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Supporting Information for "Bayesian Functional Covariance Regression"

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1. Web Appendix A: Markov-chain monte carlo sampling algorithm

In this section we give a detailed Markov-Chain Monte Carlo (MCMC) algorithm to sample from the posterior. Let N be the number of independent functional responses and assume all response functions are observed on a common grid $T = \{t_1, \ldots, t_n\}$. Let B be an $n \times p$ matrix with $B_{ij} = b_j(t_i)$. Let X be an $N \times r(d_1)$ matrix with row i equal to $\boldsymbol{b}^x(\boldsymbol{x}_i)$. Let Y be an $N \times n$ matrix with $Y_{ij} = y_i(t_j)$, so that each row represents one discretized functional response. Let Γ_j be an $N \times N$ diagonal matrix with rth diagonal element equal to η_{rj} for $j = 1, \ldots, k$.

(1) Update β:

Let $\Omega_r = \tau_{1xr}\tilde{K}_r + \tau_{1tr}\tilde{K}$ if $p_r > 1$. Otherwise set $\Omega_r = \tau_{1tr}K$. Construct

$\Omega = \text{blkdiag}(\Omega_1, \ldots, \Omega_R)$.

Let $C = \sigma^{-2}X^\top X \otimes B^\top B + \Omega$

Let $A = \sigma^{-2}\text{vec}[\{B^\top Y^\top - B^\top B(\sum_{j=1}^k \Lambda_j X^\top \Gamma_j)\}X]$

Sample $\text{vec}(\beta) \sim N(C^{-1}A, C^{-1})$

(2) Update Λ_j:

Let $\Omega_r = \tau_{2xr}\tilde{K}_r + \tau_{2tr}\tilde{K} + \tau^*_{rj}\phi_{rj}$ if $p_r > 1$. Otherwise set $\Omega_r = \tau_{2tr}K + \tau^*_{rj}\phi_{rj}$.

Construct $\Omega = \text{blkdiag}(\Omega_1, \ldots, \Omega_R)$

Let $C = \sigma^{-2}X^\top \Gamma_j^2 X \otimes B^\top B + \Omega$

Let $A = \sigma^{-2}\text{vec}[\{B^\top Y^\top - B^\top B(\beta + \sum_{j' \neq j} \Lambda_{j'} X^\top \Gamma_{j'})\}\Gamma_j X]$

Sample $\Lambda_j \sim N(C^{-1}A, C^{-1})$

(3) Update η_{ij}:

Let $\boldsymbol{\eta}_i = (\eta_{i1}, \ldots, \eta_{ik})$.

Let $\ddot{X}_i$ be a $p \times k$ matrix with column j equal to $\Lambda_j \boldsymbol{b}^x(\boldsymbol{x}_i)$.

Let $C = \sigma^{-2}\ddot{X}_i^\top B^\top B \ddot{X}_i + I_k$, where I_k is the $k \times k$ identity matrix.

Let $A = \sigma^{-2}\ddot{X}_i^\top\{B^\top Y_{i\cdot} - B^\top B\beta \boldsymbol{b}^x(\boldsymbol{x}_i)\}$

Sample $\boldsymbol{\eta}_i \sim N(C^{-1}A, C^{-1})$

(4) Update σ^2:

Let $A = Y^\top - B\beta X^\top + \sum_{j=1}^k B\Lambda_j X^\top \Gamma_j$

Sample $\sigma^{-2} \sim \text{Gamma}(Nn/2 + a_\epsilon, A \odot A/2 + b_\epsilon)$, where $\odot$ denotes element-wise multiplication.

(5) Update τ_{1tr}, τ_{1xr}, τ_{2tr}, τ_{2xr}:

Sample $\tau_{1tr} \sim \text{Gamma}\{\text{rank}(\tilde{K})/2 - 0.5, \text{vec}(\beta_r)^\top \tilde{K}\text{vec}(\beta_r)/2\}$

Sample $\tau_{1xr} \sim \text{Gamma}\{\text{rank}(\tilde{K}_r)/2 - 0.5, \text{vec}(\beta_r^\top)\tilde{K}_r\text{vec}(\beta_r)/2\}$ (if $p_r > 1$)

Sample $\tau_{2trj} \sim \text{Gamma}\{\text{rank}(\tilde{K})/2 - 0.5, \text{vec}(\Lambda_{rj})^\top \tilde{K}\text{vec}(\Lambda_{rj})/2\}$

Sample $\tau_{2xrj} \sim \text{Gamma}\{\text{rank}(\tilde{K}_r)/2 - 0.5, \text{vec}(\Lambda_{rj}^\top)\tilde{K}_r\text{vec}(\Lambda_{rj})/2\}$ (if $p_r > 1$)

(6) Update ϕ_{rj}:

Let ϕ_{irj} denote the ith diagonal element of ϕ_{rj}.

Let λ_{irj} be the ith element of $\text{vec}(\Lambda_{rj})$.

