# Partial Separability and Functional Graphical Models for Multivariate Gaussian Processes

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We present a new notion of separability for multivariate functional data called **partial separability**. This notion provides parsimonious Karhunen-Loève type expansion an invertible covariance operator yielding a well-defined Gaussian graphical model that can be identified with a sequence of finite-dimensional graphical models, each of fixed dimension.

## Partial Separability

Multivariate Gaussian Process $X$ is ***partially separable*** if there exists an orthonormal basis $\{\varphi_\ell\}_{\ell=1}$ of $L^2[0,1]$ such that the random vectors $\theta_\ell = (\langle X_1,\varphi_\ell\rangle, \ldots, \langle X_p,\varphi_\ell\rangle)$ for $\ell \geq 1$, are mutually uncorrelated.

### Partial Separability Karhunen-Loève expansion

$$X(t) = \sum_{l=1}^{\infty} \theta_l \varphi_l(t),$$

$$\theta_{lj} = \int_0^1 X_j(s)\varphi_l(s)\mathrm{d}s$$

$$\begin{array}{c} \begin{array}{cccc} l=1 & l=2 & \cdots & l=L \\ \theta_{11}\ldots\theta_{1p} & \theta_{21}\ldots\theta_{2p} & & \theta_{L1}\ldots\theta_{Lp} \end{array} \\ \begin{bmatrix} \Sigma_1 & 0 & \cdots & 0 \\ 0 & \Sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Sigma_L \end{bmatrix} \end{array}$$

### Univariate Karhunen-Loève expansion

$$X_j(t) = \sum_{l=1}^{\infty} \xi_{jl}\phi_{jl}(t),$$

$$\xi_{jl} = \int_0^1 X_j(t)\phi_{jl}(t)\mathrm{d}t$$

$$\begin{array}{c} \begin{array}{cccc} j=1 & j=2 & \cdots & j=p \\ \xi_{11}\ldots\xi_{1L} & \xi_{21}\ldots\xi_{2L} & & \xi_{p1}\ldots\xi_{pL} \end{array} \\ \begin{bmatrix} 0 & \Gamma_{12} & \cdots & \Gamma_{1p} \\ \Gamma_{21} & 0 & \cdots & \Gamma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \Gamma_{p1} & \Gamma_{p2} & \cdots & 0 \end{bmatrix} \end{array}$$

- Univariate KL expansion possesses a potentially full inverse covariance structure. Under partial separability it remains block-diagonal.

## Functional Gaussian Graphical Model

- In many problems, the object of interest is the inverse covariance matrix describing conditional independencies (under Gaussianity)
- A functional Gaussian graphical model for $X$ is the graph G=(V,E) with conditional covariance functions:

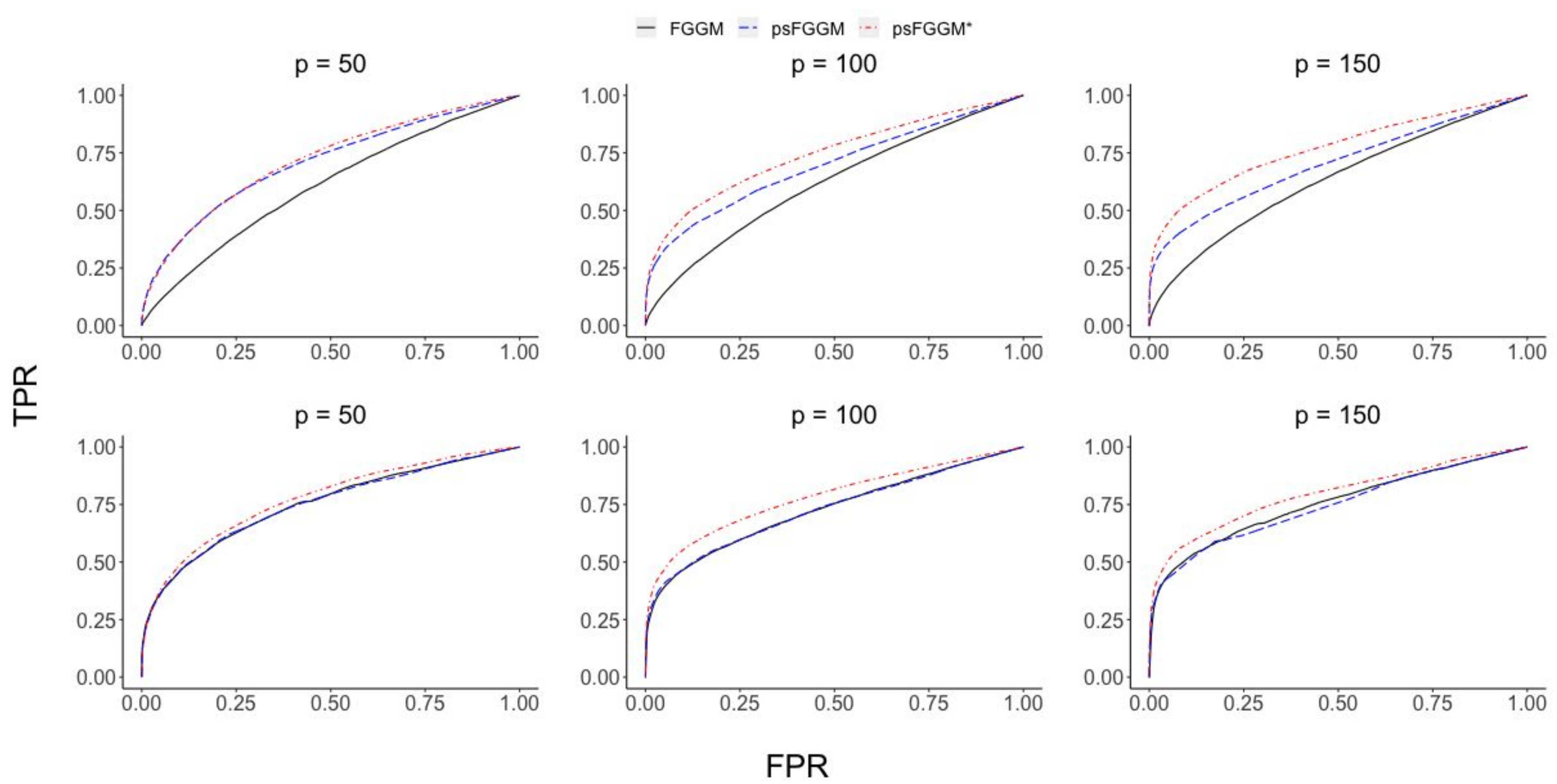
$$C_{jk}(s,t) = \mathrm{cov}(X_j(s), X_k(t) | X_{-(j,k)}), \quad j,k \in V, j \neq k,$$

- Functional graph edge set $E$ relates to edge sets $E_\ell$ by $E = \bigcup_{l=1}^{\infty} E_l$
- **psFGGM**: a group graphical lasso estimator for functional gaussian graphical models.

$$(\hat{\Xi}_1, \ldots, \hat{\Xi}_L) = \underset{\Upsilon_l \succ 0}{\mathrm{argmin}} \sum_{l=1}^{L} \left\{ \mathrm{trace}(\hat{R}_l \Upsilon_l) - \log(|\Upsilon_l|) \right\} + P(\Upsilon_1, \ldots, \Upsilon_l).$$

