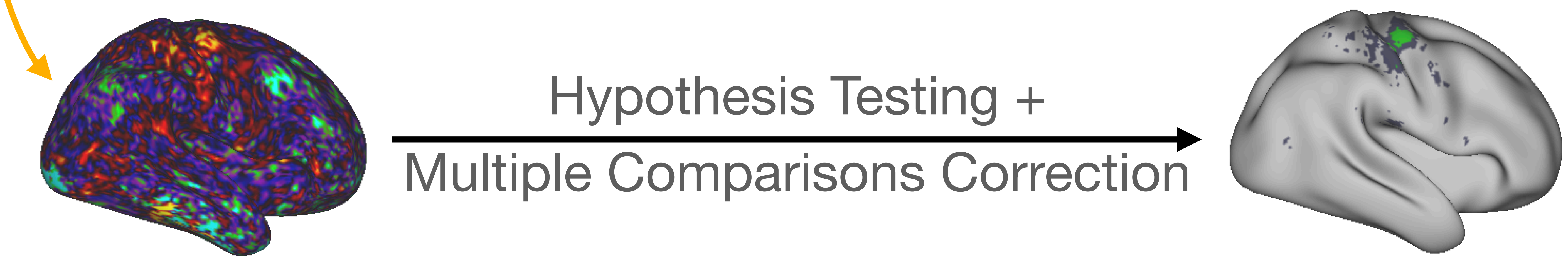
Several assumptions being made for simplicity

Classical GLM Activations

$$\mathbf{y}(1) = \sum_{k=0}^{K} \beta_k(1)\mathbf{x}_k + \boldsymbol{\epsilon}(1), \quad \boldsymbol{\epsilon}(1) \sim MVN(\mathbf{0}, \sigma^2\mathbf{I})$$

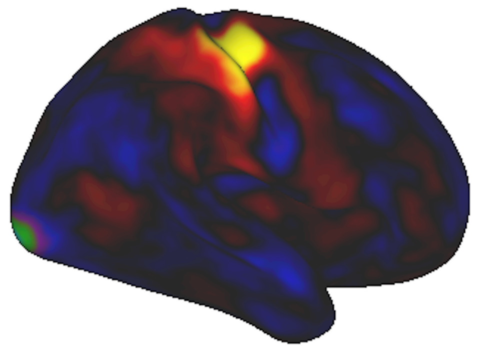
$$\vdots \qquad \vdots \qquad \qquad \vdots \qquad \qquad \vdots$$

$$\mathbf{y}(V) = \sum_{k=0}^{K} \beta_k(V)\mathbf{x}_k + \boldsymbol{\epsilon}(V), \ \boldsymbol{\epsilon}(V) \sim MVN(\mathbf{0}, \sigma^2\mathbf{I})$$



The Spatial Bayesian GLM

$$\mathbf{X}_k = \begin{pmatrix} \mathbf{x}_k & 0 & \cdots & 0 \\ 0 & \mathbf{x}_k & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{x}_k \end{pmatrix}$$



Observed BOLD signal, concatenated across all locations

Expected BOLD response to task k

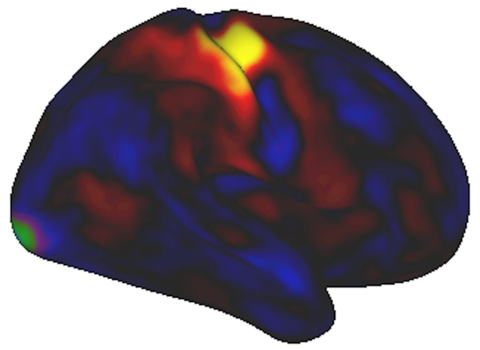
Activation amplitude for task k, concatenated across all locations

The classical GLM, concatenated across all locations

$$\underset{(TV \times 1)}{\mathbf{y}} = \sum_{k=1}^{K} \underset{(TV \times V)}{\mathbf{X}_k} \underset{(V \times 1)}{\boldsymbol{\beta}_k} + \boldsymbol{\epsilon}, \; \boldsymbol{\epsilon} \sim MVN(\mathbf{0}, \sigma^2 \mathbf{I}_{TV})$$

The Spatial Bayesian GLM

$$\mathbf{X}_k = \begin{pmatrix} \mathbf{x}_k & 0 & \cdots & 0 \\ 0 & \mathbf{x}_k & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{x}_k \end{pmatrix}$$



Observed BOLD signal, concatenated across all locations

Expected BOLD response to task k

Activation amplitude for task k, concatenated across all locations

$$\underset{(TV \times 1)}{\mathbf{y}} = \sum_{k=1}^{K} \underset{(TV \times V)}{\mathbf{X}_k} \underset{(V \times 1)}{\boldsymbol{\beta}_k} + \boldsymbol{\epsilon}, \; \boldsymbol{\epsilon} \sim MVN(\mathbf{0}, \sigma^2 \mathbf{I}_{TV})$$

