Appendix

Appendix

The following paragraphs contain additional information about the **simulation studies** that were covered in chapter **??**.

Section ??: Correlated Predictor Variables

The simulation design was chosen in the following way:

- The design matrix $\mathbf{X} = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 \end{pmatrix}$ is simulated from a three dimensional normal distribution $\mathcal{N}_3\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$ with mean vector $\boldsymbol{\mu} = \begin{pmatrix} -5 & 2 & 0 \end{pmatrix}^T$ and covariance matrix $\begin{pmatrix} 1 & \rho & \rho \\ \rho & 3 & \rho \\ \rho & \rho & 5 \end{pmatrix}$. Hence, the dependence among the regressors is fully determined by the parameter ρ.

- The design matrix $\mathbf{Z} = \begin{pmatrix} \mathbf{z}_1 & \mathbf{z}_2 \end{pmatrix}$ consists of linear combinations of the regressors $\mathbf{x}_1$ up to $\mathbf{x}_3$, more specifically $\mathbf{z}_1 = 0.8 \cdot \mathbf{x}_1 + 0.2 \cdot \mathbf{x}_2$ and $\mathbf{z}_2 = \mathbf{x}_2 - 0.5 \cdot \mathbf{x}_3$. In both design matrices intercept columns are added for estimation purposes.

- The true coefficient vectors are given by $\boldsymbol{\beta} = \begin{pmatrix} \beta_0 & \beta_1 & \beta_2 & \beta_3 \end{pmatrix}^T = \begin{pmatrix} 0 & 3 & -1 & 1 \end{pmatrix}^T$ and $\boldsymbol{\gamma} = \begin{pmatrix} \gamma_0 & \gamma_1 & \gamma_2 \end{pmatrix}^T = \begin{pmatrix} 0 & 2 & 0 \end{pmatrix}^T$.

- The outcome variable $\mathbf{y}$ is generated according to the correctly specified location-scale model $y_i \overset{iid}{\sim} \mathcal{N}\left(\mathbf{x}_i^T \boldsymbol{\beta}, \exp\left(\mathbf{z}_i^T \boldsymbol{\gamma}\right)^2\right)$ for $i = 1, \ldots, n$ with sample size $n = 50$. Before data generation all columns in $\mathbf{X}$ and $\mathbf{Z}$ are standardized, i.e. mean-centered around 0 and scaled to unit variance.

- Three different values were chosen for $\rho \in \{0, -0.5, 0.9\}$ to compare the 'nice' case of uncorrelated predictors with the performance for negative and positive dependence. For each covariance structure the three models `mcmc_ridge()`, `mcmc()` and `lmls()` are fitted to the standardized covariates, where each Posterior Mean estimate from both of the Markov Chain Monte Carlo samplers is based on 10.000 samples.

Section ??: Sample Size

Section ??: Redundant Covariates

We again state the conditions that the simulation study is based on:

- The design matrix $\mathbf{X} = \begin{pmatrix} \mathbf{1}_n & \mathbf{x}_1 & \cdots & \mathbf{x}_{20} \end{pmatrix}$ consists of one intercept column plus 10 *pairs* of successive regressors, starting with the pair $(\mathbf{x}_1, \mathbf{x}_2)$. Each pair $(\mathbf{x}_i, \mathbf{x}_{i+1})$ for $i \in \{1, 3, \ldots, 19\}$ is (independently from all remaining pairs) drawn from a bivariate normal distribution with mean vector $\boldsymbol{\mu} = \begin{pmatrix} 0 & 0 \end{pmatrix}^T$ and correlation matrix $\begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$.

- The design matrix $\mathbf{Z} = \begin{pmatrix} \mathbf{1}_n & \mathbf{x}_1 & \mathbf{x}_3 \end{pmatrix}$ is of minor interest in this case and consists of an intercept column plus two uncorrelated columns chosen from $\mathbf{X}$.

- The true coefficients of $\boldsymbol{\beta}$ are determined by the pattern $\beta_i = 0$, if i is even and $\beta_i = 1$, if i is odd. Thus, all covariates with even subscript are redundant, whereas those with odd subscript contribute to

y. The true $\boldsymbol{\gamma}$, again of minor interest here, is given by $\boldsymbol{\gamma} = \begin{pmatrix} 0 & 1 & 1 \end{pmatrix}^T$.

- The outcome variable **y** is generated according to the correctly specified location-scale model $y_i \overset{iid}{\sim} \mathcal{N}\left(\mathbf{x}_i^T\boldsymbol{\beta}, \exp\left(\mathbf{z}_i^T\boldsymbol{\gamma}\right)^2\right)$ for $i = 1, \ldots, n$, where the covariates are used on their original scale.

- The sample size $n = 50$ is deliberately chosen small compared to the number of regressors. Before fitting each of the three models, all columns of $\mathbf{X}$ except the intercept column is standardized to zero mean and unit variance. Both of the Bayesian models generate 10.000 values for each coefficient.

Section ??: Challenging the Model Assumptions

The data for this simulation study is generated by the following conventions:

- The design matrix $\mathbf{X} = \begin{pmatrix} \mathbf{1}_n & \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \mathbf{x}_4 \end{pmatrix}$ contains four independently sampled regressor variables plus one intercept column:

  - $\mathbf{x}_1 \overset{iid}{\sim} \mathcal{N}(5, 16)$,
  - $\mathbf{x}_2 \overset{iid}{\sim} \mathrm{Exp}(5)$,
  - $\mathbf{x}_3 \overset{iid}{\sim} \mathcal{U}([-2,\ 12])$,
  - $\mathbf{x}_4 \overset{iid}{\sim} \mathrm{Ber}(0.3)$.

- The design matrix $\mathbf{Z} = \begin{pmatrix} \mathbf{1}_n & \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{z}_3 \end{pmatrix}$ contains the additional regressor variable $\mathbf{z}_3 \overset{iid}{\sim} t_{10}$, which is independently sampled from all other columns.

- The true coefficient vectors are given by $\boldsymbol{\beta} = \begin{pmatrix} \beta_0 & \beta_1 & \beta_2 & \beta_3 & \beta_4 \end{pmatrix}^T = \begin{pmatrix} 0 & -3 & -1 & -1 & 2 \end{pmatrix}^T$ and $\boldsymbol{\gamma} = \begin{pmatrix} \gamma_0 & \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}^T = \begin{pmatrix} 0 & 1 & 2 & 3 \end{pmatrix}^T$.

- Three different specifications for the outcome distribution were chosen:

  - $y_i \sim \mathcal{N}\left(\mu, \sigma^2\right)$,
  - $y_i \sim \mu + \left(\sigma \cdot \sqrt{\frac{3}{5}}\right) T$, where $T \sim t_5$,
  - $y_i \sim \mu + \sigma \cdot U$, where $U \sim \mathcal{U}([0,\ 1])$. In all cases, the outcome vectors are generated with the covariates on their original (unstandardized) scale.

- In order to isolate the impact of the different shapes of the three probability distributions from the effect of varying moment structures, the mean $\mu = \mathbf{x}_i^T\boldsymbol{\beta}$ and the variance $\sigma^2 = \exp\left(\mathbf{z}_i^T\boldsymbol{\gamma}\right)^2$ are held constant across the models.

- All three models `mcmc_ridge()`, `mcmc()` and `lmls()` are fitted with standardized covariates. The sample size is set to $n = 50$ and the result of both Bayesian samplers are based on 10.000 simulations.

Section ??: Hyperparameters