Multilevel hybrid principal components analysis for region-referenced functional EEG data

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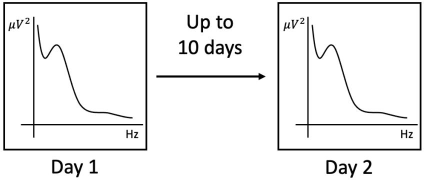
Application to Autism Spectrum Disorder (ASD)

- ASD: developmental disorder that affects communication and behavior
- Resting state: Feasibility study of Autism Biomarkers Consortium for Clinical Trials (ABC-CT) (McPartland et al. 2020; Levin et al. 2020)
  - Goal: study the day-to-day test-retest reliability of power spectral density (PSD)

Resting state EEG: Day-to-day test-retest reliability of PSD

- Study cohort: 47 children aged 5-11 years old (25 TD, 22 ASD)



  - Multilevel: Participants were shown screensaver-like videos on two separate days, a median of 6 days apart
  - Region-referenced: 18 electrodes
  - Functional: PSD

Multilevel region-referenced functional EEG data

- Generated data viewed as functional objects collected across the scalp across varying experimental conditions within a single longitudinal visit or across multiple visits

- Common analysis of EEG reduces the data complexity by collapsing one of the dimensions
  - Functional: average power within a specified frequency band
  - Regional: analysis in pre-determined scalp region (or a scalp average)

Current methods for high-dimensional functional data

- Hybrid PCA (HPCA) for region-referenced EEG data: uses the concept of weak separability for dimension reduction along regional and functional dimensions (Scheffler et al. 2020)
  - Weak separability (weaker then strong seperability): assumes the direction of variation along one of the dimensions stays constant across slices of the other dimension
  - Uses both vector and functional PCA

- Multilevel FPCA (M-FPCA) for multilevel functional data: functional ANOVA model (Di et al. 2009)
  - Decomposes total variation in functional data into between- and within-subjects variation
  - Assumes repetitions are exchangeable

M-HPCA algorithm for multilevel region-referenced functional EEG data

- Borrows ideas from HPCA and M-FPCA
- Decomposes total variation into between- ($K_{d,B}$) and within-subjects ($K_{d,W}$) variation
- Utilizes weak seperability on $K_{d,B}$ and $K_{d,W}$ for dimension reduction via product components
- Involves only one-dimensional PCA and FPCA (along regional and functional dimensions)

Proposed M-HPCA Algorithm

- Scores and variance components targeted within a mixed effects modeling framework
- **Major computational challenge:** Standard packages fail to scale up to the size of data considered
- M-HPCA addresses the computational challenge by coupling representation of the high-dimensional covariance matrices as weighted sums of lower dimensional building blocks, under the weak separability assumption, with an efficient minorization-maximization (MM) algorithm

Model

- $Y_{dij}(r,t)$ denotes the functional observation for subject i, $i = 1, \ldots, n_d$, from group d, $d = 1, \ldots, D$, for repetition j, $j = 1, \ldots, J$, in region r, $r = 1, \ldots, R$, at time t, $t \in \mathcal{T}$ and is modeled as

$$Y_{dij}(r,t) = \mu(t) + \eta_{dj}(r,t) + Z_{di}(r,t) + W_{dij}(r,t) + \epsilon_{dij}(r,t)$$

  - $\mu(t)$: overall mean function
  - $\eta_{dj}(r,t)$: group-region-repetition-specific shift from the overall mean
  - $Z_{di}(r,t)$: subject-region-specific deviation
  - $W_{dij}(r,t)$: subject-region-repetition deviation
  - $\epsilon_{dij}(r,t)$: independent measurement error

Covariances

- Total covariance:

$$K_{d,\text{Total}}\{(r,t),(r',t')\} = \text{cov}\{Y_{dij}(r,t), Y_{dij}(r',t')\}$$