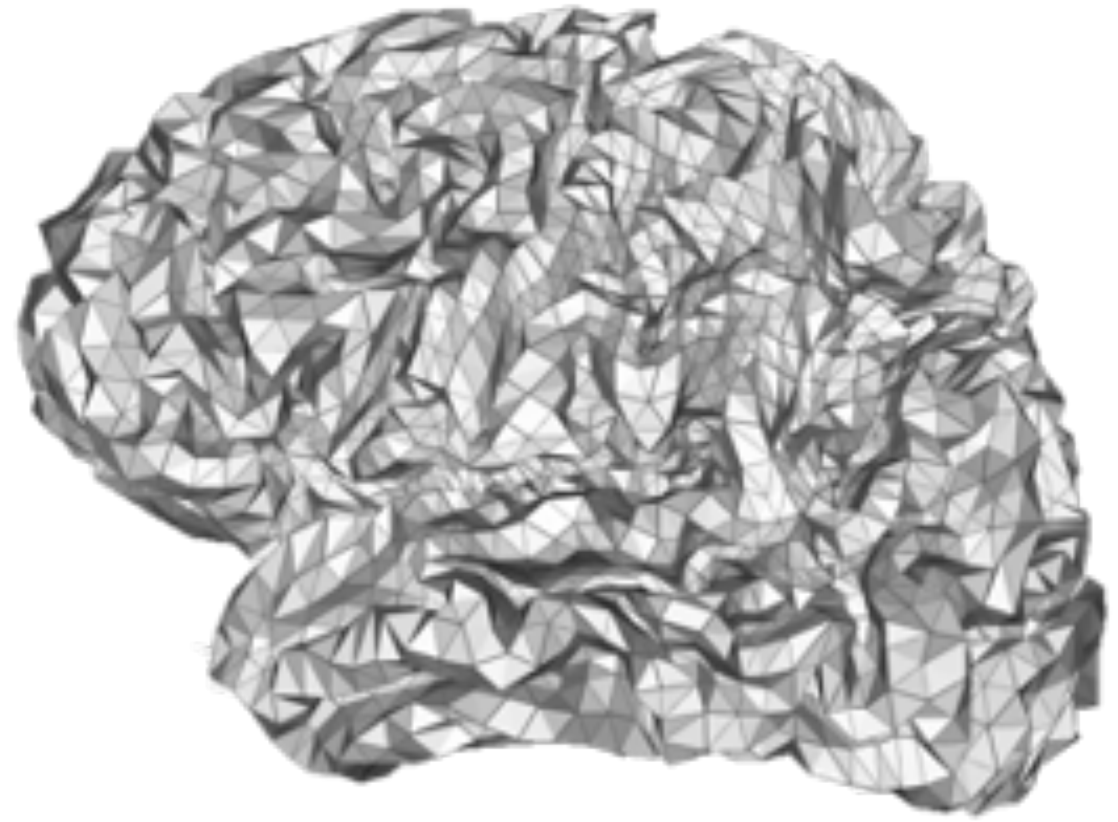
$$\boldsymbol{\beta}_k \sim N(\mathbf{0}, \mathbf{Q}_k^{-1})$$

spatial Bayesian GLM

Spatial priors for cortical surface task fMRI

We need/want a spatial prior that:

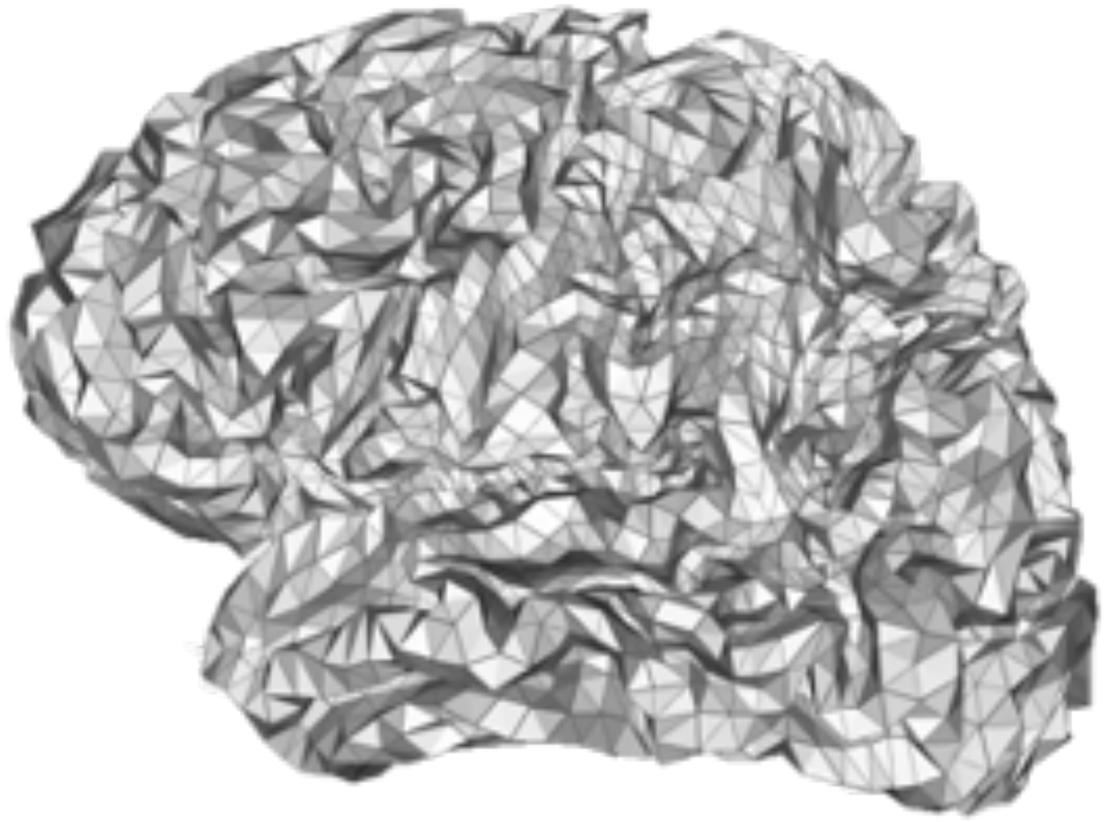
- Have sparse inverse covariance
- Is applicable to triangular mesh data
- Has a Gaussian distribution



Stochastic partial differential equation (SPDE) priors (Lindgren et al. 2011) check all the boxes!

Lindgren, et al. (2011). "An explicit link between Gaussian fields and Gaussian Markov random fields: the SPDE approach." *Journal of the Royal Statistical Society Series B: Statistical Methodology*.

SPDE Prior



$$\boldsymbol{\beta} \sim MVN(\mathbf{0}, \mathbf{Q}_{\kappa,\tau}^{-1})$$

$$\mathbf{Q}_{\kappa,\tau} = \tau^2(\kappa^4\mathbf{F} + 2\kappa^2\mathbf{G} + \mathbf{G}\mathbf{F}^{-1}\mathbf{G})$$

A fixed diagonal matrix

A fixed sparse matrix with non-zero entries for neighboring locations in mesh

κ controls the spatial correlation (must be estimated)

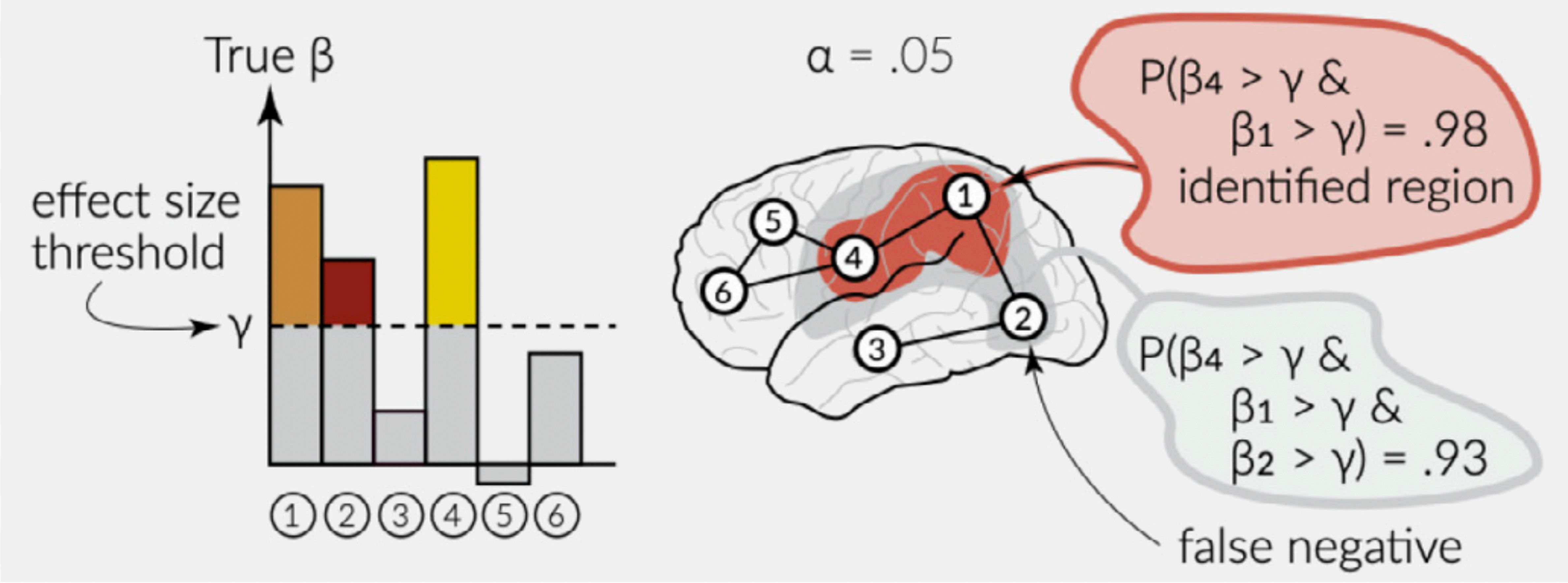
τ controls the variance (must be estimated)

