

# User's Guide for **norm2**

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## ABSTRACT

The R package **norm2** provides functions for analyzing incomplete multivariate data under a normal model, including likelihood-based parameter estimation, Bayesian posterior simulation, and multiple imputation. This document gives detailed information about **norm2**'s model and procedures, with step-by-step instructions and example analyses using datasets included with the package.

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# 1 Overview

The R package `norm2` provides methods for analyzing numeric data with missing values. These methods are based on the multivariate normal model from which the package name is derived. Although real-world data rarely conform to assumptions of normality, these techniques have proven to be surprisingly useful and may often be adapted to non-normal situations (for example, by transforming variables prior to analysis).

Source code written by the author for a much older version of this package called `norm` was ported to R by Alvaro A. Novo and submitted to the Comprehensive R Archive Network (CRAN), the collection of web servers that disseminates R. The old package is still available on CRAN, but it has major limitations and the author does not recommend its use. The new package offers better syntax, greater numerical stability, improved exception and error handling, and many other enhancements.

- Variables that are completely observed can now be included as unmodeled predictors rather than responses, eliminating unnecessary parameters and making the computations more efficient.
- The two most important functions, `emNorm` and `mcmcNorm`, return objects of new class "`norm`" which can be used as an arguments to other function calls.
- Models may now be specified using a standard formula syntax used in R's linear regression modeling procedure `lm`. Data frames and factors are handled seamlessly.

In Sections 2–4, we present the model used by `norm2` and describe our algorithms for likelihood-based parameter estimation, Bayesian posterior simulation and multiple imputation. Section 5 reviews some general concepts from R that will help new users to understand package functions and documentation. Sections 6–8 illustrate the use of `norm2` functions with three data examples taken from Schafer (1997) which are distributed with the package.

We assume that readers have basic familiarity with the R programming environment. Overviews of R can be found in the manual *An Introduction to R* written by the R Core Team and distributed with the software, in numerous books and articles, and other resources available on the Internet.

## 2 The model

### 2.1 Model for the complete data

The **norm2** model describes an  $n \times r$  data matrix

$$\mathbf{Y} = \begin{bmatrix} \mathbf{y}_1^\top \\ \mathbf{y}_2^\top \\ \vdots \\ \mathbf{y}_n^\top \end{bmatrix} = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1r} \\ y_{21} & y_{22} & \cdots & y_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ y_{n1} & y_{n2} & \cdots & y_{nr} \end{bmatrix},$$

where  $\mathbf{y}_i = (y_{i1}, \dots, y_{ir})^\top$  denotes a vector of responses for unit  $i$ , and the units  $i = 1, \dots, n$  are randomly sampled from a population. Throughout this document, we follow the convention of displaying vectors and matrices in boldface type; all vectors are assumed to be columns; and the superscript “ $\top$ ” denotes a transpose. We allow arbitrary portions of  $\mathbf{Y}$  to be missing, which is why the **norm2** package was created.

In earlier releases of this software, we had assumed that  $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n$  were independent and identically distributed as  $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , where  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_r)^\top$  is a vector of means and  $\boldsymbol{\Sigma}$  is a positive-definite covariance matrix. In that framework, if one wanted to include completely observed covariates in an analysis, they would have to be placed among the columns of  $\mathbf{Y}$ . That approach was sometimes computationally inefficient, because the joint distribution of the covariates became part of the model formulation even if it was not needed, inflating the number of unknown parameters unnecessarily (Schafer, 1997, Sec. 2.6.2). The new **norm2** model still places incomplete variables into the columns of  $\mathbf{Y}$ , but completely observed variables may now be included in a matrix of predictors,

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix},$$

which is not modeled. Responses are related to predictors by a standard multivariate regression,

$$\mathbf{y}_i \mid \mathbf{x}_i \sim N(\boldsymbol{\beta}^\top \mathbf{x}_i, \boldsymbol{\Sigma}), \quad (1)$$

where  $\boldsymbol{\beta}$  is a  $p \times r$  matrix of regression coefficients. This model can also be written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where  $\boldsymbol{\epsilon}$  is an  $n \times r$  matrix distributed as  $\text{vec}(\boldsymbol{\epsilon}) \sim N(\mathbf{0}, \boldsymbol{\Sigma} \otimes \mathbf{I}_n)$ , and  $\mathbf{I}_n$  is the  $n \times n$  identity matrix. In most applications, the first column of  $\mathbf{X}$  will be a constant,  $x_{i1} \equiv 1$ . If  $\mathbf{X}$  consists of a single column  $(1, 1, \dots, 1)^\top$ , then this new model reduces to the old one with  $\boldsymbol{\beta} = \boldsymbol{\mu}^\top$ . If desired, completely observed covariates may also be placed into the columns of  $\mathbf{Y}$ , because a joint normal model for the augmented vector  $(\mathbf{y}_i^\top, \mathbf{x}_i^\top)^\top$  implies a conditional model of the form (1) for  $\mathbf{y}_i$  given  $\mathbf{x}_i$ .

## 2.2 Estimation with complete data

Before describing our missing-data routines, it is helpful to consider how the parameters of this model (1) could be estimated if there were no missing values. Given  $\mathbf{Y}$ , the complete-data loglikelihood function for  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$  is

$$\begin{aligned} l(\boldsymbol{\beta}, \boldsymbol{\Sigma} | \mathbf{Y}, \mathbf{X}) &= -\frac{n}{2} \log |\boldsymbol{\Sigma}| - \frac{1}{2} \sum_{i=1}^n (\mathbf{y}_i - \boldsymbol{\beta}^\top \mathbf{x}_i)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{y}_i - \boldsymbol{\beta}^\top \mathbf{x}_i) \\ &= -\frac{n}{2} \log |\boldsymbol{\Sigma}| - \frac{1}{2} \text{tr} \boldsymbol{\Sigma}^{-1} \left\{ \sum_{i=1}^n (\mathbf{y}_i - \boldsymbol{\beta}^\top \mathbf{x}_i)(\mathbf{y}_i - \boldsymbol{\beta}^\top \mathbf{x}_i)^\top \right\} \\ &= -\frac{n}{2} \log |\boldsymbol{\Sigma}| - \frac{1}{2} \text{tr} \boldsymbol{\Sigma}^{-1} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}). \end{aligned} \quad (2)$$

This loglikelihood is a linear function of the sufficient statistics  $\mathbf{T}_1 = \mathbf{X}^\top \mathbf{Y}$  and  $\mathbf{T}_2 = \mathbf{Y}^\top \mathbf{Y}$ , whose expectations are  $E(\mathbf{T}_1 | \mathbf{X}) = \mathbf{X}^\top \mathbf{X} \boldsymbol{\beta}$  and  $E(\mathbf{T}_2 | \mathbf{X}) = \boldsymbol{\beta}^\top \mathbf{X}^\top \mathbf{X} \boldsymbol{\beta} + n\boldsymbol{\Sigma}$ . Setting the realized values of  $\mathbf{T}_1$  and  $\mathbf{T}_2$  equal to their expectations and solving for  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$  leads immediately to the maximum-likelihood (ML) estimates,

$$\begin{aligned} \hat{\boldsymbol{\beta}} &= (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y} \\ &= (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{T}_1, \end{aligned} \quad (3)$$

$$\begin{aligned} \hat{\boldsymbol{\Sigma}} &= n^{-1} (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \\ &= n^{-1} (\mathbf{T}_2 - \mathbf{T}_1^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{T}_1). \end{aligned} \quad (4)$$

Another useful expression for the complete-data loglikelihood function is

$$\begin{aligned} l(\boldsymbol{\beta}, \boldsymbol{\Sigma} | \mathbf{Y}, \mathbf{X}) &= -\frac{n}{2} \log |\boldsymbol{\Sigma}| - \frac{1}{2} \text{tr} \boldsymbol{\Sigma}^{-1} (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \\ &\quad - \frac{1}{2} \text{vec}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^\top \left[ \boldsymbol{\Sigma} \otimes (\mathbf{X}^\top \mathbf{X})^{-1} \right]^{-1} \text{vec}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}). \end{aligned} \quad (5)$$

## 3 ML estimation with ignorable nonresponse

### 3.1 An EM algorithm

Now suppose that some elements of  $\mathbf{Y}$  are missing at random (MAR) in the sense defined by Rubin (1976). Let  $\mathbf{Y}_!$  and  $\mathbf{Y}_?$  denote the observed and missing parts of  $\mathbf{Y}$ , respectively, and let  $\mathbf{y}_{i!}$  and  $\mathbf{y}_{i?}$  denote the observed and missing parts of  $\mathbf{y}_i$ . Let  $\boldsymbol{\beta}_{i!}$  and  $\boldsymbol{\beta}_{i?}$  denote the submatrices of  $\boldsymbol{\beta}$  corresponding to  $\mathbf{y}_{i!}$  and  $\mathbf{y}_{i?}$ . That is,  $\boldsymbol{\beta}_{i!}$  contains the columns of  $\boldsymbol{\beta}$  for predicting the observed elements of  $\mathbf{y}_i$ , and  $\boldsymbol{\beta}_{i?}$  contains the columns for predicting the missing elements. Similarly, suppose we partition  $\boldsymbol{\Sigma}$  into submatrices corresponding to the observed and missing parts of  $\mathbf{y}_i$ , calling the submatrices  $\boldsymbol{\Sigma}_{i!!}$ ,  $\boldsymbol{\Sigma}_{i!?}$ ,  $\boldsymbol{\Sigma}_{i?!$  and  $\boldsymbol{\Sigma}_{i??}$ .

For example, if the first  $r_1$  elements of  $\mathbf{y}_i$  are observed and the remaining  $r_2 = r - r_1$  elements of  $\mathbf{y}_i$  are missing, then

$$\begin{bmatrix} \mathbf{y}_{i!} \\ \mathbf{y}_{i?} \end{bmatrix} \mid \mathbf{x}_i \sim N \left( [\boldsymbol{\beta}_{i!}, \boldsymbol{\beta}_{i?}]^\top \mathbf{x}_i, \begin{bmatrix} \boldsymbol{\Sigma}_{i!!} & \boldsymbol{\Sigma}_{i!?} \\ \boldsymbol{\Sigma}_{i?!} & \boldsymbol{\Sigma}_{i??} \end{bmatrix} \right),$$

where  $\boldsymbol{\beta}_{i!}$  is  $p \times r_1$ ,  $\boldsymbol{\beta}_{i?}$  is  $p \times r_2$ ,  $\boldsymbol{\Sigma}_{i!!}$  is  $r_1 \times r_1$ ,  $\boldsymbol{\Sigma}_{i!?}$  is  $r_1 \times r_2$ ,  $\boldsymbol{\Sigma}_{i?!}$  is  $r_2 \times r_1$  and  $\boldsymbol{\Sigma}_{i??}$  is  $r_2 \times r_2$ .