- Between-subject covariance:

$$K_{d,B}\{(r,t),(r',t')\} = \text{cov}\{Y_{dij_1}(r,t), Y_{dij_2}(r',t')\} = \text{cov}\{Z_{di}(r,t), Z_{di}(r',t')\}$$

- Within-subject covariance

$$\begin{aligned} K_{d,W}\{(r,t),(r',t')\} &:= K_{d,\text{Total}}\{(r,t),(r',t')\} - K_{d,B}\{(r,t),(r',t')\} \\ &= \text{cov}\{W_{dij}(r,t), W_{dij}(r',t')\} \end{aligned}$$

Marginal covariances

- Functional marginal between and within covariance surfaces

$$\Sigma_{d,\mathcal{T},B}(t,t') = \sum_{r=1}^{R} K_{d,B}\{(r,t),(r,t')\} = \sum_{\ell=1}^{\infty} \tau_{d\ell,\mathcal{T}}^{(1)} \phi_{d\ell}^{(1)}(t)\phi_{d\ell}^{(1)}(t')$$

$$\Sigma_{d,\mathcal{T},W}(t,t') = \sum_{r=1}^{R} K_{d,W}\{(r,t),(r,t')\} = \sum_{m=1}^{\infty} \tau_{dm,\mathcal{T}}^{(2)} \phi_{dm}^{(2)}(t)\phi_{dm}^{(2)}(t'),$$

- Regional marginal between and within covariance matrices

$$(\Sigma_{d,\mathcal{R},B})_{r,r'} = \int_{\mathcal{T}} K_{d,B}\{(r,t),(r',t)\}dt = \sum_{k=1}^{R} \tau_{dk,\mathcal{R}}^{(1)} \mathrm{v}_{dk}^{(1)}(r)\mathrm{v}_{dk}^{(1)}(r')$$

$$(\Sigma_{d,\mathcal{R},W})_{r,r'} = \int_{\mathcal{T}} K_{d,W}\{(r,t),(r',t)\}dt = \sum_{p=1}^{R} \tau_{dp,\mathcal{R}}^{(2)} \mathrm{v}_{dp}^{(2)}(r)\mathrm{v}_{dp}^{(2)}(r'),$$

- $\phi_{d\ell}^{(1)}(t)$ and $\phi_{dm}^{(2)}(t)$ are the level 1 and level 2 eigenfunctions, $\mathrm{v}_{dk}^{(1)}(r)$ and $\mathrm{v}_{dp}^{(2)}(r)$ are the level 1 and level 2 eigenvectors, and $\tau_{d\ell,\mathcal{T}}^{(1)}$, $\tau_{dm,\mathcal{T}}^{(2)}$, $\tau_{dk,\mathcal{R}}^{(1)}$, and $\tau_{dp,\mathcal{R}}^{(2)}$ are the respective eigenvalues

M-HPCA decomposition

- Utilizing the marginal eigenfunctions and eigenvectors

$$\begin{aligned} Y_{dij}(r,t) &= \mu(t) + \eta_{dj}(r,t) + Z_{di}(r,t) + W_{dij}(r,t) + \epsilon_{dij}(r,t) \\ &= \mu(t) + \eta_{dj}(r,t) + \sum_{k=1}^{K}\sum_{\ell=1}^{L} \zeta_{di,k\ell} \mathrm{v}_{dk}^{(1)}(r)\phi_{d\ell}^{(1)}(t) \\ &\quad + \sum_{p=1}^{P}\sum_{m=1}^{M} \xi_{dij,pm} \mathrm{v}_{dp}^{(2)}(r)\phi_{dm}^{(2)}(t) + \epsilon_{dij}(r,t) \end{aligned}$$