Areas of Activation via Excursion Sets

For each task k, we use the ***joint posterior distribution of*** $\boldsymbol{\beta}_k$ to identify areas of statistically significant activation above a minimum effect size of interest

This approach ***avoids the need to correct for multiple comparisons***, which would be required if we used the marginal posterior distribution at each location to identify areas of activation

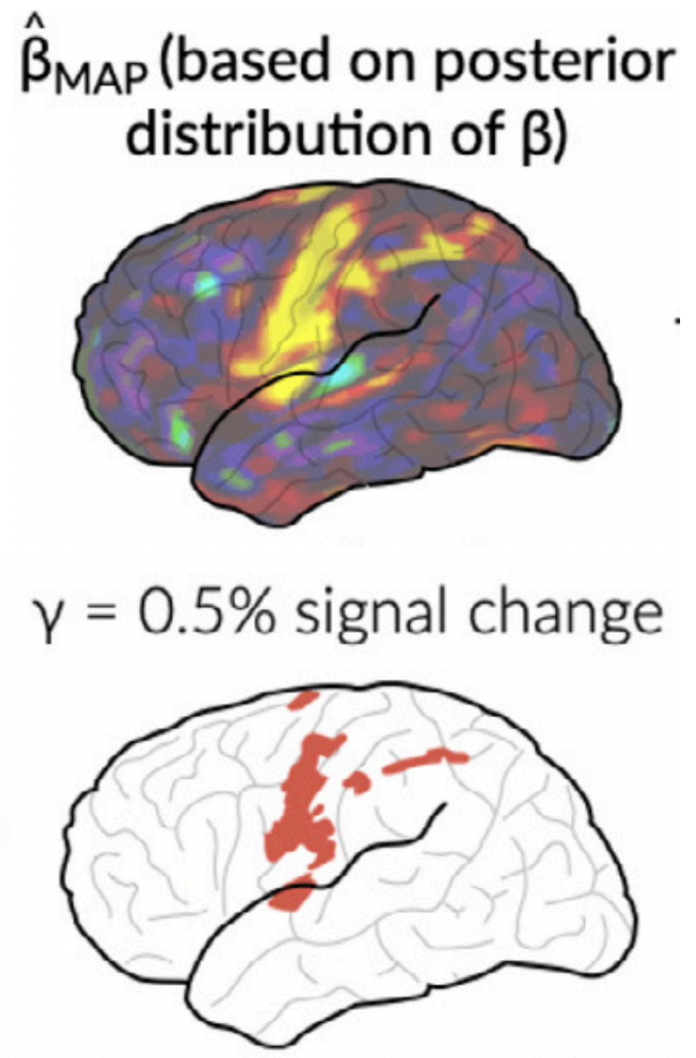
There is a ***dramatic gain in power*** over massive univariate modeling, facilitating the use of a scientifically meaningful minimum effect size



Bolin, D., & Lindgren, F. (2015). Excursion and contour uncertainty regions for latent Gaussian models. *Journal of the Royal Statistical Society Series B: Statistical Methodology.*
Mejia, A. F., Yue, Y., Bolin, D., Lindgren, F., & Lindquist, M. A. (2020). A Bayesian general linear modeling approach to cortical surface fMRI data analysis. *Journal of the American Statistical Association.*