The loglikelihood function ignoring the missing-data mechanism is

$$\begin{aligned} l(\boldsymbol{\beta}, \boldsymbol{\Sigma} \mid \mathbf{Y}_1, \mathbf{X}) &= \sum_{i=1}^n \log \left\{ \int |\boldsymbol{\Sigma}|^{-1/2} \exp -\frac{1}{2} (\mathbf{y}_i - \boldsymbol{\beta}^\top \mathbf{x}_i)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{y}_i - \boldsymbol{\beta}^\top \mathbf{x}_i) d\mathbf{y}_{i?} \right\} \\ &= \sum_{i=1}^n \left\{ -\frac{1}{2} \log |\boldsymbol{\Sigma}_{i!!}| - \frac{1}{2} (\mathbf{y}_{i!} - \boldsymbol{\beta}_{i!}^\top \mathbf{x}_i)^\top \boldsymbol{\Sigma}_{i!!}^{-1} (\mathbf{y}_{i!} - \boldsymbol{\beta}_{i!}^\top \mathbf{x}_i) \right\}. \end{aligned} \quad (6)$$

We maximize this function by an extension of the EM algorithm for multivariate normal data described by Schafer (1997), Little and Rubin (2002) and others. In the E-step, we accumulate the expectations of  $\mathbf{T}_1 = \sum_i \mathbf{x}_i \mathbf{y}_i^\top$  and  $\mathbf{T}_2 = \sum_i \mathbf{y}_i \mathbf{y}_i^\top$  with respect to the conditional distribution of  $\mathbf{Y}_?$  given  $\mathbf{Y}_1$ , fixing  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$  equal to their current estimates. In the M-step, we update the estimates by substituting the expected values of  $\mathbf{T}_1$  and  $\mathbf{T}_2$  into (3)–(4). When computing the expectations, we use the formulas

$$\begin{aligned} E(\mathbf{y}_{i!} \mid \mathbf{y}_{i!}) &= \mathbf{y}_{i!}, \\ E(\mathbf{y}_{i?} \mid \mathbf{y}_{i!}) &= \boldsymbol{\beta}_{i?}^\top \mathbf{x}_i + \boldsymbol{\Sigma}_{i?!} \boldsymbol{\Sigma}_{i!!}^{-1} (\mathbf{y}_{i!} - \boldsymbol{\beta}_{i!}^\top \mathbf{x}_i), \\ E(\mathbf{y}_{i!} \mathbf{y}_{i!}^\top \mid \mathbf{y}_{i!}) &= \mathbf{y}_{i!} \mathbf{y}_{i!}^\top, \\ E(\mathbf{y}_{i!} \mathbf{y}_{i?}^\top \mid \mathbf{y}_{i!}) &= \mathbf{y}_{i!} E(\mathbf{y}_{i?} \mid \mathbf{y}_{i!})^\top, \\ E(\mathbf{y}_{i?} \mathbf{y}_{i?}^\top \mid \mathbf{y}_{i!}) &= E(\mathbf{y}_{i?} \mid \mathbf{y}_{i!}) E(\mathbf{y}_{i?} \mid \mathbf{y}_{i!})^\top + \boldsymbol{\Sigma}_{i??} - \boldsymbol{\Sigma}_{i?!} \boldsymbol{\Sigma}_{i!!}^{-1} \boldsymbol{\Sigma}_{i!?}, \end{aligned}$$

where conditioning on  $\mathbf{x}_i$ ,  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$  is assumed but suppressed in the notation. We compute  $\boldsymbol{\Sigma}_{i?!} \boldsymbol{\Sigma}_{i!!}^{-1}$  and  $\boldsymbol{\Sigma}_{i??} - \boldsymbol{\Sigma}_{i?!} \boldsymbol{\Sigma}_{i!!}^{-1} \boldsymbol{\Sigma}_{i!?}$  using the sweep operator (Goodnight, 1979), sweeping  $\boldsymbol{\Sigma}$  on the positions corresponding to  $\mathbf{y}_{i!}$ . At the outset, we group the sample units by their missingness patterns to avoid unnecessary sweeps.

This EM algorithm is implemented in `norm2` in a function called `emNorm`, which will be described in Section 6. Each iteration of this algorithm increases the loglikelihood function (6) until it converges to a local maximum (or, rarely, a saddlepoint) or until it reaches a boundary of the parameter space where  $\boldsymbol{\Sigma}$  is no longer positive definite. If no elements of  $\mathbf{Y}$  are missing, the algorithm converges after a single iteration.

### 3.2 Starting values

The EM routine in `emNorm` allows the user to provide starting values for  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$ . If none are given, the software chooses its own. The default starting values are obtained as

follows. The observed values in each column of  $\mathbf{Y}$  are regressed on the corresponding rows of  $\mathbf{X}$ , and the ordinary least-squares (OLS) coefficients from this regression are placed in the appropriate column of  $\boldsymbol{\beta}$ . The usual estimate of the residual variance, commonly known as the mean squared error or MSE, is placed in the appropriate diagonal position of  $\boldsymbol{\Sigma}$ , and the off-diagonal elements are set to zero. If the predictor matrix happens to be rank-deficient, the OLS coefficients are not unique, and a convenient solution is chosen. If the model happens to have perfect fit (for example, because the number of predictors exceeds the number of available cases), the residual variance is arbitrarily set to one-half the value of the sample variance of the observed responses.

### 3.3 Detecting convergence

Suppose we arrange the parameters of our model into a vector

$$\boldsymbol{\theta} = \left[ \text{vec}(\boldsymbol{\beta})^\top, \text{vech}(\boldsymbol{\Sigma})^\top \right]^\top,$$

where “vec” stacks the columns of a matrix into a single column, and “vech” stacks the nonredundant elements (the lower triangle) of a symmetric matrix into a single column. Let  $\theta_j$  denote an element of  $\boldsymbol{\theta}$ , and let  $\theta_j^{(t)}$  denote the estimate of  $\theta_j$  after  $t$  iterations of EM. We say that the algorithm has converged by iteration  $t$  if  $\theta_j^{(t)}$  is sufficiently close to  $\theta_j^{(t-1)}$  for all  $j$ . The convergence criterion used by `emNorm` requires

$$\frac{|\theta_j^{(t)} - \theta_j^{(t-1)}|}{|\theta_j^{(t-1)}|} \leq \delta$$

for all  $j$ , where the default value of  $\delta$  is  $1.0 \times 10^{-5}$ . In the unlikely event that  $\theta_j^{(t-1)}$  happens to be exactly zero, that parameter is ignored when assessing convergence at that iteration.

### 3.4 Elementwise rates of convergence

When EM has nearly converged, the rate of convergence for  $\theta_j$  can be estimated by

$$\hat{\lambda}_j = \frac{|\theta_j^{(t+1)} - \theta_j^{(t)}|}{|\theta_j^{(t)} - \theta_j^{(t-1)}|}. \quad (7)$$

If there happens to be no missing information regarding  $\theta_j$  (e.g., if  $\theta_j$  is the mean or variance of a variable that has no missing values), then EM converges for that parameter in a single step, and  $\hat{\lambda}_j$  will be zero or undefined. In most other situations,  $\hat{\lambda}_j$  estimates the “worst fraction of missing information” for the problem—not the rate of missing

information for  $\theta_j$  itself, but the supremum of the rate of missing information over all linear combinations of the elements of  $\boldsymbol{\theta}$  (Meng and Rubin, 1994; Schafer, 1997, Sec. 3.3).

The worst fraction of missing information can sometimes be approximated by the  $\hat{\lambda}_j$ 's over the final iterations of EM. Unfortunately, those quantities can be notoriously unstable, especially in problems where EM converges quickly. A better technique was developed by Fraley (1998). Suppose we view the E- and M-steps of EM as a function that updates the parameter vector at each iteration,

$$\boldsymbol{\theta}^{(t+1)} = \mathcal{M}(\boldsymbol{\theta}^{(t)}),$$

where  $\mathcal{M}$  maps the parameter space onto itself. The algorithm stops at a fixed point  $\hat{\boldsymbol{\theta}}$  if  $\hat{\boldsymbol{\theta}} = \mathcal{M}(\hat{\boldsymbol{\theta}})$ . The convergence behavior of EM and rates of missing information are determined by the Jacobian matrix

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{\partial}{\partial \boldsymbol{\theta}^\top} \mathcal{M}(\boldsymbol{\theta}).$$

More specifically, the worst fraction of missing information  $\hat{\lambda}$  is the largest eigenvalue of  $\hat{\mathcal{J}} = \mathcal{J}(\hat{\boldsymbol{\theta}})$ , and the eigenvector  $\hat{\mathbf{v}}$  corresponding to  $\hat{\lambda}$  approximates the trajectory of EM as it approaches  $\hat{\boldsymbol{\theta}}$ . Fraley (1998) obtained a numerical estimate of  $\hat{\lambda}$  using power iteration, a well known technique for computing dominant eigenvalues that dates back to the 1920's. Fraley's method does not require the full Jacobian matrix, but only the vector

$$\frac{d}{d\delta} \mathcal{M}(\hat{\boldsymbol{\theta}} + \delta \hat{\mathbf{v}})$$

in the neighborhood of  $\delta = 0$ . In **emNorm**, we apply Fraley's power method with a numerical estimate of this derivative vector obtained from a second-order finite differencing sequence. In well behaved problems, the procedure gives reasonably accurate estimates of  $\hat{\lambda}$  and  $\hat{\mathbf{v}}$ . If the procedure fails, it suggests that the loglikelihood function (6) may be oddly shaped, with a maximum that is not unique or a solution on the boundary of the parameter space where  $\boldsymbol{\Sigma}$  is singular.

### 3.5 Prior information for $\boldsymbol{\Sigma}$

Depending on the rates and patterns of missing observations in  $\mathbf{Y}$ , certain aspects of  $\boldsymbol{\Sigma}$  may be poorly estimated. For example, if there are no cases having joint responses for variables  $j$  and  $j'$ , then functions of  $\boldsymbol{\Sigma}$  pertaining to the partial correlation between  $y_{ij}$  and  $y_{ij'}$  given  $\mathbf{x}_i$  and the other variables will be inestimable (Rubin, 1974). In other cases, multicollinearity among the response variables may push the ML estimate of  $\boldsymbol{\Sigma}$  toward a boundary of the parameter space. When this occurs, instability in the estimation of  $\boldsymbol{\Sigma}$  may make it difficult to draw inferences based only on the likelihood function. One remedy for this problem is to introduce prior information to smooth the estimate of  $\boldsymbol{\Sigma}$  toward a guess.



Suppose that we apply an improper uniform prior distribution to  $\boldsymbol{\beta}$  and an inverted Wishart prior distribution to  $\boldsymbol{\Sigma}$ , so that

$$\boldsymbol{\Sigma}^{-1} \sim W(\xi, \boldsymbol{\Lambda}),$$

where  $\xi$  and  $\boldsymbol{\Lambda}$  denote the degrees of freedom and the scale matrix, respectively. The prior density function is

$$p(\boldsymbol{\beta}, \boldsymbol{\Sigma}) \propto |\boldsymbol{\Sigma}|^{-\left(\frac{\xi+r+1}{2}\right)} \exp\left\{-\frac{1}{2} \text{tr } \boldsymbol{\Sigma}^{-1} \boldsymbol{\Lambda}^{-1}\right\}, \quad (8)$$

which has the same functional form as the complete-data likelihood. If we add the logarithm of this density to the complete-data loglikelihood function, the joint mode for  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$  is given by

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{T}_1$$

and

$$\begin{aligned} \hat{\boldsymbol{\Sigma}} &= \frac{1}{n + \xi + r + 1} \left[ (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \boldsymbol{\Lambda}^{-1} \right] \\ &= \frac{1}{n + \xi + r + 1} \left[ \mathbf{T}_2 + \mathbf{T}_1^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{T}_1 + \boldsymbol{\Lambda}^{-1} \right]. \end{aligned} \quad (9)$$

If we change the M-step by computing (9) rather than (4), with  $\mathbf{T}_1$  and  $\mathbf{T}_2$  replaced by their expectations, then the modified EM algorithm will maximize the observed-data log-posterior density, which is equal to (6) plus the logarithm of (8).