- $\zeta_{di,k\ell} = \langle Z_{di}(r,t), \mathrm{v}_{dk}^{(1)}(r)\phi_{d\ell}^{(1)}(t)\rangle$, $\xi_{dij,pm} = \langle W_{dij}(r,t), \mathrm{v}_{dp}^{(2)}(r)\phi_{dm}^{(2)}(t)\rangle$
- Number of product components: level 1 ($G = KL$), level 2 ($H = PM$)
- $\mathrm{var}(\zeta_{dig}) = \lambda_{dg}^{(1)}$, $\mathrm{var}(\xi_{dijh}) = \lambda_{dh}^{(2)}$

Mixed effects modeling to target scores + variance components

$$Y_{di} = Z_{di}\boldsymbol{\zeta}_{di} + W_{di}\boldsymbol{\xi}_{di} + \boldsymbol{\epsilon}_{di} \text{ for } i = 1, \ldots, n_d$$

$$\boldsymbol{\zeta}_{di} \sim \text{MVN}\left(0, \boldsymbol{\Lambda}_d^{(1)}\right),\ \boldsymbol{\xi}_{di} \sim \text{MVN}\left(0, I_{J_i} \otimes \boldsymbol{\Lambda}_d^{(2)}\right),\ \boldsymbol{\epsilon}_{di} \sim \text{MVN}\left(0, \sigma_d^2 I_{TRJ_i}\right)$$

- $Y_{di} \sim \text{MVN}(\mathbf{0}, \boldsymbol{\Sigma}_{di})$, where $\boldsymbol{\Sigma}_{di} = Z_{di}\boldsymbol{\Lambda}_d^{(1)} Z_{di}^{\mathrm{T}} + W_{di}\left(I_{J_i} \otimes \boldsymbol{\Lambda}_d^{(2)}\right) W_{di}^{\mathrm{T}} + \sigma_d^2 I_{TRJ_i}$
- Log-likelihood: $\ell_d\left(\boldsymbol{\Lambda}_d^{(1)}, \boldsymbol{\Lambda}_d^{(2)}, \sigma_d^2\right) = -\frac{1}{2}\sum_{i=1}^{n_d} \log\det \boldsymbol{\Sigma}_{di} + Y_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-1}Y_{di}$
- Major computational challenge: $\boldsymbol{\Sigma}_{di}$ is $TRJ_i \times TRJ_i$
- ABC-CT feasibility-study: $T = 108$, $R = 18$, $J = 2 \Rightarrow TRJ > 3800$

MM Algorithm

- Minorizing function of log-likelihood:

$$\sum_{i=1}^{n_d} f_{di}\left(\boldsymbol{\Lambda}_d^{(1)}, \boldsymbol{\Lambda}_d^{(2)}, \sigma_d^2 \middle| \boldsymbol{\Lambda}_d^{(1)(c)}, \boldsymbol{\Lambda}_d^{(2)(c)}, \sigma_d^{2(c)}\right)$$
$$= \sum_{i=1}^{n_d} -\frac{1}{2}\Bigg[\mathrm{tr}\left(Z_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-1(c)}Z_{di}\boldsymbol{\Lambda}_d^{(1)(c)}\right) + \boldsymbol{\zeta}_{di}^{(c)\mathrm{T}}\boldsymbol{\Lambda}_d^{-(1)(c)}\boldsymbol{\zeta}_{di}^{(c)}$$
$$+ \mathrm{tr}\left\{W_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-1(c)}W_{di}\left(I_{J_i}\otimes\Lambda_d^{(2)(c)}\right)\right\} + \boldsymbol{\xi}_{di}^{(c)\mathrm{T}}\left(I_{J_i}\otimes\boldsymbol{\Lambda}_d^{-1(2)(c)}\right)\xi_{di}^{(c)}$$
$$+ \mathrm{tr}\left(\sigma_d^2\boldsymbol{\Sigma}_{di}^{-1(c)}\right) + \frac{\sigma_d^{4(c)}}{\sigma_d^2}Y_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-2(c)}Y_{di}\Bigg] + q^{(c)}$$