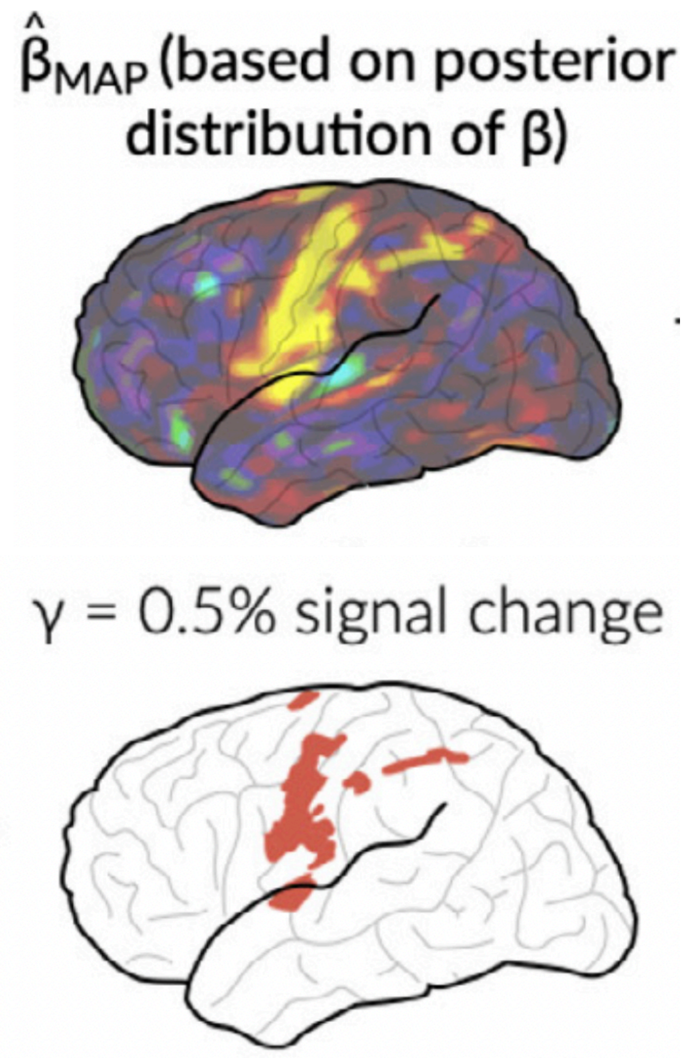
Excursions Set Procedure

- A location v is defined as *truly activated* if $\beta_k(v) > \gamma$ (activation threshold)



Mejia, A. F., Yue, Y., Bolin, D., Lindgren, F., & Lindquist, M. A. (2020). A Bayesian general linear modeling approach to cortical surface fMRI data analysis. *Journal of the American Statistical Association.*

Excursions Set Procedure

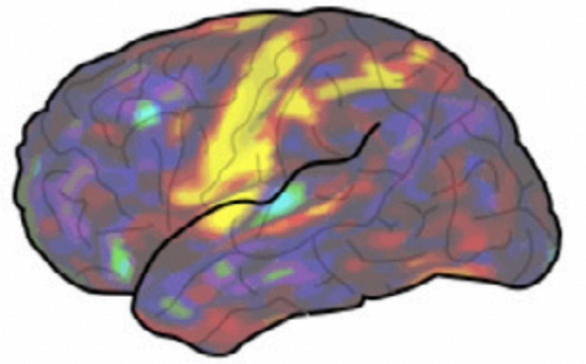


- A location v is defined as *truly activated* if $\beta_k(v) > \gamma$ (activation threshold)

- We aim to identify the *excursion region* $E_{\gamma,\alpha}$, the largest set of locations where with joint posterior probability $1 - \alpha$, every location is truly activated (above γ)

Excursions Set Procedure

$\hat{\beta}_{MAP}$ (based on posterior distribution of β)

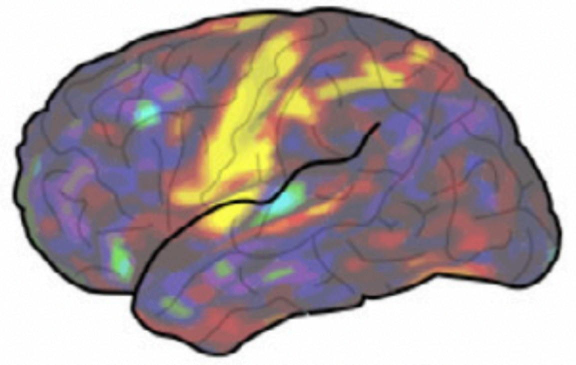


γ = 0.5% signal change

- A location v is defined as *truly activated* if $\beta_k(v) > \gamma$ (activation threshold)
- We aim to identify the *excursion region* $E_{\gamma,\alpha}$, the largest set of locations where with joint posterior probability $1 - \alpha$, every location is truly activated (above γ)
- We estimate the *excursion function*, the largest value of $1 - \alpha$ for which a location v would be included in $E_{\gamma,\alpha}$ (assuming locations are added in order of their marginal posterior probabilities)