In choosing values for the hyperparameters, we may think of  $\xi^{-1} \boldsymbol{\Lambda}^{-1}$  as a prior guess for  $\boldsymbol{\Sigma}$  and  $\xi$  as the degrees of freedom on which this guess is based. In that case,  $\boldsymbol{\Lambda}^{-1}$  can be regarded as the prior sums of squares and cross-products (SSCP) matrix. The function `emNorm` allows the user to supply values for  $\xi$  and  $\boldsymbol{\Lambda}^{-1}$ . It also implements three special cases of this prior distribution:

- the uniform prior, which sets  $\xi = -(r + 1)$  and  $\boldsymbol{\Lambda}^{-1} = 0$ ;
- the Jeffreys prior, which sets  $\xi = 0$  and  $\boldsymbol{\Lambda}^{-1} = 0$ ; and
- a data-dependent “ridge” prior, which smooths all of the estimated correlations toward zero (Schafer, 1997, pp. 155–156). The ridge prior requires the user to specify  $\xi$ , which determines the amount of smoothing. The prior guess for  $\boldsymbol{\Sigma}$  is set equal to the ad hoc diagonal estimate used for default starting values as described in Section 3.2.

The default prior used by `emNorm` is the uniform prior, for which the posterior mode is the ML estimate.

## 4 Posterior simulation and multiple imputation

### 4.1 A Markov chain Monte Carlo procedure

With some modification, the EM algorithm described above can be turned into a Markov chain Monte Carlo (MCMC) procedure for simulating draws of  $\mathbf{Y}_?$ ,  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$  from their joint posterior distribution given  $\mathbf{Y}_!$  and  $\mathbf{X}$ . The MCMC algorithm proceeds as follows. Given the current random draws  $\mathbf{Y}_?^{(t)}$ ,  $\boldsymbol{\beta}^{(t)}$  and  $\boldsymbol{\Sigma}^{(t)}$ , we first

$$\text{draw } \mathbf{y}_{i?}^{(t+1)} \text{ from } P(\mathbf{y}_{i?} | \mathbf{y}_{i!}, \boldsymbol{\beta}^{(t)}, \boldsymbol{\Sigma}^{(t)}, \mathbf{x}_i) \quad (10)$$

independently for  $i = 1, \dots, n$  to create  $\mathbf{Y}_?^{(t+1)}$ . We call this the Imputation or I-step; it is very closely related to the E-step of the previous section. Given  $\mathbf{y}_{i!}$ ,  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$ , the distribution of  $\mathbf{y}_{i?}$  is normal with mean vector

$$\boldsymbol{\beta}_{i?}^\top \mathbf{x}_i + \boldsymbol{\Sigma}_{i?!} \boldsymbol{\Sigma}_{i!!}^{-1} (\mathbf{y}_{i!} - \boldsymbol{\beta}_{i!}^\top \mathbf{x}_i)$$

and covariance matrix

$$\boldsymbol{\Sigma}_{i??} - \boldsymbol{\Sigma}_{i?!} \boldsymbol{\Sigma}_{i!!}^{-1} \boldsymbol{\Sigma}_{i!?}.$$

After the I-step has been completed, we

$$\text{draw } \boldsymbol{\Sigma}^{(t+1)} \text{ from } P(\boldsymbol{\Sigma} | \mathbf{Y}_!, \mathbf{Y}_?^{(t+1)}, \mathbf{X}) \quad (11)$$

and then

$$\text{draw } \boldsymbol{\beta}^{(t+1)} \text{ from } P(\boldsymbol{\beta} | \mathbf{Y}_!, \mathbf{Y}_?^{(t+1)}, \boldsymbol{\Sigma}^{(t+1)}, \mathbf{X}), \quad (12)$$

which is called the Posterior or P-step. Repeating (10)–(12) many times generates a sequence of random draws  $(\mathbf{Y}_?^{(t)}, \boldsymbol{\beta}^{(t)}, \boldsymbol{\Sigma}^{(t)}), t = 1, 2, \dots$  whose limiting distribution is  $P(\mathbf{Y}_?, \boldsymbol{\beta}, \boldsymbol{\Sigma} | \mathbf{Y}_!, \mathbf{X})$  regardless of the starting values.

Steps (11) and (12) require us to specify a joint prior distribution for  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$ . Once again, we apply an improper uniform prior to  $\boldsymbol{\beta}$  and an inverted Wishart prior to  $\boldsymbol{\Sigma}$ . Combining the prior density (8) with the likelihood function implied by (5), and using the fact that

$$\left| \boldsymbol{\Sigma} \otimes (\mathbf{X}^\top \mathbf{X})^{-1} \right| = |\boldsymbol{\Sigma}|^p |\mathbf{X}^\top \mathbf{X}|^{-r},$$

the joint posterior density for  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$  given  $\mathbf{Y}$  and  $\mathbf{X}$  is

$$\begin{aligned} p(\boldsymbol{\beta}, \boldsymbol{\Sigma} | \mathbf{Y}, \mathbf{X}) &\propto |\boldsymbol{\Sigma}|^{-\left(\frac{n-p+\xi+r+1}{2}\right)} \\ &\times \exp \left\{ -\frac{1}{2} \text{tr} \boldsymbol{\Sigma}^{-1} \left[ \boldsymbol{\Lambda}^{-1} + (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \right] \right\} \\ &\times \left| \boldsymbol{\Sigma} \otimes (\mathbf{X}^\top \mathbf{X})^{-1} \right|^{-\frac{1}{2}} \\ &\times \exp \left\{ -\frac{1}{2} \text{vec}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^\top \left[ \boldsymbol{\Sigma} \otimes (\mathbf{X}^\top \mathbf{X})^{-1} \right]^{-1} \text{vec}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) \right\}. \end{aligned}$$

From this it immediately follows that

$$\begin{aligned}\boldsymbol{\Sigma}^{-1} \mid \mathbf{Y}, \mathbf{X} &\sim W(\xi', \boldsymbol{\Lambda}'), \\ \text{vec}(\boldsymbol{\beta}) \mid \mathbf{Y}, \mathbf{X}, \boldsymbol{\Sigma} &\sim N\left(\text{vec}(\hat{\boldsymbol{\beta}}), \boldsymbol{\Sigma} \otimes (\mathbf{X}^\top \mathbf{X})^{-1}\right),\end{aligned}$$

where  $\xi' = \xi + n - p$  and

$$\boldsymbol{\Lambda}' = \left[ \boldsymbol{\Lambda}^{-1} + (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \right]^{-1}.$$

Under the Jeffreys prior

$$p(\boldsymbol{\beta}, \boldsymbol{\Sigma}) \propto |\boldsymbol{\Sigma}|^{-\left(\frac{r+1}{2}\right)},$$

which can be regarded as the limit of (8) as  $\xi \rightarrow 0$  and  $\boldsymbol{\Lambda}^{-1} \rightarrow 0$ , the posterior becomes

$$\begin{aligned}\boldsymbol{\Sigma}^{-1} \mid \mathbf{Y}, \mathbf{X} &\sim W\left(n - p, \left[(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})\right]^{-1}\right), \\ \text{vec}(\boldsymbol{\beta}) \mid \mathbf{Y}, \mathbf{X}, \boldsymbol{\Sigma} &\sim N\left(\text{vec}(\hat{\boldsymbol{\beta}}), \boldsymbol{\Sigma} \otimes (\mathbf{X}^\top \mathbf{X})^{-1}\right).\end{aligned}$$

To simulate  $\boldsymbol{\beta}$ , we apply the Cholesky factorizations  $\boldsymbol{\Sigma} = \mathbf{G}\mathbf{G}^\top$  and  $(\mathbf{X}^\top \mathbf{X})^{-1} = \mathbf{H}\mathbf{H}^\top$ , where  $\mathbf{G}$  and  $\mathbf{H}$  are lower-triangular. Using elementary properties of Kronecker products, we get

$$\begin{aligned}\boldsymbol{\Sigma} \otimes (\mathbf{X}^\top \mathbf{X})^{-1} &= (\mathbf{G}\mathbf{G}^\top) \otimes (\mathbf{H}\mathbf{H}^\top) \\ &= (\mathbf{G} \otimes \mathbf{H})(\mathbf{G}^\top \otimes \mathbf{H}) \\ &= (\mathbf{G} \otimes \mathbf{H})(\mathbf{G} \otimes \mathbf{H})^\top,\end{aligned}$$

where  $\mathbf{G} \otimes \mathbf{H}$  is lower-triangular. A random draw of  $\text{vec}(\boldsymbol{\beta})$  is obtained as  $\text{vec}(\hat{\boldsymbol{\beta}}) + (\mathbf{G} \otimes \mathbf{H})\mathbf{z}$ , where  $\mathbf{z}$  is a vector of independent standard normal variates of length  $p \times r$ .

We implemented this procedure in a function called `mcmcNorm`, which will be described in Section 6. When calling `mcmcNorm`, the user must supply starting values for  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$ . A good choice for starting values is an ML estimate or posterior mode obtained from `emNorm`. If `emNorm` is run first, then the result from `emNorm` may be supplied as the main argument to `mcmcNorm`, in which case the EM estimates automatically become the starting values for MCMC. The result from `mcmcNorm` may also be supplied as the main argument in another call to `mcmcNorm`, so that the final simulated values of  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$  from the first chain become the starting values for the second chain.

## 4.2 Assessing convergence

Proper use of MCMC requires us to judge how many iterations are required before the simulated parameters can be regarded as draws from the observed-data posterior distribution. In general, we would like to know whether the algorithm achieves stationarity by

$k$  iterations, which means that  $\boldsymbol{\theta}^{(t+k)}$ , the simulated value after iteration  $t + k$ , is independent of  $\boldsymbol{\theta}^{(t)}$ . Like EM, the convergence of this MCMC procedure is related to missing information. If there were no missing values in  $\mathbf{Y}$ , then the algorithm would converge in one iteration. When the rates of missing information are high, many iterations may be needed.

Users of MCMC typically assess convergence by examining time-series plots and autocorrelation functions (ACF's) for the series

$$\theta_j^{(t+1)}, \theta_j^{(t+2)}, \theta_j^{(t+3)}, \dots$$

for individual parameters  $j = 1, 2, \dots$ . By default, `mcmcNorm` saves the entire output stream consisting of the simulated elements of  $\boldsymbol{\beta}$  and  $\boldsymbol{\Sigma}$  from all iterations, returning them as multivariate time-series objects.

In large problems with many parameters, saving the full output stream from all iterations may be impractical. The `mcmcNorm` function has two options that allow us to make the output more manageable. An option called `multicycle` instructs `mcmcNorm` to perform multiple cycles of MCMC per iteration (one cycle consists of an I-step followed by a P-step). By specifying `multicycle = k` for some  $k \geq 2$ , `mcmcNorm` will save only the subsampled stream  $\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta}^{(2k)}, \boldsymbol{\theta}^{(3k)}, \dots$

Another option for output analysis is to save and examine the simulated values of scalar functions of  $\boldsymbol{\theta}$  for which the serial dependence tends to be high. Schafer (1997, Section 4.4) recommends using the inner product

$$\hat{\mathbf{v}}^\top \boldsymbol{\theta} = \sum_j \hat{v}_j \theta_j,$$

where  $\hat{\mathbf{v}} = (\hat{v}_1, \hat{v}_2, \dots)^\top$  is the eigenvector corresponding to the dominant eigenvalue of the Jacobian matrix in Section 3.5. This is the worst linear function of  $\boldsymbol{\theta}$ , the linear combination of  $\theta_j$ 's in the vicinity of  $\hat{\boldsymbol{\theta}}$  for which the missing information is highest. For interpretability, we this function as

$$g(\boldsymbol{\theta}) = \frac{\hat{\mathbf{v}}^\top \boldsymbol{\theta}}{\sqrt{\hat{\mathbf{v}}^\top \hat{\mathbf{v}}} \sqrt{\boldsymbol{\theta}^\top \boldsymbol{\theta}}}, \quad (13)$$

so that it becomes the cosine of the angle between  $\hat{\mathbf{v}}$  and  $\boldsymbol{\theta}$ . In typical applications, if the serial correlation in this function has died down by  $k$  cycles, we can be reasonably sure that the correlations in other functions of  $\boldsymbol{\theta}$  have died down as well. If the result from `emNorm` is provided as input to `mcmcNorm`, the elements of  $\hat{\mathbf{v}}$  (the so-called worst linear coefficients) are carried over to `mcmcNorm` automatically, and values of  $g(\boldsymbol{\theta})$  are then saved for all iterations of MCMC.

