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Implementation

The file normal.semipar.sim.R simulates data according to the model statement presented below, and normal.semipar.mcmc.R contains the MCMC algorithm for model fitting.

Model statement

Let $\mathbf{y} = (y_1, \dots, y_T)'$ be a vector of observations. Also let \mathbf{X} be a design matrix containing covariates for which inference is desired, and \mathbf{Z} be a design matrix containing some basis expansion. The vectors $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$ are the corresponding 'fixed' and 'random' effects, respectively. Note that $\mathbf{Z}\boldsymbol{\alpha}$ models non-linear patterns or dependence non-parametrically.

$$\begin{array}{lcl} \mathbf{y} & \sim & \mathcal{N}(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\alpha}, \sigma^2\mathbf{I}) \\ \boldsymbol{\beta} & \sim & \mathcal{N}(\mathbf{0}, \sigma^2_{\boldsymbol{\beta}}\mathbf{I}) \\ \boldsymbol{\alpha} & \sim & \mathcal{N}(\mathbf{0}, \sigma^2_{\boldsymbol{\alpha}}\mathbf{I}) \\ \sigma^2 & \sim & \mathrm{IG}(r,q) \end{array}$$

Models of this type are typically fit using a large number of basis vectors, more than necessary to approximate non-linear trends or dependence. Regularization (e.g., a ridge penalty) is subsequently conducted to shrink the coefficients toward 0 where appropriate. Therefore, the parameter σ_{α}^2 must be selected using cross-validation or some model selection criterion. Model-based estimation of σ_{α}^2 , i.e., $\sigma_{\alpha}^2 \sim \mathrm{IG}(r,q)$, results in a mixed effects model similar to that implemented by the function lme in the R package nlme.

Full conditional distributions

Fixed effects (β) :

$$\begin{split} [\boldsymbol{\beta}|\cdot] & \propto & [\mathbf{y}|\boldsymbol{\beta},\boldsymbol{\alpha},\sigma^2][\boldsymbol{\beta}] \\ & \propto & \mathcal{N}(\mathbf{y}|\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\alpha},\sigma^2\mathbf{I})\mathcal{N}(\boldsymbol{\beta}|\mathbf{0},\sigma_{\boldsymbol{\beta}}^2\mathbf{I}) \\ & \propto & \exp\left\{-\frac{1}{2}\left(\mathbf{y} - (\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\alpha})\right)'\left(\sigma^2\mathbf{I}\right)^{-1}\left(\mathbf{y} - (\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\alpha})\right)\right\} \\ & \exp\left\{-\frac{1}{2}\left(\boldsymbol{\beta} - \mathbf{0}\right)'\left(\sigma_{\boldsymbol{\beta}}^2\mathbf{I}\right)^{-1}\left(\boldsymbol{\beta} - \mathbf{0}\right)\right\} \\ & \propto & \exp\left\{-\frac{1}{2}\left((\mathbf{y} - \mathbf{Z}\boldsymbol{\alpha}) - \mathbf{X}\boldsymbol{\beta}\right)'\left(\sigma^2\mathbf{I}\right)^{-1}\left((\mathbf{y} - \mathbf{Z}\boldsymbol{\alpha}) - \mathbf{X}\boldsymbol{\beta}\right)\right\} \\ & \propto & \exp\left\{-\frac{1}{2}\left(\boldsymbol{\beta} - \mathbf{0}\right)'\left(\sigma_{\boldsymbol{\beta}}^2\mathbf{I}\right)^{-1}(\boldsymbol{\beta} - \mathbf{0})\right\} \\ & \propto & \exp\left\{-\frac{1}{2}\left(-2(\mathbf{y} - \mathbf{Z}\boldsymbol{\alpha})'\left(\sigma^2\mathbf{I}\right)^{-1}\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}'\mathbf{X}'\left(\sigma^2\mathbf{I}\right)^{-1}\mathbf{X}\boldsymbol{\beta}\right)\right\} \times \\ & \exp\left\{-\frac{1}{2}\left(\boldsymbol{\beta}'\left(\sigma_{\boldsymbol{\beta}}^2\mathbf{I}\right)^{-1}\boldsymbol{\beta}\right)\right\} \\ & \propto & \exp\left\{-\frac{1}{2}\left(-2\left((\mathbf{y} - \mathbf{Z}\boldsymbol{\alpha})'\left(\sigma^2\mathbf{I}\right)^{-1}\mathbf{X}\right)\boldsymbol{\beta} + \boldsymbol{\beta}'\left(\mathbf{X}'\left(\sigma^2\mathbf{I}\right)^{-1}\mathbf{X} + \left(\sigma_{\boldsymbol{\beta}}^2\mathbf{I}\right)^{-1}\right)\boldsymbol{\beta}\right)\right\} \times \\ & = & \mathcal{N}(\mathbf{A}^{-1}\mathbf{b}, \mathbf{A}^{-1}) \end{split}$$