Mejia, A. F., Yue, Y., Bolin, D., Lindgren, F., & Lindquist, M. A. (2020). A Bayesian general linear modeling approach to cortical surface fMRI data analysis. *Journal of the American Statistical Association.*

Excursions Set Procedure



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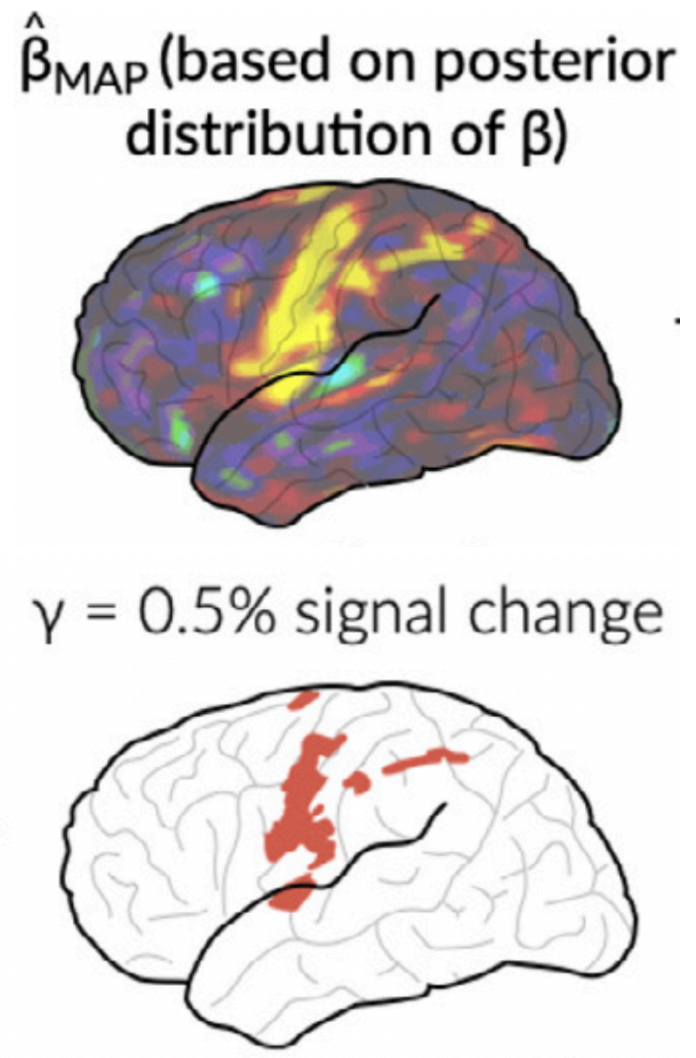
- Thresholding the excursion function at, e.g., 0.95 yields the excursion region for $\alpha = 0.05$

Mejia, A. F., Yue, Y., Bolin, D., Lindgren, F., & Lindquist, M. A. (2020). A Bayesian general linear modeling approach to cortical surface fMRI data analysis. *Journal of the American Statistical Association.*