### 4.3 Inferences about the normal model parameters

After a suitable burn-in period to achieve stationarity, the output stream from the MCMC algorithm may be used for direct Bayesian inferences about model parameters. For example, the parameter series  $\theta_j^{(t+1)}, \theta_j^{(t+2)}, \theta_j^{(t+3)}, \dots$  may be averaged to obtain a simulated posterior mean for  $\theta_j$ . A simulated 95% Bayesian credible interval runs from the 2.5th to the 97.5th percentiles of the sampled values of  $\theta_j$ . For more discussion on the use of simulated parameters from MCMC, see Section 4.2 of Schafer (1997).

### 4.4 Imputation of missing values

Perhaps the most important feature of `mcmcNorm` is that it enables us to easily create multiple imputations for missing values. Multiple imputations, as described by Rubin (1987), Schafer (1997) and others, are independent draws from a Bayesian posterior predictive distribution for the missing values given the observed values under an assumed model,

$$P(\mathbf{Y}_? \mid \mathbf{Y}_!, \mathbf{X}) = \int P(\mathbf{Y}_? \mid \mathbf{Y}_!, \mathbf{X}, \boldsymbol{\theta}) P(\boldsymbol{\theta} \mid \mathbf{Y}_!, \mathbf{X}) d\boldsymbol{\theta}.$$

To create multiple imputations  $\mathbf{Y}_?^{(1)}, \mathbf{Y}_?^{(2)}, \dots, \mathbf{Y}_?^{(M)}$ , we first generate  $M$  independent draws of the parameters,  $\boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)}, \dots, \boldsymbol{\theta}^{(M)}$ , from the posterior distribution  $P(\boldsymbol{\theta} \mid \mathbf{Y}_!, \mathbf{X})$ . Then, given the simulated parameters, we draw  $\mathbf{Y}_?^{(m)}$  from  $P(\mathbf{Y}_? \mid \mathbf{Y}_!, \mathbf{X}, \boldsymbol{\theta} = \boldsymbol{\theta}^{(m)})$  for  $m = 1, \dots, M$ . Multiple imputations can be generated by a single chain or by multiple chains. In the single-chain method, we run the MCMC procedure for  $Mk$  cycles, where  $k$  is large enough to ensure that  $\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta}^{(2k)}, \dots, \boldsymbol{\theta}^{(Mk)}$  are essentially independent, and save the simulated values of  $\mathbf{Y}_?$  from every  $k$ th I-step. This is accomplished by supplying an argument `impute.every = k` to the function `mcmcNorm`. In the multiple-chain method, we call the `mcmcNorm` function  $M$  times, running it for  $k$  cycles each time, to create  $M$  sets of simulated parameters. Each set of simulated parameters is then supplied to another function, `impNorm`, which draws the missing values from  $P(\mathbf{Y}_? \mid \mathbf{Y}_!, \mathbf{X}, \boldsymbol{\theta})$ . Whether using a single chain or multiple chains, it is advisable to first examine the output stream from an exploratory MCMC run to make sure that serial correlations in all parameters have died down by  $k$  cycles.

### 4.5 Prediction of missing values

In certain situations, it may be desirable to predict the missing values without random noise. That is, rather than simulating a random draw of  $\mathbf{Y}_?$  from  $P(\mathbf{Y}_? \mid \mathbf{Y}_!, \mathbf{X}, \boldsymbol{\theta})$ , we may want to compute the expected value  $E(\mathbf{Y}_? \mid \mathbf{Y}_!, \mathbf{X}, \boldsymbol{\theta})$  for a given  $\boldsymbol{\theta}$  using the formulas given in Section 3.1. This can be accomplished by calling the function `impNorm` with the option `method = "predict"`. The default procedure for `impNorm`, which is `method = "random"`, draws the missing values from  $P(\mathbf{Y}_? \mid \mathbf{Y}_!, \mathbf{X}, \boldsymbol{\theta})$ .

## 4.6 Combining results from analyses after multiple imputation

An attractive feature of multiple imputation is that, after the imputations have been created, the resulting datasets may be handled using routines designed for complete data. We may analyze each of the completed versions of  $(\mathbf{X}, \mathbf{Y})$  separately, saving the  $M$  sets of estimates and standard errors, and then combine them by rules developed by Rubin (1987) and others.

In the basic procedure described by Rubin (1987, Chap. 3), there is a scalar quantity  $Q$  for which we need an estimate and measure of uncertainty. Suppose that, if there were no missing data, we could calculate a point estimate  $\hat{Q} = \hat{Q}(\mathbf{X}, \mathbf{Y})$  and a variance estimate  $U = U(\mathbf{X}, \mathbf{Y})$ . Suppose that we have imputed datasets  $(\mathbf{X}, \mathbf{Y}_1, \mathbf{Y}_?^{(m)})$  for  $m = 1, \dots, M$ , and let  $\hat{Q}^{(m)}$  and  $U^{(m)}$  denote the point and variance estimate from the  $m$ th imputed dataset. The overall point estimate for  $Q$  is simply the mean of the repeated estimates,

$$\bar{Q} = M^{-1} \sum_{m=1}^M \hat{Q}^{(m)},$$

and the overall variance estimate is

$$T = (1 + M^{-1}) B + \bar{U},$$

where

$$B = (M - 1)^{-1} \sum_{m=1}^M (\hat{Q}^{(m)} - \bar{Q})^2$$

and

$$\bar{U} = M^{-1} \sum_{m=1}^M U^{(m)}$$

are the between- and within-imputation variances, respectively. The relative increase in variance due to nonresponse is

$$\hat{r} = \frac{(1 + M^{-1}) B}{\bar{U}},$$

and the approximate rate of missing information is

$$\hat{\gamma} = \frac{(1 + M^{-1}) B}{T} = \frac{\hat{r}}{\hat{r} + 1}.$$

Intervals and tests for  $Q$  are based on the result that  $(\hat{Q} - Q)/\sqrt{T}$  is approximately distributed as Student's  $t$  with degrees of freedom

$$\nu_M = (M - 1) \hat{\gamma}^{-2}. \tag{14}$$

Rubin (1987) assumed that the sample size was large enough that, if there were no missing data, it would be appropriate to base intervals and tests on the normal approximation

$$(\hat{Q} - Q)/\sqrt{U} \sim N(0, 1). \quad (15)$$

When the sample is too small for (15) to be plausible, better results are available from a modified procedure described by Barnard and Rubin (1999). If we suppose that  $(\hat{Q} - Q)/\sqrt{U}$  with complete data is distributed as Student's  $t$  with  $\nu_{com}$  degrees of freedom, Barnard and Rubin (1999) show that  $(\hat{Q} - Q)/\sqrt{T}$  is approximately Student's  $t$  with degrees of freedom

$$\tilde{\nu}_M = \left( \frac{1}{\nu_M} + \frac{1}{\hat{\nu}} \right)^{-1}, \quad (16)$$

where

$$\hat{\nu} = \frac{\nu_{com}(\nu_{com} + 1)(1 - \hat{\gamma})}{(\nu_{com} + 3)}.$$

When  $\nu_{com} = \infty$ , (16) reduces to (14), yielding Rubin's (1987) rules as a special case. The rules of Rubin (1987) and Barnard and Rubin (1999) are implemented in the **norm2** package as a function called **miInference**.

## 5 Preliminaries

[In this section, we review some important concepts from R that are helpful for understanding **norm2** functions and documentation. Experienced users of R may want to lightly skim this material or skip ahead to Section 6.]

### 5.1 Loading the package

An R package is a collection of functions, data and documentation that is not part of the basic R distribution and needs to be installed separately. Once a package has been installed on an R user's system, it becomes a library that can be attached and used in any R session. Procedures for downloading and installing packages from CRAN vary slightly depending on your version of R and your computer's operating system, but they are quite simple. For example, in a typical Windows session of R, you would select the "Install package(s)" from the "Packages" menu at the top of the R user interface. For more details on package installation, refer to the documentation and help files for your particular version of R.

Before you can use any of the **norm2** functions or datasets within an R session, you will have to load it by issuing the command

```
> library(norm2)
```

from the R console.

## 5.2 Documentation and data examples

Once the library has been loaded, you can view its documentation files in the usual R fashion, as in the following examples:

```
> help(norm2)      # overview of the package
> ?norm2           # same thing as above
> help(emNorm)     # documentation for the function emNorm
```

The `norm2` package also includes several datasets that were used by Schafer (1997) to illustrate techniques of estimation and imputation. If you issue the command

```
> data(package="norm2")
```

then a list of these datasets will appear. Each dataset has its own documentation; for example,

```
> help(flas)
```

will display the page for the `flas` dataset. To gain access to these datasets, use the `data` function with the name of the dataset as its argument. For example, if you type

```
> data(flas)
```

then a copy of the `flas` dataset will be loaded into your current workspace.

## 5.3 Objects, classes and generic methods

Objects in R are self-documenting in the sense that each object carries important information about itself: what types of data it contains, how large it is, and so on. These pieces of information about an object are called its attributes. One of the most important attributes of an object is its class. The class of an object is a character string that tells us what kind of object it is. We can discover the class of an object by using the function `class`, as in the following examples.



```

> ivec <- 1:10                      # a vector of integers 1, ..., 10
> converged <- T                    # a single logical value
> y <- matrix(rnorm(10), 5, 2)      # a 5 x 2 matrix of random numbers
> mylist <- list(ivec, converged, y) # a list with 3 components
> class(ivec)
[1] "integer"
> class(y)
[1] "matrix"
> class(mylist)
[1] "list"

```

The reason why classes are so important is that R has generic methods that do different things depending on what kind of arguments are supplied to it. More precisely, a generic method is a group of functions called by the same name but distinguished by the class of the first argument. To see how this works, consider the most widely used generic method in R, which is `print`. In an interactive R session, whenever you look at an object by typing its name, you are implicitly calling `print`.

```

> ivec          # look at ivec
[1] 1 2 3 4 5 6 7 8 9 10

> print(ivec)   # exactly the same thing
[1] 1 2 3 4 5 6 7 8 9 10

```

Here is a part of the R documentation file for `print`.

```

print                                package:base                                R Documentation

Print Values

Description:

  'print' prints its argument and returns it _invisibly_ (via
  'invisible(x)'). It is a generic function which means that new
  printing methods can be easily added for new 'class'es.

Usage:

print(x, ...)

## S3 method for class 'factor':
print(x, quote = FALSE, max.levels = NULL,
      width = getOption("width"), ...)

```

```
## S3 method for class 'table':
print(x, digits = getOption("digits"), quote = FALSE,
      na.print = "", zero.print = "0", justify = "none", ...)
```

The first two arguments to `print` are:

Arguments:

`x`: an object used to select a method.

`...:` further arguments passed to or from other methods.

When you invoke a generic method, R examines your first argument and decides what action to take. If the first argument to `print` is an object of class `"factor"`, then `print` passes the first argument and all subsequent arguments to another function called `print.factor`. If the first argument to `print` is an object of class `"table"`, then `print` passes the first argument and all subsequent arguments to another function called `print.table`. You may call the functions `print.factor` and `print.table` directly if you like, but users rarely do; it's easier to just refer to all of these functions by their generic name `print`.