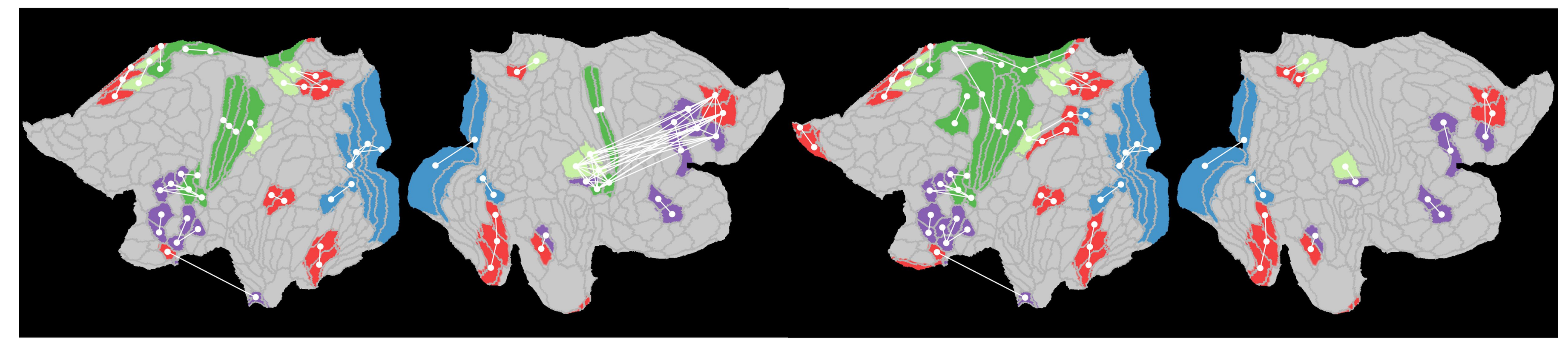
$$P(\Upsilon_1, \ldots, \Upsilon_l) = \gamma \left[ \alpha \sum_{l=1}^{L} \sum_{j \neq k} |v_{ljk}| + (1-\alpha) \sum_{j \neq k} \sqrt{\sum_{l=1}^{L} v_{ljk}^2} \right], \quad (\Upsilon_l)_{jk} = v_{ljk}$$

- **Simulations:** Mean ROC curves. Case n=p/2, with partial separable covariance (top) and non-separable (bottom).

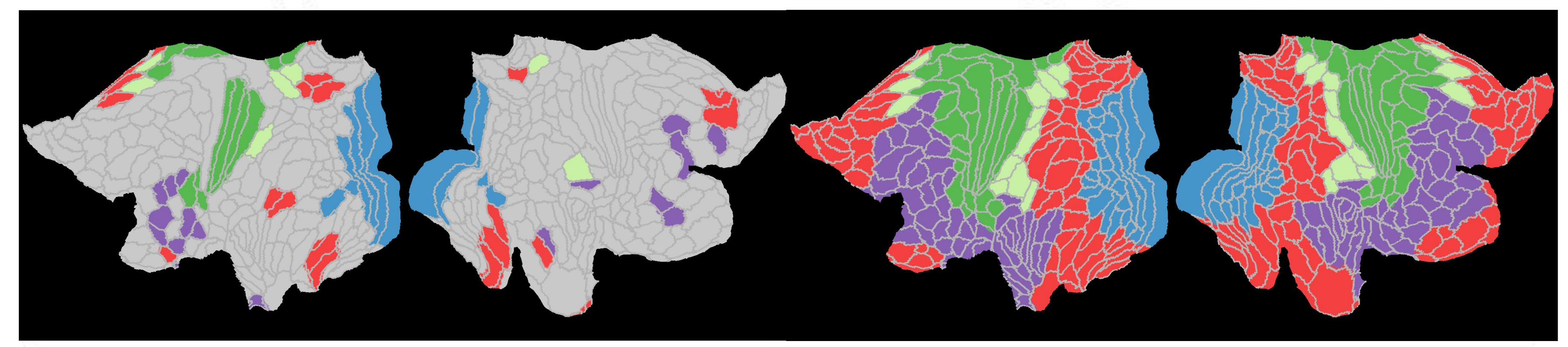



## Application: Functional Bain Connectivity

- psFGGM is used to reconstruct the functional brain connectivity structure of left and right-hand taks using functional magnetic resonance imaging data from the Human Connectome Project.



(a) Left-hand task (b) Right-hand task



(c) Activated ROIs common to both tasks (d) ROI task activation map Glasser et al. (2016)

Figure 4: *psFGGM estimated functionally connected cortical ROIs for the left- and right-hand motor tasks. Each sub-figure shows a flat brain map of the left and right hemispheres (in that order). ROIs having a positive degree of connectivity in each estimated graph are colored based on their functionality Glasser et al. (2016): visual (blue), motor (green), mixed motor (light green), mixed other (red) and other (purple).*

- **Uniqueness and Optimality:** Maximum variance explained by truncated FPCA of covariance operator.
- **Well-defined conditional covariance operator:** It allows for infinite dimensional basis expansion.
- **Consistency:** fully observed functional data and α=1
- **Doesn't saturate:** psFGGM can accommodate high number functional basis in the KL expansion.