MM Algorithm

- Minorizing function of log-likelihood:

$$\sum_{i=1}^{n_d} f_{di}\left(\mathbf{\Lambda}_d^{(1)}, \mathbf{\Lambda}_d^{(2)}, \sigma_d^2 \middle| \mathbf{\Lambda}_d^{(1)(c)}, \mathbf{\Lambda}_d^{(2)(c)}, \sigma_d^{2(c)}\right)$$

$$= \sum_{i=1}^{n_d} -\frac{1}{2}\Big[\mathrm{tr}\left(Z_{di}^{\mathrm{T}} \mathbf{\Sigma}_{di}^{-1(c)} Z_{di} \mathbf{\Lambda}_d^{(1)(c)}\right) + \zeta_{di}^{(c)\mathrm{T}} \mathbf{\Lambda}_d^{-(1)(c)} \zeta_{di}^{(c)}$$

$$+ \mathrm{tr}\left\{ W_{di}^{\mathrm{T}} \mathbf{\Sigma}_{di}^{-1(c)} W_{di} \left(I_{J_i} \otimes \Lambda_d^{(2)(c)} \right) \right\} + \xi_{di}^{(c)\mathrm{T}} \left(I_{J_i} \otimes \mathbf{\Lambda}_d^{-1(2)(c)} \right) \xi_{di}^{(c)}$$

$$+ \mathrm{tr}\left(\sigma_d^2 \mathbf{\Sigma}_{di}^{-1(c)} \right) + \frac{\sigma_d^{4(c)}}{\sigma_d^2} Y_{di}^{\mathrm{T}} \mathbf{\Sigma}_{di}^{-2(c)} Y_{di} \Big] + q^{(c)}$$

Level 1 variance components

MM Algorithm

- Minorizing function of log-likelihood:

$$\sum_{i=1}^{n_d} f_{di}\left(\mathbf{\Lambda}_d^{(1)}, \mathbf{\Lambda}_d^{(2)}, \sigma_d^2 \middle| \mathbf{\Lambda}_d^{(1)(c)}, \mathbf{\Lambda}_d^{(2)(c)}, \sigma_d^{2(c)}\right)$$

$$= \sum_{i=1}^{n_d} -\frac{1}{2}\Big[\mathrm{tr}\left(Z_{di}^{\mathrm{T}} \mathbf{\Sigma}_{di}^{-1(c)} Z_{di} \mathbf{\Lambda}_d^{(1)(c)}\right) + \boldsymbol{\zeta}_{di}^{(c)\mathrm{T}} \mathbf{\Lambda}_d^{-(1)(c)} \boldsymbol{\zeta}_{di}^{(c)}$$

Level 2 variance components

$$+ \mathrm{tr}\left\{W_{di}^{\mathrm{T}} \mathbf{\Sigma}_{di}^{-1(c)} W_{di}\left(I_{J_i} \otimes \Lambda_d^{(2)(c)}\right)\right\} + \boldsymbol{\xi}_{di}^{(c)\mathrm{T}}\left(I_{J_i} \otimes \mathbf{\Lambda}_d^{-1(2)(c)}\right)\xi_{di}^{(c)}$$

$$+ \mathrm{tr}\left(\sigma_d^2 \mathbf{\Sigma}_{di}^{-1(c)}\right) + \frac{\sigma_d^{4(c)}}{\sigma_d^2} Y_{di}^{\mathrm{T}} \mathbf{\Sigma}_{di}^{-2(c)} Y_{di}\Big] + q^{(c)}$$