What happens if you apply a generic method to an object for which no specific method exists? For example, suppose `x` is an object of class `"boogeyman"`. If you invoke `print(x)`, then R searches for a function named `print.boogeyman`. If none can be found, R tries to find another specific method that may be appropriate. As a last resort, it calls a default method which is called `print.default`. In R, every generic method is supposed to have a default method that is invoked as a last resort.

## 5.4 User-defined classes

Experienced users of R, especially those who write their own packages, are fond of developing new object classes. R makes this very easy to do. For example, if you issue these commands,

```
> x <- rnorm(100)
> class(x) <- "randomVector"
```

then you have just created a new object class `"randomVector"`. If you then create a new function called `"summary.randomVector"`, then

```
> summary(x)
```

will invoke your new function automatically.

In the `norm2` package, we have defined a new object class called `norm`. A `norm` object is simply a list whose `class` attribute has been set to `"norm"`. Most of the functions in `norm2` can operate either on raw data or on a `norm` object, which makes them easier to remember and use.

## 5.5 A note on data frames and factors

In R, a basic two-dimensional array is a matrix, an object whose `class` attribute is `"matrix"`. All of the elements of a matrix are the same type of data (numeric values, character strings or logical values). A more general type of two-dimensional array is the data frame, whose `class` attribute is `"data.frame"`. One column of a data frame may contain numbers, while another may contain logical values, another may contain character strings, and so on. A column of a data frame may also be a factor, which is R's terminology for a categorical variable. In a factor, data values are stored as integer codes, and character labels corresponding to these codes (e.g., `"Male"` and `"Female"`) are carried along via an attribute called `levels`. If a  $k$ -level factor appears in a as a predictor in a call to the regression modeling functions `lm` or `glm`, R automatically converts it to a set of  $k - 1$  contrasts or dummy codes. An ordered is similar to a factor except that the levels are assumed to be ordered, and R converts it to a set of contrasts representing effects that are linear, quadratic, cubic, etc.

We have been assuming that response variables are jointly normal. In practice, missing-data procedures designed for variables that are normal are sometimes applied to variables that are not. Binary and ordinal variables are sometimes imputed under a normal model, and the imputed values may be classified or rounded (Schafer, 1997, Chap. 6). If `norm2` functions are applied to variables that are categorical, it is up to the user to decide how to do it. For example, consider a factor for race/ethnicity coded as 1=Black, 2=non-Black Hispanic and 3=Other. It would make little sense to enter this factor into a model as is, treating the internal codes 1, 2 and 3 as numeric values, because the categories are not intrinsically ordered. A better strategy would be to convert this variable into a pair of dummy variables, e.g. an indicator for Black (1 if Black, 0 otherwise) and an indicator for non-Black Hispanic (1 if non-Black Hispanic, 0 otherwise). If the race/ethnicity were completely observed, then the two dummy variables could enter the model as columns of  $X$ . If race/ethnicity had missing values, the dummy variables could be included as columns of  $Y$  and imputed, but then the user would have to decide how to convert the continuously distributed imputed values for these dummy codes back into categories of race/ethnicity.

Various ad hoc procedures for converting continuous imputed values into categories have been tried, and no single method seems to dominate the others (Bernaards, Belin, and Schafer, 2007). Because we have no firmly recommended strategy for applying normal

distributions to categorical variables, `norm2` makes no serious attempt to handle factors or ordered factors. If a data frame is supplied as an argument to a `norm2` function, the data frame is converted to a numeric matrix using the R conversion function `data.matrix`. If any factors or ordered factors are present, they are replaced by their internal codes, which may or may not be sensible.

## 6 Using the package: Example 1

### 6.1 Cholesterol data

In the remaining sections, we show by example how to use all the major functions in `norm2`. Our first dataset, which was originally published by Ryan and Joiner (1994), reports cholesterol levels for 28 patients treated for heart attack at a Pennsylvania medical center. These data, which were previously analyzed by Schafer (1997, Chap. 5), are distributed with the `norm2` package and stored in a data frame called `cholesterol`:

```
> data(cholesterol)
> cholesterol
   Y1  Y2  Y3
1  270 218 156
2  236 234  NA
3  210 214 242
4  142 116  NA
5  280 200  NA
6  272 276 256
7  160 146 142
8  220 182 216
9  226 238 248
10 242 288  NA
11 186 190 168
12 266 236 236
13 206 244  NA
14 318 258 200
15 294 240 264
16 282 294  NA
17 234 220 264
18 224 200  NA
19 276 220 188
20 282 186 182
21 360 352 294
22 310 202 214
23 280 218  NA
```

```

24 278 248 198
25 288 278 NA
26 288 248 256
27 244 270 280
28 236 242 204

```

The three variables correspond to cholesterol levels observed 2 days (Y1), 4 days (Y2) and 14 days (Y3) after attack. Nine patients have missing values for Y3.

## 6.2 Listwise deletion

The first step in our analysis is to estimate the means and the covariance matrix for Y1, Y2 and Y3. The R generic method `summary`, when applied to a data frame, displays univariate summary statistics for each variable, ignoring any missing values for that variable.

```

> summary(cholesterol, na.rm=F)
      Y1      Y2      Y3
Min.   :142.0 Min.   :116.0 Min.   :142.0
1st Qu.:225.5 1st Qu.:201.5 1st Qu.:193.0
Median :268.0 Median :235.0 Median :216.0
Mean   :253.9 Mean   :230.6 Mean   :221.5
3rd Qu.:282.0 3rd Qu.:250.5 3rd Qu.:256.0
Max.   :360.0 Max.   :352.0 Max.   :294.0
      NA's   :9

```

The R function `var` computes a sample covariance matrix. If `var` is called with the argument `use="complete.obs"`, it omits any row of the dataset that contains missing values. In the missing-data literature, this method is known as listwise deletion or complete-case analysis (Little and Rubin, 2002).

```

> var(cholesterol, use="complete.obs")
      Y1      Y2      Y3
Y1 2299.0409 1448.912  813.2632
Y2 1448.9123 1924.585 1348.9123
Y3  813.2632 1348.912 1864.8187

```

Multivariate methods based on case deletion may be inefficient, because data are being discarded unnecessarily. In this example, listwise deletion omits the observed values of Y1 and Y2 for the nine patients with missing values for Y3. Estimates from listwise deletion may also be biased if the complete cases and incomplete cases are systematically different. A better alternative is to compute ML estimates for the means and covariances using the `norm2` function `emNorm`.

## 6.3 Applying the EM algorithm

One technique for calling `emNorm`, as explained in its documentation file, is shown below:

```
## Default S3 method:
emNorm(obj, x = NULL, intercept = TRUE,
       iter.max = 1000, criterion = NULL, estimate.worst = TRUE,
       prior = "uniform", prior.df = NULL, prior.sscp = NULL,
       starting.values = NULL, ...)
```

The only only required argument is:

`obj`: an object used to select a method. It may be 'y', a numeric matrix, vector or data frame containing response variables to be modeled as multivariate normal. Missing values ('NA's) are allowed. If 'y' is a data frame, any factors or ordered factors will be replaced by their internal codes, and a warning will be given. Alternatively, this first argument may be a 'formula' as described below, or an object of class 'norm' resulting from a call to 'emNorm' or 'mcmcNorm'; see DETAILS.

If we call `emNorm` with `cholesterol` as its first argument, the data frame is coerced into a numeric data matrix (via the function `data.matrix`) and becomes `y`. If no value is supplied for the argument `x`, the matrix of predictors defaults to a single column of 1's, and the three variables in `cholesterol` will be regressed on a constant.

```
> emResult <- emNorm(cholesterol)
```

The result from `emNorm` is an object of class "norm". Important information in this object can be viewed with `summary`.

```
> summary(emResult)
Predictor (X) variables:
      Mean SD Observed Missing Pct.Missing
CONST   1  0         28        0          0

Response (Y) variables:
      Mean      SD Observed Missing Pct.Missing
Y1 253.9286 47.71049         28        0    0.00000
Y2 230.6429 46.96745         28        0    0.00000
```

```
Y3 221.4737 43.18355      19      9      32.14286
```

```
Missingness patterns for response (Y) variables
  (. denotes observed value, m denotes missing value)
  (variable names are displayed vertically)
  (rightmost column is the frequency):
```

```
YYY
123
... 19
..m  9
```

```
Method:                EM
Prior:                  "uniform"
Convergence criterion:  1e-05
Iterations:             15
Converged:              TRUE
Max. rel. difference:   8.5201e-06
-2 Loglikelihood:       615.9902
-2 Log-posterior density: 615.9902
Worst fraction missing information: 0.4617
```

```
Estimated coefficients (beta):
      Y1      Y2      Y3
CONST 253.9286 230.6429 222.2371
```

```
Estimated covariance matrix (sigma):
      Y1      Y2      Y3
Y1 2194.9949 1454.617  835.3973
Y2 1454.6173 2127.158 1515.4584
Y3  835.3973 1515.458 1952.2182
```

The section above titled "Missingness patterns for response (Y) variables" has a matrix that displays in compact form the patterns of missing values that appear in the dataset and the frequency of each pattern. The next section below it provides basic information about the EM run. Using the default starting values and the default convergence criterion, the algorithm converged in just 15 iterations, suggesting that the rates of missing information are low. The rate of convergence, which estimates the worst fraction of missing information, is approximately 0.46.

More results from EM are available by examining the components of the object directly. The names of the components are:

```
> names(emResult)
[1] "y"                "x"                "method"
```

[4]	"prior"	"prior.df"	"prior.sscp"
[7]	"starting.values"	"iter"	"converged"
[10]	"criterion"	"estimate.worst"	"loglik"
[13]	"logpost"	"param"	"param.rate"
[16]	"y.mean.imp"	"miss.patt"	"miss.patt.freq"
[19]	"n.obs"	"which.patt"	"rel.diff"
[22]	"ybar"	"ysdv"	"em.worst.ok"
[25]	"worst.frac"	"worst.linear.coef"	"msg"

Some of these components are described in the documentation for `emNorm`. The component `iter` is the number of iterations actually performed.

```
> emResult$iter
[1] 15
```

Perhaps the most important component is `param`, which contains the final parameter estimates. This is list of two components whose names are `beta` and `sigma`, corresponding to the matrices  $\beta$  and  $\Sigma$ .

```
> emResult$param
$beta
      Y1      Y2      Y3
CONST 253.9286 230.6429 222.2371

$sigma
      Y1      Y2      Y3
Y1 2194.9949 1454.617  835.3973
Y2 1454.6173 2127.158 1515.4584
Y3  835.3973 1515.458 1952.2182
```

The component `loglik` is a vector that reports, for each iteration, the value of the loglikelihood function at the start of that iteration. A property of EM is that the loglikelihood function (or log-posterior density, if a non-uniform prior is applied) will increase at each iteration.

```
> emResult$loglik
[1] -323.5527 -310.3163 -308.5807 -308.1113 -308.0162 -307.9990 -307.9958
[8] -307.9952 -307.9951 -307.9951 -307.9951 -307.9951 -307.9951 -307.9951
[15] -307.9951
```

The last element of `loglik` is not the loglikelihood evaluated at the final parameter estimates, but at the parameter estimates just before the start of the final iteration. If



the algorithm has converged, the two are essentially the same. If for some reason you need the precise value of the loglikelihood at the final parameter estimates, you can compute it using the function `loglikNorm`. One technique for calling `loglikNorm`, as shown in its documentation file, is

```
## Default S3 method:
loglikNorm(obj, x = NULL, intercept = TRUE, param, ...)
```

where the data are supplied through `obj` and `x`, and the parameters are supplied through `param`. Let's compute the value of the loglikelihood at the final parameter estimates from EM and compare it to the value just before the final iteration.

```
> llmax <- loglikNorm(cholesterol, param=emResult$param)
> llmax - emResult$loglik[ emResult$iter ]
[1] 2.375202e-09
```