where
$$\mathbf{A} = (\mathbf{y} - \mathbf{Z}\boldsymbol{\alpha})' (\sigma^2 \mathbf{I})^{-1} \mathbf{X}$$
 and $\mathbf{b}' = \mathbf{X}' (\sigma^2 \mathbf{I})^{-1} \mathbf{X} + (\sigma_{\beta}^2 \mathbf{I})^{-1}$.

Random effects (α) :

$$\begin{aligned} [\boldsymbol{\alpha}|\cdot] & \propto & [\mathbf{y}|\boldsymbol{\beta}, \boldsymbol{\alpha}, \sigma^2][\boldsymbol{\alpha}] \\ & \propto & \mathcal{N}(\mathbf{y}|\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\alpha}, \sigma^2\mathbf{I})\mathcal{N}(\boldsymbol{\alpha}|\mathbf{0}, \sigma_{\alpha}^2\mathbf{I}) \\ & = & \mathcal{N}(\mathbf{A}^{-1}\mathbf{b}, \mathbf{A}^{-1}) \end{aligned}$$

where
$$\mathbf{A} = \mathbf{Z}' \left(\sigma^2 \mathbf{I}\right)^{-1} \mathbf{Z} + \left(\sigma_{\alpha}^2 \mathbf{I}\right)^{-1}$$
 and $\mathbf{b}' = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \left(\sigma^2 \mathbf{I}\right)^{-1} \mathbf{Z}$.

Observation error (σ^2) :

$$\begin{split} & [\sigma^2|\cdot] \quad \propto \quad [\mathbf{y}|\boldsymbol{\beta}, \boldsymbol{\alpha}, \sigma^2][\sigma^2] \\ & \propto \quad \mathcal{N}(\mathbf{y}|\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\alpha}, \sigma^2\mathbf{I})\mathrm{IG}(r,q) \\ & \propto \quad |\sigma^2\mathbf{I}|^{-1/2}\exp\left\{-\frac{1}{2}\left((\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\alpha})'\left(\sigma^2\mathbf{I}\right)^{-1}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\alpha})\right)\right\} \times \\ & \quad \left(\sigma^2\right)^{-(q+1)}\exp\left\{-\frac{1}{r\sigma^2}\right\} \\ & \propto \quad \left(\sigma^2\right)^{-T/2}\exp\left\{-\frac{1}{2\sigma^2}\left((\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\alpha})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\alpha})\right)\right\} \\ & \quad \left(\sigma^2\right)^{-(q+1)}\exp\left\{-\frac{1}{r\sigma^2}\right\} \\ & \propto \quad \left(\sigma^2\right)^{-(T/2+q+1)}\exp\left\{-\frac{1}{\sigma^2}\left(\frac{(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\alpha})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\alpha})}{2} + \frac{1}{r}\right)\right\} \\ & = \quad \mathrm{IG}\left(\left(\frac{(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\alpha})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\alpha})}{2} + \frac{1}{r}\right)^{-1}, \frac{T}{2} + q\right) \end{split}$$