MM Algorithm

- Minorizing function of log-likelihood:

$$\sum_{i=1}^{n_d} f_{di}\left(\boldsymbol{\Lambda}_d^{(1)}, \boldsymbol{\Lambda}_d^{(2)}, \sigma_d^2 \middle| \boldsymbol{\Lambda}_d^{(1)(c)}, \boldsymbol{\Lambda}_d^{(2)(c)}, \sigma_d^{2(c)}\right)$$

$$= \sum_{i=1}^{n_d} -\frac{1}{2}\Big[\mathrm{tr}\left(Z_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-1(c)}Z_{di}\boldsymbol{\Lambda}_d^{(1)(c)}\right) + \zeta_{di}^{(c)\mathrm{T}}\boldsymbol{\Lambda}_d^{-(1)(c)}\zeta_{di}^{(c)}$$

$$+ \mathrm{tr}\left\{W_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-1(c)}W_{di}\left(I_{J_i} \otimes \Lambda_d^{(2)(c)}\right)\right\} + \boldsymbol{\xi}_{di}^{(c)\mathrm{T}}\left(I_{J_i} \otimes \boldsymbol{\Lambda}_d^{-1(2)(c)}\right)\xi_{di}^{(c)}$$

$$+ \mathrm{tr}\left(\sigma_d^2\boldsymbol{\Sigma}_{di}^{-1(c)}\right) + \frac{\sigma_d^{4(c)}}{\sigma_d^2}Y_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-2(c)}Y_{di}\Big] + q^{(c)}$$

Measurement error variance component

MM Algorithm

- Minorizing function of log-likelihood:

$$\sum_{i=1}^{n_d} f_{di}\left(\boldsymbol{\Lambda}_d^{(1)}, \boldsymbol{\Lambda}_d^{(2)}, \sigma_d^2 \middle| \boldsymbol{\Lambda}_d^{(1)(c)}, \boldsymbol{\Lambda}_d^{(2)(c)}, \sigma_d^{2(c)}\right)$$

$$= \sum_{i=1}^{n_d} -\frac{1}{2}\Bigg[\mathrm{tr}\left(Z_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-1(c)}Z_{di}\boldsymbol{\Lambda}_d^{(1)(c)}\right) + \zeta_{di}^{(c)\mathrm{T}}\boldsymbol{\Lambda}_d^{-(1)(c)}\zeta_{di}^{(c)}$$

$$+ \mathrm{tr}\left\{W_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-1(c)}W_{di}\left(I_{J_i}\otimes\Lambda_d^{(2)(c)}\right)\right\} + \boldsymbol{\xi}_{di}^{(c)\mathrm{T}}\left(I_{J_i}\otimes\boldsymbol{\Lambda}_d^{-1(2)(c)}\right)\xi_{di}^{(c)}$$

$$+ \mathrm{tr}\left(\sigma_d^2\boldsymbol{\Sigma}_{di}^{-1(c)}\right) + \frac{\sigma_d^{4(c)}}{\sigma_d^2}Y_{di}^{\mathrm{T}}\boldsymbol{\Sigma}_{di}^{-2(c)}Y_{di}\Bigg] + q^{(c)}$$

- Variance components separated $\Rightarrow$ derivatives are easy!

MM algorithm and computational savings

- Minorization function is much easier to maximize with respect to the variance components, due to the additive structure
- Taking advantage of weak separability, the high-dimensional covariance matrices are represented as weighted sums of lower dimensional building blocks
- Instead of inverting $TRJ_i \times TRJ_i$ covariance matrix, $\boldsymbol{\Sigma}_{di}$, we only invert matrices of size $G \times G$ and $H \times H$

M-HPCA ICC and inference via parametric bootstrap

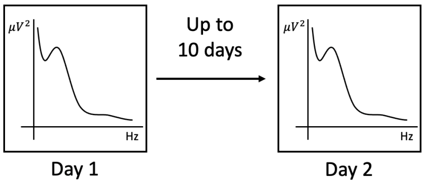
- Compare the variability explained at each level of the data (subject vs. repetition) across the functional and regional dimensions

$$\widehat{\rho}_{dW} = \frac{\sum_{g=1}^{G} \widehat{\lambda}_{dg}^{(1)}}{\sum_{g=1}^{G} \widehat{\lambda}_{dg}^{(1)} + \sum_{h=1}^{H} \widehat{\lambda}_{dh}^{(2)}}$$