The first argument to `loglikNorm` may also be an object of class `"norm"`, as shown in this section of the documentation file:

```
## S3 method for class 'norm'
loglikNorm(obj, param = obj$param, ...)
```

If we invoke `loglikNorm` with the object returned by `emNorm` (in this case, `emResult`) as its only argument, then the parameter estimates from EM (in this case, `emResult$param`) are automatically passed to `loglikNorm` as the parameter values at which the loglikelihood is to be evaluated. Therefore, we could have achieved the same effect with this easier syntax:

```
> llmax <- loglikNorm(emResult)
```

## 6.4 Completely observed variables as predictors

In this example, `Y1` and `Y2` have no missing values. Variables that are completely observed may be treated either as responses (columns of the matrix  $Y$ ) or as predictors (columns of the matrix  $X$ ). If we treat `Y1` and `Y2` as predictors, then the model becomes a simple linear regression of `Y3` on `Y1`, `Y2` and a constant.

```

> x <- cholesterol[,1:2]
> y <- cholesterol[,3]
> emResult <- emNorm(y,x)
> summary(emResult)
Predictor (X) variables:
      Mean      SD Observed Missing Pct.Missing
CONST  1.0000  0.00000      28      0          0
Y1     253.9286 47.71049      28      0          0
Y2     230.6429 46.96745      28      0          0

Response (Y) variables:
      Mean      SD Observed Missing Pct.Missing
Y1 221.4737 43.18355      19      9     32.14286

Missingness patterns for response (Y) variables
  (. denotes observed value, m denotes missing value)
  (variable names are displayed vertically)
  (rightmost column is the frequency):
Y
1
. 19
m 9

Method:                EM
Prior:                  "uniform"
Convergence criterion:  1e-05
Iterations:
      10
Converged:              TRUE
Max. rel. difference:   4.6597e-06
-2 Loglikelihood:       146.9102
-2 Log-posterior density: 146.9102
Worst fraction missing information: 0.3214

Estimated coefficients (beta):
      Y1
CONST 74.0236337
Y1    -0.1673990
Y2     0.8269102

Estimated covariance matrix (sigma):
      Y1
Y1 838.9239

```

## 6.5 Other ways to invoke EM

Many users of R are familiar with linear regression using the `lm` function and the syntax `lm( formula, data )`, where `formula` is a symbolic representation of the model to be fit, and `data` is a data frame where the model's variables reside. For example,

```
> lmResult <- lm( Y3 ~ Y1 + Y2, data=cholesterol )
```

will regress the variable `Y3` on `Y1`, `Y2` and a constant using the data contained in `cholesterol`. We can invoke `emNorm` in a similar fashion, by supplying a model formula and data frame.

```
> emResult <- emNorm( Y3 ~ Y1 + Y2, data=cholesterol )
```

If there are multiple response variables, these variables should be placed on the left-hand side of the model formula and glued together using `cbind`. For example, the expressions

```
emNorm( cholesterol )
```

and

```
emNorm( cbind(Y1,Y2,Y3) ~ 1, data=cholesterol )
```

are equivalent.

The documentation for `emNorm` describes yet another technique for calling the function, in which the first argument is an object of class `"norm"`.

```
## S3 method for class 'norm'
emNorm(obj, iter.max = 1000,
       criterion = obj$criterion, estimate.worst = obj$estimate.worst,
       prior = obj$prior, prior.df = obj$prior.df,
       prior.sscp = obj$prior.sscp, starting.values = obj$param, ...)
```

This may be useful in a problem where EM did not converge by `iter.max` iterations. If we supply the result from `emNorm` in another call to `emNorm`, then the data, model and specification of the prior distribution from the first EM run are automatically carried over, and the final parameter estimates from the first run become the starting values for the second. See what happens when we do this with the `cholesterol` data.

```

> emResult <- emNorm(cholesterol)
> emResult <- emNorm(emResult)
> summary(emResult, show.variables=F, show.patterns=F)

```

```

Method:                EM
Prior:                 "uniform"
Convergence criterion: 1e-05
Iterations:           1
Converged:             TRUE
Max. rel. difference:  3.9456e-06
-2 Loglikelihood:      615.9902
-2 Log-posterior density: 615.9902
Worst fraction missing information: 0.4652

```

```

Estimated coefficients (beta):
              Y1          Y2          Y3
CONST 253.9286 230.6429 222.2371

```

```

Estimated covariance matrix (sigma):
              Y1          Y2          Y3
Y1 2194.9949 1454.617  835.3977
Y2 1454.6173 2127.158 1515.4631
Y3  835.3977 1515.463 1952.2259

```

Because the first run of EM had already converged according to the default convergence criterion, the second run stopped after a single iteration, and the parameter estimates are essentially unchanged.

## 6.6 Running MCMC and assessing convergence

The function `mcmcNorm` is another generic method that calls different functions depending on the class of its first argument. The default method syntax is shown below.

```

## Default S3 method:
mcmcNorm(obj, x = NULL, intercept = TRUE,
  starting.values, iter = 1000, multicycle = NULL,
  seeds = NULL, prior = "uniform",
  prior.df = NULL, prior.sscp = NULL, save.all.series = TRUE,
  save.worst.series = FALSE, worst.linear.coef = NULL,
  impute.every = NULL, ...)

```

The only required inputs are a matrix of response variables, which may be provided as the first argument, and starting values for the parameters provided as `starting.values`.

Unlike `emNorm`, there is no default starting-value procedure; some starting values must be specified by the user. An easy way to get them is to run `emNorm` first and use the final parameter estimates from EM as the starting values for MCMC, as in the example below.

```
> emResult <- emNorm( cholesterol )
> mcmcResult <- mcmcNorm( cholesterol,
+   starting.values = emResult$param )
```

A second way to call `mcmcNorm` is to provide a model formula, a data frame in which the variables reside, and starting values for the parameters.

```
> mcmcResult <- mcmcNorm( cbind(Y1,Y2,Y3) ~ 1,
+   data = cholesterol,
+   starting.values = emResult$param )
```

The third and easiest way to call `mcmcNorm` is to supply an object of class "norm" produced by a previous call to `emNorm` or `mcmcNorm`. If we run `emNorm` first and then use its result as the first argument to `mcmcNorm`, the data, model, and prior distributions are carried over, and the final estimates from EM automatically become the starting values for MCMC.

```
> emResult <- emNorm(cholesterol)
> set.seed(92561) # so that you can reproduce these results
> mcmcResult <- mcmcNorm(emResult)
> summary(mcmcResult)
```

```
Method:                MCMC
Prior:                  "uniform"
Iterations:             1000
Cycles per iteration:   1
Impute every k iterations, k = NULL
No. of imputations created: 0
series.worst present:   TRUE
series.beta present:    TRUE
series.sigma present:   TRUE
```

Using estimates from EM as the starting values for MCMC has an additional benefit. Notice that the output from `summary` tells us that `mcmcResult` contains an object called `series.worst`. This is a time series that records the value of the worst linear function of the parameters at every iteration. The coefficients that determine the worst linear function were automatically computed by `emNorm` after the EM algorithm converged. Plotting `series.worst` and its autocorrelation (ACF) function helps us to assess the convergence behavior of MCMC.

```

> par(mfrow=c(3,2)) # arrange plots on page in a 3x2 matrix
> plot(mcmcResult$series.worst)
> acf(mcmcResult$series.worst)

```

These plots, which are shown in Figure 1, suggest that the algorithm approaches stationarity very quickly, with no appreciable serial dependence beyond lag 5.

Checking the behavior of the worst linear function is a sensible first step in judging convergence. Our experience with many data examples has shown that this series often behaves like a worst-case scenario; when the serial dependence in this series has died down, the dependence in other parameters has also died down. But counterexamples to this rule do exist, so after examining the worst linear function, it is best to look at other parameters as well. By default, the `mcmcNorm` function will save the full series for all nonredundant model parameters in objects called `series.beta` and `series.sigma`. Each of these is a multivariate time series with rows corresponding to the iterations of MCMC and columns corresponding to the individual parameters. In the example below, we plot the ACF's for all parameters, and the resulting plots are displayed in Figure 2.

```

> dim(mcmcResult$series.beta) # check dimensions of beta series
[1] 1000    3
> dim(mcmcResult$series.sigma) # check dimensions of sigma series
[1] 1000    6
> par(mfrow=c(3,3)) # nine plots per page
> for(i in 1:3)
+   acf(mcmcResult$series.beta[,i],
+       main=colnames(mcmcResult$series.beta)[i])
> for(i in 1:6)
+   acf(mcmcResult$series.sigma[,i],
+       main=colnames(mcmcResult$series.sigma)[i])

```

## 6.7 Inferences from simulated parameters

In this data example, it may be of interest to draw inferences about changes in mean cholesterol over time. Let  $\mu_j$ ,  $j = 1, 2, 3$  denote the mean cholesterol levels at the three occasions, and let  $\delta_{31} = \mu_3 - \mu_1$  be the average change from occasion 1 to occasion 3. The ML estimate of this parameter is

```

> emResult$param$beta[1,3] - emResult$param$beta[1,1]
[1] -31.69151

```

but because EM does not provide measures of uncertainty, we do not know whether this difference is statistically significant. The parameter series from MCMC, which contain

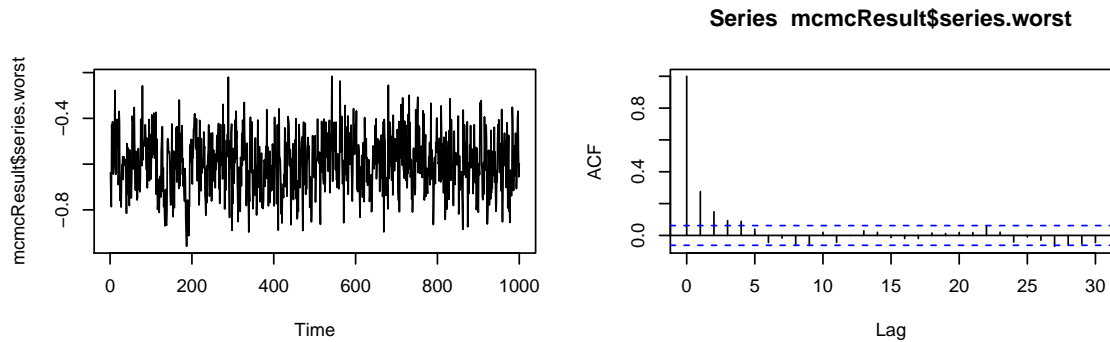


Figure 1: Time-series and ACF plots for the worst linear function of the parameters from 1,000 iterations of MCMC applied to the cholesterol data.

simulated draws from their posterior distribution, can be used to compute simulated Bayesian estimates and intervals for  $\delta_{31}$  or any other function of the parameters.