Excursions Set Procedure

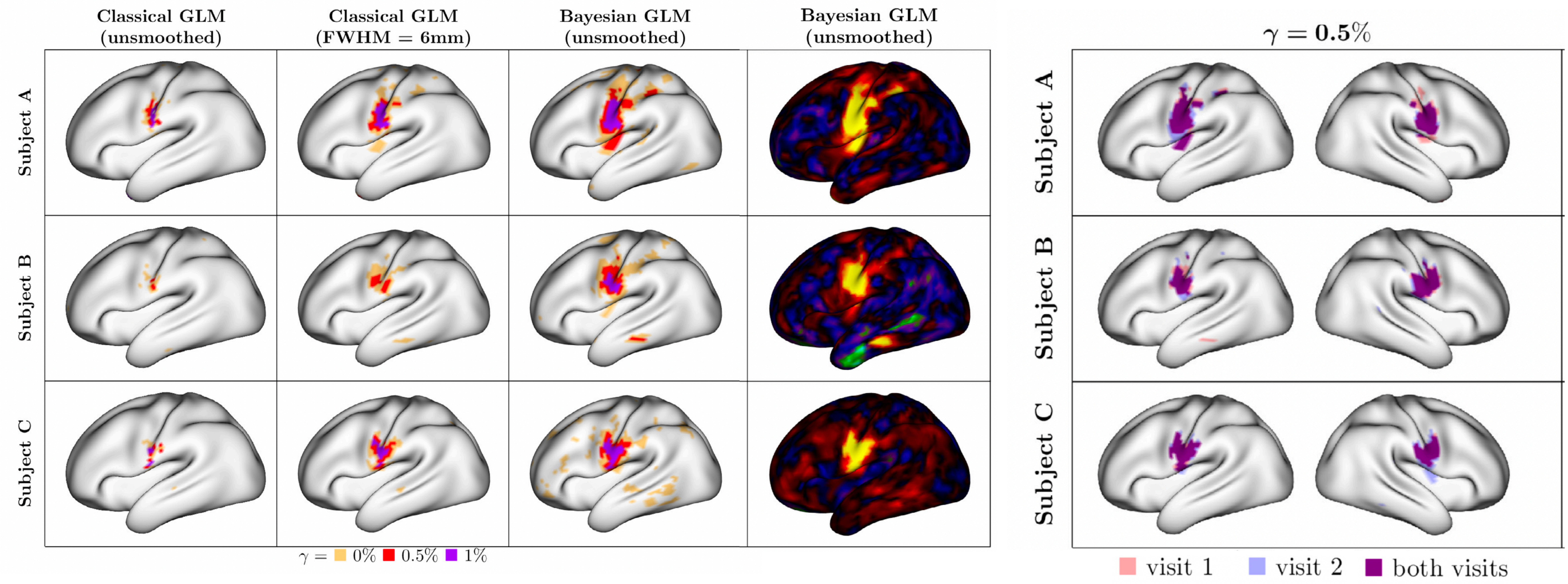


- A location v is defined as *truly activated* if $\beta_k(v) > \gamma$ (activation threshold)
- We aim to identify the *excursion region* $E_{\gamma,\alpha}$, the largest set of locations where with joint posterior probability $1 - \alpha$, every location is truly activated (above γ)
- We estimate the *excursion function*, the largest value of $1 - \alpha$ for which a location v would be included in $E_{\gamma,\alpha}$ (assuming locations are added in order of their marginal posterior probabilities)
- Thresholding the excursion function at, e.g., 0.95 yields the excursion region for $\alpha = 0.05$
- **<u>This approach controls the FWER</u>**, since the probability that *all* locations in the excursion set are truly activated is $1 - \alpha$, so the probability of at least one false positive is α

Mejia, A. F., Yue, Y., Bolin, D., Lindgren, F., & Lindquist, M. A. (2020). A Bayesian general linear modeling approach to cortical surface fMRI data analysis. *Journal of the American Statistical Association.*

Bayesian GLM is powerful in individuals

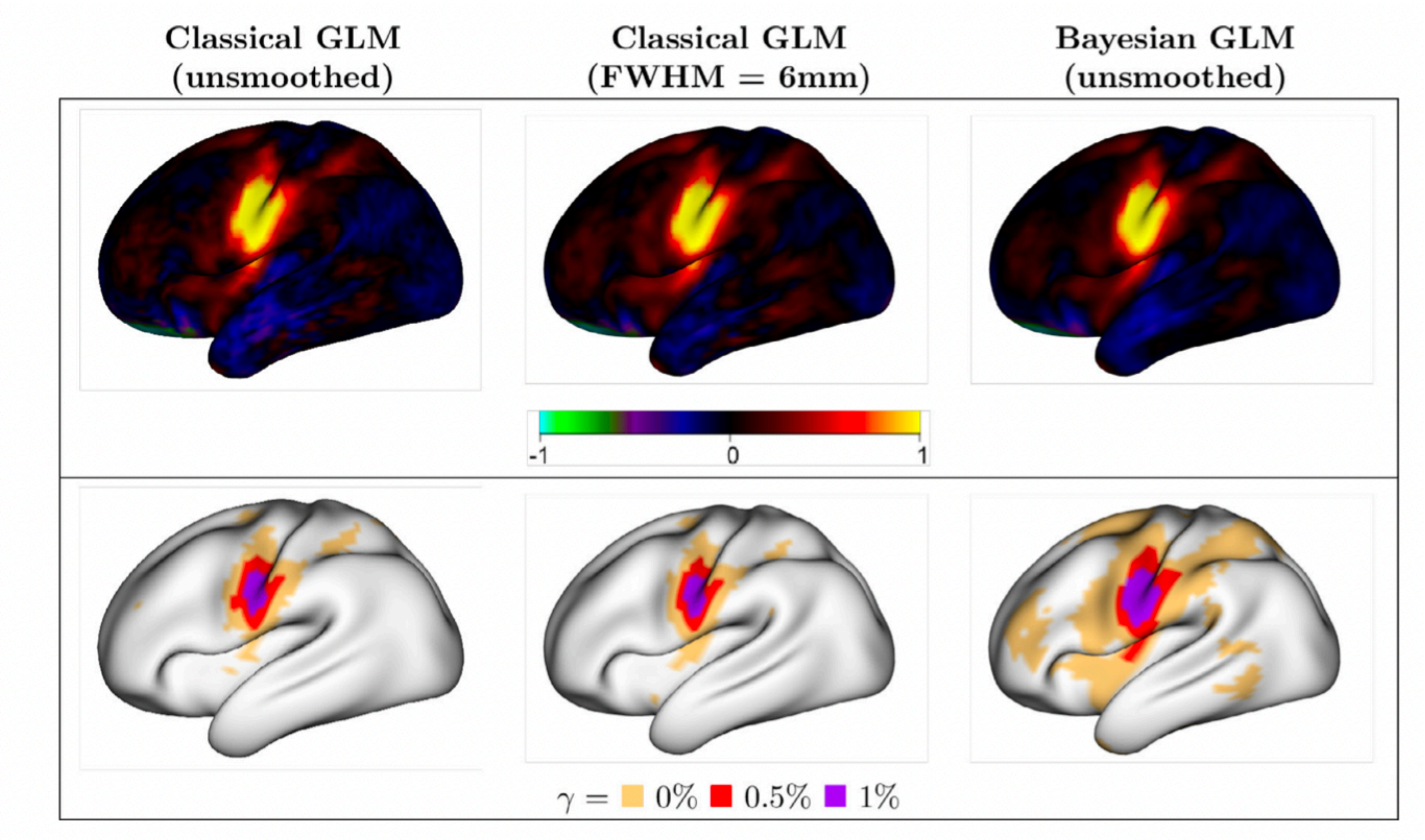
Tongue task activations in the motor task fMRI study for 3 individuals in the HCP. The LR + RL runs for each session were analyzed together for each subject.

