Semiparametric Regression for Normally Distributed Data

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07 August 2015

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 $\mathbf{y} = (y_1, \ldots, y_T)'$ 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.

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

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 $\boldsymbol{\alpha}$ toward 0 where appropriate. Therefore, the parameter σ^2_α must be selected using cross-validation or some model selection criterion. Model-based estimation of σ^2_α , i.e., $\sigma^2_\alpha \sim \text{IG}(r, q)$, results in a mixed effects model similar to that implemented by the function `lme` in the R package `nlme`.

Full conditional distributions

Fixed effects ($\boldsymbol{\beta}$):

$$\begin{aligned}
[\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^2_\beta\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\} \\
&\qquad \exp\left\{-\frac{1}{2}\left(\boldsymbol{\beta} - \mathbf{0}\right)'\left(\sigma^2_\beta\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\} \\
&\qquad \exp\left\{-\frac{1}{2}\left(\boldsymbol{\beta} - \mathbf{0}\right)'\left(\sigma^2_\beta\mathbf{I}\right)^{-1}\left(\boldsymbol{\beta} - \mathbf{0}\right)\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 \\
&\qquad \exp\left\{-\frac{1}{2}\left(\boldsymbol{\beta}'\left(\sigma^2_\beta\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^2_\beta\mathbf{I}\right)^{-1}\right)\boldsymbol{\beta}\right)\right\} \times \\
&= \mathcal{N}(\mathbf{A}^{-1}\mathbf{b}, \mathbf{A}^{-1})
\end{aligned}$$

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

Random effects ($\boldsymbol{\alpha}$):

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

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):

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