- High M-HPCA ICC $\Rightarrow$ more of the total variation is explained by heterogeneity at the subject level, implying repeatedly observed region-referenced functional data are similar within subjects
- Inference via parametric bootstrap is proposed using estimated variance components and the low dimensional representation provided by M-HPCA

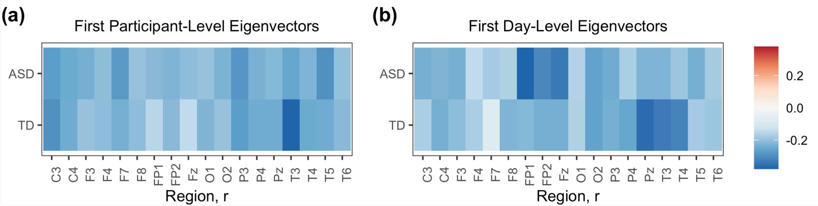
Day-to-day test-retest reliability of PSD

- Study cohort: 47 children aged 5-11 years old (25 TD, 22 ASD)



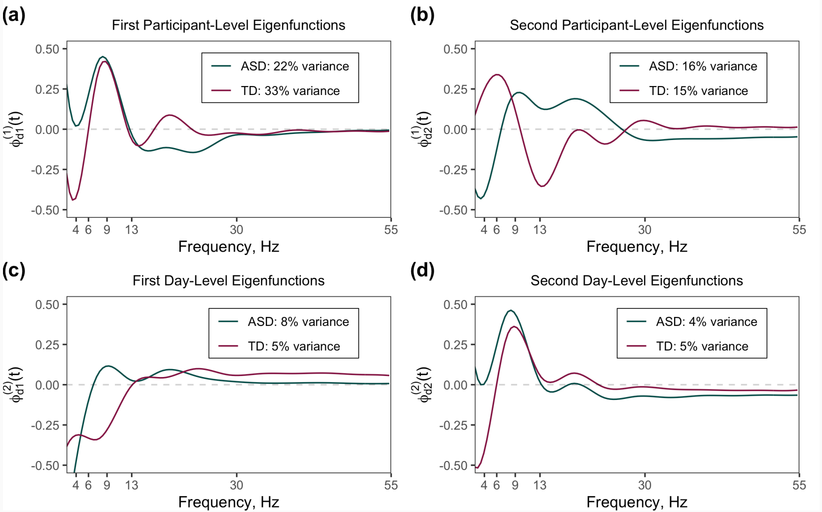
  - Multilevel: Participants were shown screensaver-like videos on two separate days, a median of 6 days apart
  - Region-referenced: 18 electrodes
  - Functional: PSD

Marginal eigenvectors



- Leading eigenvector explains most of the variation across both groups and levels and signals constant variation across the scalp

Marginal eigenfunctions



Marginal eigenfunctions

- Leading participant-level eigenfunctions: most of the variation *across subjects* is observed in the alpha peak amplitude in both groups
- Second leading participant-level eigenfunction signals variation in location of the dominant peak across subjects (TD: low and high alpha, ASD: high alpha to beta)
- Leading day-level eigenfunctions: variation *across days* is in the dominant peak location within alpha to beta bands in ASD, within theta to alpha in TD
- Second leading day-level eigenfunctions signal peak alpha amplitude variation in both groups

M-HPCA ICC

$$\widehat{\rho}_{dW} = \frac{\sum_{g=1}^{G} \widehat{\lambda}_{dg}^{(1)}}{\sum_{g=1}^{G} \widehat{\lambda}_{dg}^{(1)} + \sum_{h=1}^{H} \widehat{\lambda}_{dh}^{(2)}}$$

- Estimated to be 0.673 [95% CI (0.626, 0.793)] for ASD and 0.656 for TD [95% CI (0.639, 0.776)]
- Signals moderate agreement in within subject day-to-day PSD, where most of the variation is explained at the subject level
- Results consistent with findings of Levin et al. (2020) who reported moderate aggreement for scalp averaged PSDs across days within subjects

- M-HPCA models EEG data in its full complexity, including the functional and regional features as well as the repeated observations over experimental conditions or visits
- Both time and the frequency domains are targeted under the umbrella of multilevel region-referenced functional data
- Computationally efficient MM algorithm that is specifically designed to take advantage of the lower dimensional representation provided by M-HPCA
- Major savings in computational time as the number of product components increase: 100 fold savings over lme4 at 16 product components

Thank you!