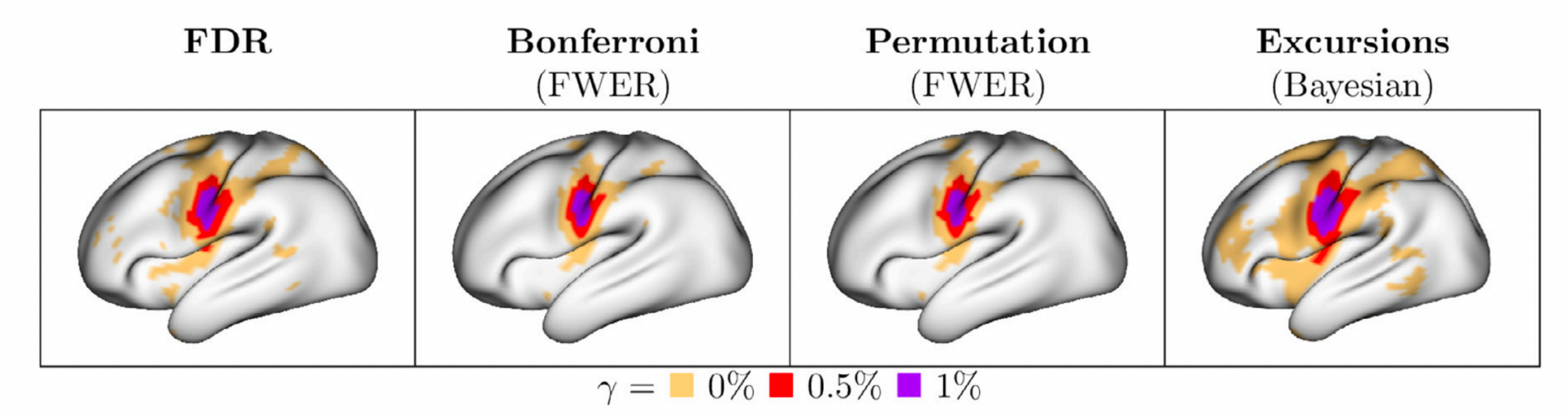


Spencer, Yue, Bolin, Ryan,& Mejia (2022). Spatial Bayesian GLM on the cortical surface produces reliable task activations in individuals and groups. *NeuroImage*, 249, 118908.

Bayesian Group Averages and Contrasts

We can analyze group averages and contrasts in a principled way after fitting all of the subject-level models, for **scalable & powerful** multi-subject analysis.





Mejia, A. F., Yue, Y., Bolin, D., Lindgren, F., & Lindquist, M. A. (2020). A Bayesian general linear modeling approach to cortical surface fMRI data analysis. *Journal of the American Statistical Association.*
Spencer, Yue, Bolin, Ryan,& Mejia (2022). Spatial Bayesian GLM on the cortical surface produces reliable task activations in individuals and groups. *NeuroImage*, 249, 118908.

Demo in R

BayesfMRI R Package