The default number of iterations (`iter=1000`) used by `mcmcNorm` is large enough to diagnose convergence in many problems, but it does not give very accurate estimates of posterior quantiles. So we will run `mcmcNorm` for an additional 10,000 iterations, using the simulated parameters at the end of first run as starting values, and retain only the parameter series from the new iterations. In effect, the first 1,000 iterations are being used as a burn-in period.

```
> mcmcResult <- mcmcNorm(mcmcResult, iter=10000)
```

Now we simply compute the 10,000 simulated values of  $\delta_{31}$  and summarize them.

```
> delta31 <- mcmcResult$series.beta[,3] -
+   mcmcResult$series.beta[,1]
> mean(delta31)    # simulated posterior mean
[1] -31.52694
> quantile(delta31, probs=c(.025,.975) )  # simulated 95% interval
      2.5%      97.5%
-57.190033  -5.198703
> table( delta31 < 0 )

FALSE  TRUE
  108   9892
```

The simulated 95% Bayesian posterior interval lies entirely below zero, so the drop in mean cholesterol appears to be statistically significant. About 99% of the simulated

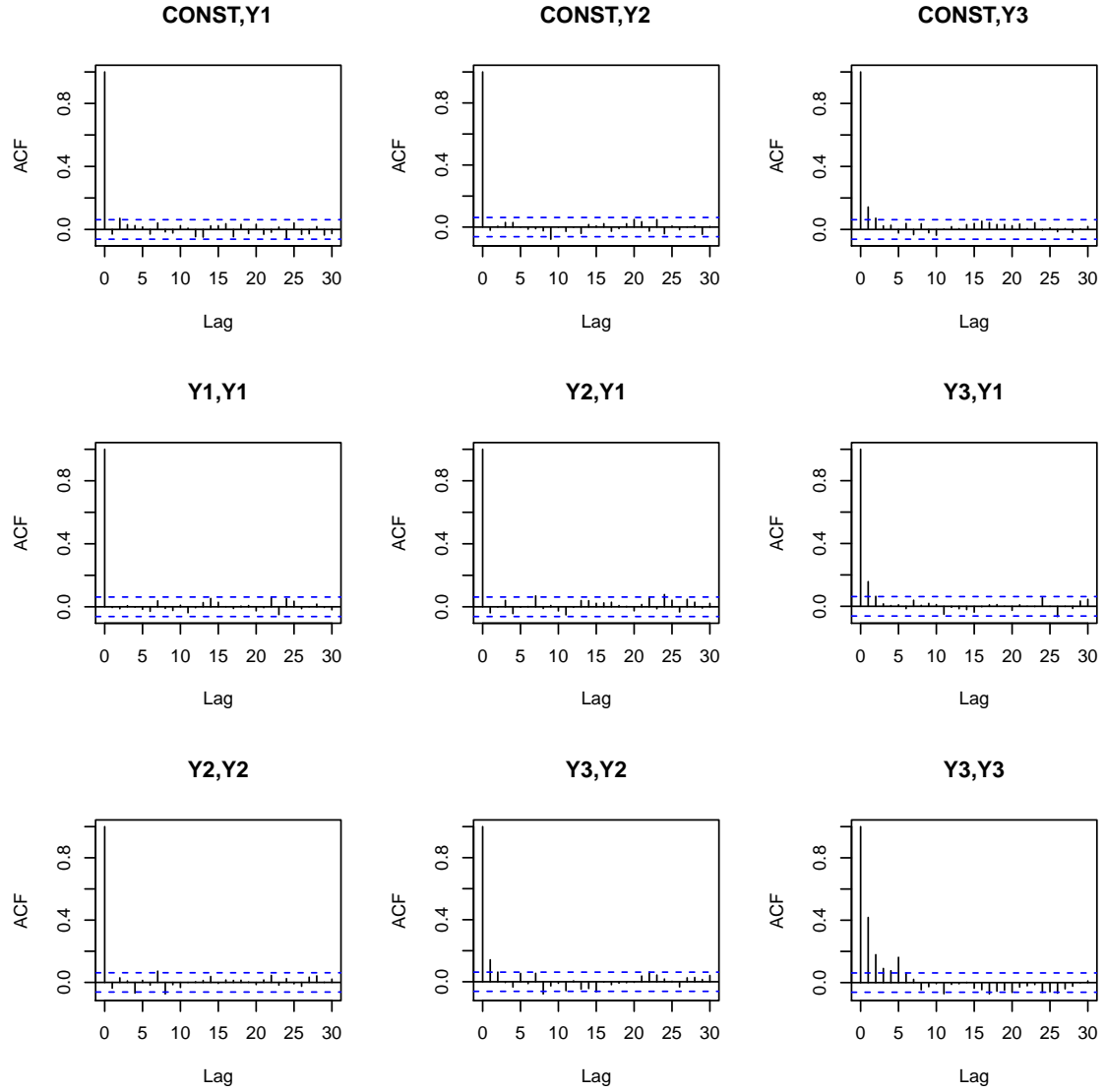


Figure 2: ACF plots for all parameters (means and covariances) from 1,000 iterations of MCMC applied to the cholesterol data.



values of  $\delta_{31}$  lie below zero, so we are about 99% sure, in the Bayesian sense, that the average level of cholesterol has declined between occasions 1 and 3.

Simulated parameters from successive iterations of MCMC tend to be positively correlated, so these 10,000 values of  $\delta_{31}$  carry less information than they would if they were independent draws from the posterior distribution. If independent draws are needed, the optional argument `multicycle` may be helpful. Specifying `multicycle=k` for some  $k > 1$  instructs `mcmcNorm` to perform the I- and P-step cycle  $k$  times within each iteration. Calling `mcmcNorm` with `iter=10000` and `multicycle=k` has the same effect as running the algorithm for  $10,000 \times k$  iterations and saving every  $k$ th set of simulated parameters. In this example, it is probably conservative to believe that the algorithm achieves stationarity by 10 cycles, because no significant serial correlations were seen beyond lag 5. Therefore,

```
> mcmcResult <- mcmcNorm(mcmcResult, iter=10000, multicycle=10)
```

should produce a `beta.series` and `sigma.series` that behave as 10,000 independent draws from the joint posterior distribution.

## 6.8 Creating multiple imputations

Another way to use MCMC for inference is to create multiple imputations (MI's). Simulated values of the missing observations from the I-steps of MCMC can be used as MI's, but they need to be independent of one another. The simplest way to achieve independence is to save the results from every  $k$ th I-step, where  $k$  is large enough to ensure stationarity. We do this by supplying the argument `impute.every=k` to `mcmcNorm`. In the example below, we start at the ML estimate and run the MCMC algorithm for 5,000 iterations, spacing the imputations  $k = 100$  iterations apart to create  $M = 50$  multiple imputations.

```
> emResult <- emNorm(cholesterol)
> set.seed(532) # so you can reproduce these results
> mcmcResult <- mcmcNorm(emResult, iter=5000, impute.every=100)
> summary(mcmcResult)
```

Method:	MCMC
Prior:	"uniform"
Iterations:	5000
Cycles per iteration:	1
Impute every k iterations, k =	100
No. of imputations created:	50
series.worst present:	TRUE

```

series.beta present:      TRUE
series.sigma present:     TRUE

```

The result from `mcmcNorm` now contains an object called `imp.list`. This is a list with  $M = 50$  components, where each component is a data matrix that resembles the original dataset `y`, except that the missing values have been imputed.

```

> cholesterol[1:5,] # first 5 rows of original data
   Y1  Y2  Y3
1 270 218 156
2 236 234  NA
3 210 214 242
4 142 116  NA
5 280 200  NA

> mcmcResult$imp.list[[1]][1:5,] # first 5 rows of imputed dataset 1
   Y1  Y2      Y3
[1,] 270 218 156.0000
[2,] 236 234 179.0431
[3,] 210 214 242.0000
[4,] 142 116  90.7577
[5,] 280 200 185.2721

> mcmcResult$imp.list[[2]][1:5,] # first 5 rows of imputed dataset 2
   Y1  Y2      Y3
[1,] 270 218 156.0000
[2,] 236 234 204.7819
[3,] 210 214 242.0000
[4,] 142 116 215.8521
[5,] 280 200 224.6960

```

The method described above for creating MI's relies on a single chain of  $Mk$  iterations. A slightly different method is to run  $M$  chains of  $k$  iterations each. At the end of each chain, we call the function `impNorm` to generate a single random imputation based on the final simulated parameters. In the example below, we run  $M = 50$  chains of 100 iterations each, starting each chain at the ML estimate, generate an imputed dataset at the end of each chain, and save the imputed datasets as a list.

```

> imp.list <- as.list(NULL)
> for(m in 1:50){
+   mcmcResult <- mcmcNorm(emResult, iter=100)
+   imp.list[[m]] <- impNorm(mcmcResult) }

```

## 6.9 Combining the results from post-imputation analyses

Now let's use the imputed datasets to draw inferences about the mean difference  $\delta_{31}$ . With complete data, inferences about this parameter correspond to a paired t-test. That is, we estimate  $\delta_{31}$  by the mean of the difference scores (occasion 3 minus occasion 1) among the  $N = 28$  patients. The standard error is the variance of the difference scores divided by  $N$ . In the code below, we generate  $M = 50$  imputed datasets by the single-chain method, compute the estimate and standard error from each one, and save the results as two lists.

```
> emResult <- emNorm(cholesterol)
> set.seed(532) # so you can reproduce these results
> mcmcResult <- mcmcNorm(emResult, iter=5000, impute.every=100)
> est.list <- as.list(NULL) # to hold the estimates
> std.err.list <- as.list(NULL) # to hold the standard errors
> for(m in 1:50){
+   y.imp <- mcmcResult$imp.list[[m]] # one imputed dataset
+   diff <- y.imp[,3] - y.imp[,1] # difference scores
+   est.list[[m]] <- mean(diff)
+   std.err.list[[m]] <- sqrt( var(diff) / length(diff) ) }
```

Now we combine the results across imputations using the techniques described in Section 4.6, which are implemented in the function `miInference`. The syntax for calling this function, as provided in its documentation file, is shown below.

```
miInference( est.list, std.err.list, method = "scalar",
             df.complete = NULL )
```

Arguments:

`est.list`: a list of estimates to be combined. Each component of this list should be a scalar or vector containing point estimates from the analysis of an imputed dataset. This list should have `_M_` components, where `_M_` is the number of imputations, and all components should have the same length.

`std.err.list`: a list of standard errors to be combined. Each component of this list should be a scalar or vector of standard errors associated with the estimates in `'est.list'`.

`method`: how are the estimates to be combined? At present, the only type allowed is `"scalar"`, which means that estimands are treated as one-dimensional entities. If `'est.list'` contains vectors, inference for each element of the vector is carried

out separately; covariances among them are not considered.

`df.complete`: degrees of freedom assumed for the complete-data inference. This should be a scalar or a vector of the same length as the components of `'est.list'` and `'std.err.list'`.

If there were no missing data in this example, tests and intervals for  $\delta_{31}$  would be based on a  $t$ -distribution with  $N - 1 = 27$  degrees of freedom. Therefore, when we call `miInference`, we need to supply the argument `df.complete=27`.

```
> miResult <- miInference(est.list, std.err.list, df.complete=27)
> miResult
```

	Est	SE	Est/SE	df	p	Pct.mis
[1,]	-31.84235	11.37477	-2.799383	18.9	0.011	23.3

The overall estimate of  $-31.8$  is close to the ML estimate of  $-31.7$  and the simulated posterior mean of  $-31.5$  reported earlier. The endpoints of the approximate 95% confidence interval from MI,

```
> miResult$est - miResult$std.err * qt(.975, miResult$df)
[1] -55.65734

> miResult$est + miResult$std.err * qt(.975, miResult$df)
[1] -8.02737
```

are also close to the endpoints of the simulated 95% posterior interval  $(-57.2, -5.20)$  reported earlier.

## 7 Using the package: Example 2

### 7.1 Marijuana data

We now turn to an example that is less straightforward. Weil, Zinberg, and Nelson (1968) described an experiment to investigate the effects of marijuana. Nine male subjects received three treatments each (placebo, low dose and high dose). Under each treatment, the change in heart rate (beats per minute above baseline) was recorded 15 minutes after smoking and 90 minutes after smoking, producing six measures per subject, but five of the 54 data values are missing. These data are distributed with `norm2` as a data frame called `marijuana`.

```

> data(marijuana)
> marijuana
  Plac.15 Low.15 High.15 Plac.90 Low.90 High.90
1      16    20      16      20     -6      -4
2      12    24      12      -6      4      -8
3       8     8      26      -4      4       8
4      20     8      NA      NA     20     -4
5       8     4     -8      NA     22     -8
6      10    20     28     -20     -4     -4
7       4    28     24      12      8     18
8      -8    20     24      -3      8    -24
9      NA    20     24       8     12     NA

```

Classical analysis-of-variance methods for repeated measures make strong assumptions about the covariance structure. Following the example analyses of Schafer (1997, Chap. 5), we will proceed without assuming any particular form for the within-person covariance matrix.