R package available at github.com/emjcampos/mhpca

Manuscript available at doi/10.1002/sim.9445

References

- Levin AR, Naples AJ, Scheffler AW, et al. Day-to-Day Test-Retest Reliability of EEG Profiles in Children With Autism Spectrum Disorder and Typical Development. Frontiers in Integrative Neuroscience 2020; 14(April): 1–12. doi: 10.3389/fnint.2020.00021

Covariances

- Total covariance:

$$K_{d,\text{Total}}\{(r,t),(r',t')\} = \text{cov}\{Y_{dij}(r,t), Y_{dij}(r',t')\}$$

- Between-subject covariance:

$$K_{d,B}\{(r,t),(r',t')\} = \text{cov}\{Y_{dij_1}(r,t), Y_{dij_2}(r',t')\} = \text{cov}\{Z_{di}(r,t), Z_{di}(r',t')\}$$

- Within-subject covariance

$$\begin{aligned} K_{d,W}\{(r,t),(r',t')\} &:= K_{d,\text{Total}}\{(r,t),(r',t')\} - K_{d,B}\{(r,t),(r',t')\} \\ &= \text{cov}\{W_{dij}(r,t), W_{dij}(r',t')\} \end{aligned}$$

Marginal covariances

- Functional marginal between and within covariance surfaces

$$\Sigma_{d,\mathcal{T},B}(t,t') = \sum_{r=1}^{R} K_{d,B}\{(r,t),(r,t')\} = \sum_{\ell=1}^{\infty} \tau^{(1)}_{d\ell,\mathcal{T}} \phi^{(1)}_{d\ell}(t)\phi^{(1)}_{d\ell}(t')$$

$$\Sigma_{d,\mathcal{T},W}(t,t') = \sum_{r=1}^{R} K_{d,W}\{(r,t),(r,t')\} = \sum_{m=1}^{\infty} \tau^{(2)}_{dm,\mathcal{T}} \phi^{(2)}_{dm}(t)\phi^{(2)}_{dm}(t'),$$

- Regional marginal between and within covariance matrices

$$(\Sigma_{d,\mathcal{R},B})_{r,r'} = \int_{\mathcal{T}} K_{d,B}\{(r,t),(r',t)\}dt = \sum_{k=1}^{R} \tau^{(1)}_{dk,\mathcal{R}} \mathrm{v}^{(1)}_{dk}(r)\mathrm{v}^{(1)}_{dk}(r')$$

$$(\Sigma_{d,\mathcal{R},W})_{r,r'} = \int_{\mathcal{T}} K_{d,W}\{(r,t),(r',t)\}dt = \sum_{p=1}^{R} \tau^{(2)}_{dp,\mathcal{R}} \mathrm{v}^{(2)}_{dp}(r)\mathrm{v}^{(2)}_{dp}(r'),$$

- $\phi^{(1)}_{d\ell}(t)$ and $\phi^{(2)}_{dm}(t)$ are the level 1 and level 2 eigenfunctions, $\mathrm{v}^{(1)}_{dk}(r)$ and $\mathrm{v}^{(2)}_{dp}(r)$ are the level 1 and level 2 eigenvectors, and $\tau^{(1)}_{d\ell,\mathcal{T}}$, $\tau^{(2)}_{dm,\mathcal{T}}$, $\tau^{(1)}_{dk,\mathcal{R}}$, and $\tau^{(2)}_{dp,\mathcal{R}}$ are the respective eigenvalues