Sample $\phi_{irj} \sim \text{Gamma}(a_\phi + 0.5, \tau_{rj}^*\lambda_{irj}^2/2 + b_\phi)$

(7) Update δ_{r1}:

Let $A = \text{vec}(\Lambda_{r1}^\top)\phi_{r1}\text{vec}(\Lambda_{r1})$

Let $B = \sum_{j=2}^k \tau_{rj}^*\text{vec}(\Lambda_{rj})^\top\phi_{rj}\text{vec}(\Lambda_{rj})$

Sample $\delta_{r1} \sim \text{Gamma}\{kp_r p/2 + a_{r0}, (A+B)/2 + 1\}$

(8) Update δ_{rj}:

Let $A = \sum_{j'=1}^k \tau_{rj'}^{*(j)}\text{vec}(\Lambda_{rj'})^\top\phi_{rj'}\text{vec}(\Lambda_{rj})$, where $\tau_{rj'}^{*(j)} = \tau_{rj'}^*$ if $j \neq j'$ and 1 otherwise.

Sample $\delta_{rj'} \sim \text{Gamma}\{p_r p(k - j' + 1)/2 + a_{r1}, A/2 + 1\}$

(9) Update a_{r0}:

Let $\text{Gamma}^*(x, a, b)$ denote the Gamma density evaluated at x with shape a and rate b.

Let $\phi(x)$ denote the standard normal cumulative distribution function evaluated at x.

Sample candidate $a^*_{r0} \sim N(a_{r0}, 1)$ until $a^*_{r0} > 0$.

Compute $A = \dfrac{\text{Gamma}^*(\delta_{r1}, a^*_{r0}, 1) \cdot \text{Gamma}^*(a^*_{r0}, 2, 1) \cdot \phi(a_{r0})}{\text{Gamma}^*(\delta_{r1}, a_{r0}, 1) \cdot \text{Gamma}^*(a_{r0}, 2, 1) \cdot \phi(a^*_{r0})}$

Sample $U \sim \text{Unif}(0, 1)$

If $U \leqslant A$, accept candidate a^*_{r0}.

(10) Update a_{r1}:

Let $\delta^*_{r2} = \prod_{j=2}^{k} \delta_{rj}$

Let $\text{Gamma}^*(x, a, b)$ denote the Gamma density evaluated at x with shape a and rate b.

Let $\phi(x)$ denote the standard normal cumulative distribution function evaluated at x.

Sample candidate $a^*_{r1} \sim N(a_{r1}, 1)$ until $a^*_{r1} > 0$.

Compute $A = \dfrac{\text{Gamma}^*(\delta^*_{r2}, a^*_{r1}, 1) \cdot \text{Gamma}^*(a^*_{r1}, 2, 1) \cdot \phi(a_{r1})}{\text{Gamma}^*(\delta^*_{r2}, a_{r1}, 1) \cdot \text{Gamma}^*(a_{r1}, 2, 1) \cdot \phi(a^*_{r1})}$

Sample $U \sim \text{Unif}(0, 1)$

If $U \leqslant A$, accept candidate a^*_{r1}.

(11) Update missing values of Y:

Suppose $y_i(t_j)$ is missing.

Let $\mu = \boldsymbol{b}(t_j)\beta\boldsymbol{b}^x(\boldsymbol{x}_i) + \sum_{j=1}^{k} \boldsymbol{b}(t_j)\Lambda_j\boldsymbol{b}^x(\boldsymbol{x}_i)\eta_{ij}$

Sample $y_i(t_j) \sim N(\mu, \sigma^2)$

For convenience, Table contains notation used in the main article and this document of supporting information.

[Table 1 about here.]

2. Web Appendix B: Additional details on posterior inference

3. Web Appendix C: Setting hyperparameters

4. Web Appendix D: Extended simulation results

5. Web Appendix E: Additional details on case studies

Table 1
Notation used in the main article and document of supporting information.

Name	Description	Dimension
$\boldsymbol{x}_i$	Covariate vector for the ith functional response	$d_1 \times 1$
$\boldsymbol{x}_{ir}$	rth group of covariates associated with the ith functional response	
$\boldsymbol{b}^r(\boldsymbol{x}_{ir})$	rth group of covariates expanded into basis functions evaluated at $\boldsymbol{x}_{ir}$	$p_r \times 1$
$\boldsymbol{b}^x(\boldsymbol{x}_i)$	Concatenated $\boldsymbol{b}^r(\boldsymbol{x}_{ir})$, $r = 1, \ldots, R$	$r(d_1) \times 1$
p_r	# of basis functions for rth covariate group expansion	
$r(d_1)$	Total number of covariate basis functions used equal to $\sum_{r=1}^{R} p_r$	
$\boldsymbol{b}(t)$	Basis functions for functional dimension evaluated at t	$p \times 1$
$\mu(t, \boldsymbol{x}_i)$	Covariate-adjusted functional mean equal to $\boldsymbol{b}(t)^\top \beta \boldsymbol{b}^x(\boldsymbol{x}_i)$	
β	Fixed effect parameter matrix equal to	