## 7.2 Difficulties with noninformative priors

As in the cholesterol example, we will run the EM algorithm and then use the resulting ML estimates as starting values for MCMC.

```

> emResult <- emNorm(marijuana)
Note: Finite-differencing procedure strayed outside
parameter space; solution at or near boundary.
OCCURRED IN: estimate_worst_frac in MOD norm_engine
> set.seed(543)
> mcmcResult <- mcmcNorm(emResult)
Note: Degrees of freedom not positive.
OCCURRED IN: ran_genchi in MOD random_generator
OCCURRED IN: run_pstep in MOD norm_engine
Posterior distribution may not be proper.
MCMC aborted at iteration 1, cycle 1
OCCURRED IN: run_norm_engine_mcmc in MOD norm_engine

```

What happened? The EM algorithm did converge, but the procedure for estimating the worst fraction of missing information and worst linear function failed. The warning message indicates that the EM solution lies at or near the boundary of the parameter space, meaning that the final estimate of the covariance matrix  $\Sigma$  is nearly singular. The MCMC procedure did not work and aborted at the first cycle. The problem lies with the prior distribution. The default prior density for  $\Sigma$ , which is `prior="uniform"`, looks

like an inverted Wishart density with  $\xi = -(r + 1)$  degrees of freedom, where  $r$  is the number of response variables (Section 3.5). It is not a real density function, however, because the inverted Wishart density does not exist unless the degrees of freedom exceed  $r$  (Schafer, 1997, Chap. 5). When the sample size is large, this is not a problem, because the complete-data posterior distribution for  $\Sigma$  is inverted Wishart with degrees of freedom equal  $\xi + N - p$ , where  $\xi$  is the prior degrees of freedom,  $N$  is the sample size, and  $p$  is the number of predictors. But in this particular example, we have  $r = 6$ ,  $\xi = -7$ ,  $N = 9$ , and  $p = 1$  (the only predictor is a constant), so the posterior degrees of freedom are

$$-(r + 1) + (N - p) = 1,$$

which does not yield a proper posterior distribution even with complete data.

When  $(N - p)$  is much larger than  $r$ , the choice of prior distribution tends to have little impact on the results. But with small samples like this one, the uniform prior may cause difficulty in MCMC. A better choice is the Jeffreys noninformative prior, which resembles an inverted Wishart density with prior degrees of freedom equal to 0. Under the Jeffreys prior, the posterior degrees of freedom with complete data are  $(N - p)$ , which is proper provided that  $(N - p) > r$ .

Let's see what happens if we run MCMC under the Jeffreys prior starting at the posterior mode.

```
> emResult <- emNorm(marijuana, prior="jeffreys")
Note: Finite-differencing procedure strayed outside
parameter space; solution at or near boundary.
OCCURRED IN: estimate_worst_frac in MOD norm_engine
> set.seed(543)
> mcmcResult <- mcmcNorm(emResult)
Note: Matrix not positive definite
OCCURRED IN: cholesky_saxpy in MOD matrix_methods
OCCURRED IN: run_pstep in MOD norm_engine
Posterior distribution may not be proper.
MCMC aborted at iteration 106, cycle 1
OCCURRED IN: run_norm_engine_mcmc in MOD norm_engine
```

In this run, MCMC aborted at iteration 106. The error message again suggests that the posterior distribution may not be proper. This time, however, the problem is not that the degrees of freedom are negative, but that the estimated covariance matrix became singular or negative definite. This problem arises when the pattern of missing values causes some aspects of the covariance matrix to be poorly estimated or inestimable from the observed data.

To get more insight into what is happening, let's run EM again under a uniform prior and look at the results.

```
> emResult <- emNorm(marijuana)
> summary(emResult, show.variables=F, show.patterns=F, show.params=F )
```

```
Method:                EM
Prior:                 "uniform"
Convergence criterion: 1e-05
Iterations:            288
Converged:             TRUE
Max. rel. difference:  8.810968e-06
-2 Loglikelihood:      114.3465
-2 Log-posterior density: 114.3465
Estimated rate of convergence: 0.47868
```

EM apparently converged, but the estimated covariance matrix is nearly singular, because its smallest eigenvalue is nearly zero.

```
> eigen(emResult$param$sigma, symmetric=T, only.values=T)
$values
[1] 7.510111e+02 1.483758e+02 8.574829e+01 4.563068e+01 2.783385e+01
[6] 6.523830e-10

$vectors
NULL
```

In fact, if we run EM again with a stricter convergence criterion, the procedure aborts, showing that the ML estimate does indeed lie on the boundary of the parameter space.

```
> emResult <- emNorm(marijuana, criterion=1e-06)
Note: Attempted logarithm of non-positive number
Cov. matrix became singular or negative definite.
OCCURRED IN: run_estep in MOD norm_engine
EM algorithm aborted at iteration 459
OCCURRED IN: run_norm_engine_em in MOD norm_engine
Warning message:
In emNorm.default(marijuana, criterion = 1e-06) :
Algorithm did not converge by iteration 464
```

### 7.3 Using a ridge prior

When aspects of the covariance structure are poorly estimated or inestimable, one remedy is to introduce a small amount of prior information. The ridge prior (Section 3.5), allows the variances to be estimated from the observed data, but smooths the estimated

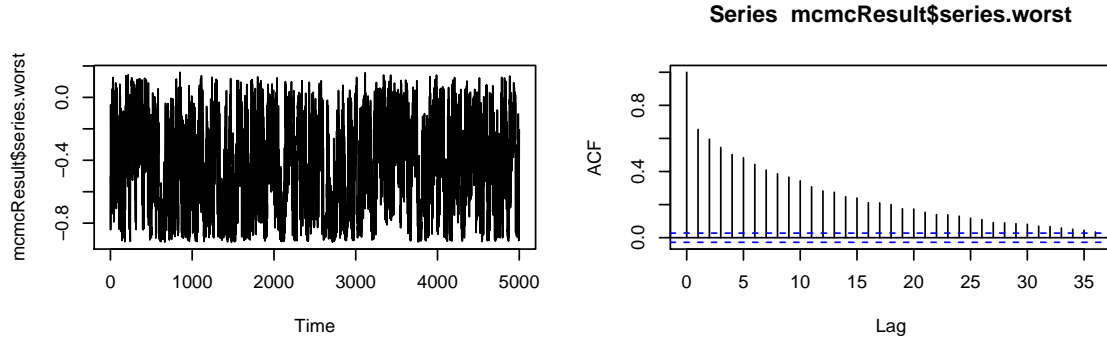


Figure 3: Time-series and ACF plots for the worst linear function of the parameters from 5,000 iterations of MCMC applied to the marijuana data under ridge prior.

correlations toward zero. The degree of smoothing is controlled by the prior degrees of freedom  $\xi$ , which is specified via the argument `prior.df`. In many cases, we can stabilize the inference with very small amounts of prior information. Here we apply a ridge prior with  $\xi = 0.5$  and run 5,000 iterations of MCMC starting from the posterior mode.

```
> emResult <- emNorm(marijuana, prior="ridge", prior.df=0.5)
> set.seed(543)
> mcmcResult <- mcmcNorm(emResult, iter=5000)
```

This time, the procedure ran without difficulty. Plots of the worst linear function (Figure 3) show that MCMC converges slowly because the rates of missing information are high.

## 7.4 Inferences by parameter simulation

The slow convergence of MCMC in this example indicates that many iterations will be required to get precise estimates for quantities of interest. Here we perform an analysis similar to that of Schafer (1997, Sec. 5.4), examining posterior distributions for contrasts among the means of the repeated measurements. Let  $\mu_j$ ,  $j = 1, \dots, 6$  denote the means for the six measurements, and let  $\delta_{jk} = \mu_j - \mu_k$  denote a contrast between two means. In the code below, we run 10,000 iterations of MCMC, cycling the procedure 100 times within each iteration, so that the simulated draws saved to the parameter series are approximately independent. From the series, we compute 10,000 simulated values for the six contrasts  $\delta_{21}$ ,  $\delta_{31}$ ,  $\delta_{32}$ ,  $\delta_{54}$ ,  $\delta_{64}$ , and  $\delta_{65}$ , and summarize them with a boxplot-like graph that, except for a minor amount of random noise, replicates the results shown in Schafer (1997, Fig. 5.9). The boxplot-like graph is shown in Figure 4.

```
> set.seed(876)
```



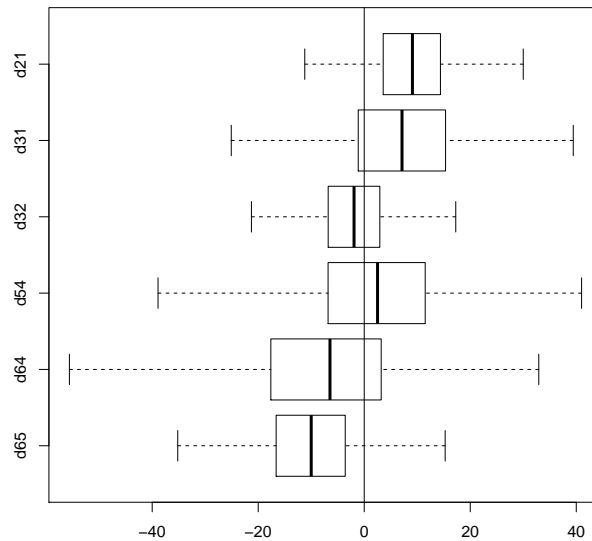


Figure 4: Simulated posterior medians, quartiles and 95% equal-tailed posterior intervals for six contrasts from the marijuana dataset.

```
> mcmcResult <- mcmcNorm(emResult, iter=10000, multicycle=100)
>
> diff.scores <- cbind(
+   d65 = mcmcResult$series.beta[,6] - mcmcResult$series.beta[,5],
+   d64 = mcmcResult$series.beta[,6] - mcmcResult$series.beta[,4],
+   d54 = mcmcResult$series.beta[,5] - mcmcResult$series.beta[,4],
+   d32 = mcmcResult$series.beta[,3] - mcmcResult$series.beta[,2],
+   d31 = mcmcResult$series.beta[,3] - mcmcResult$series.beta[,1],
+   d21 = mcmcResult$series.beta[,2] - mcmcResult$series.beta[,1] )
>
> # construct boxplot-like graph showing the posterior
> # median, quartiles and 95% interval for each contrast
> stats <- matrix( NA, 5, 6)
> for(i in 1:6)
+   stats[,i] <- quantile( diff.scores[,i], probs=c(.025,.25,.5,.75,.975))
> box.stats <- list( stats=stats, names=colnames(diff.scores) )
> bxp( box.stats, horizontal=T )
> abline(v=0)
```

## 8 Using the package: Example 3

### 8.1 FLAS data

Our third example uses the dataset `flas`. These data come from a pilot study to assess the reliability and validity of the Foreign Language Attitude Scale (FLAS), an instrument for predicting success in the study of foreign languages (Raymond and Roberts, 1983). The questionnaire was given to  $N = 279$  students enrolled in four different language courses (French, German, Spanish, Russian) at Penn State University. This dataset includes FLAS score, final grade in the course, and other variables relevant to academic achievement. The variables in the dataset, as shown in its documentation file, are:

```
'LAN2' 1=Spanish, 0=other.  
  
'LAN3' 1=German, 0=other.  
  
'LAN4' 1=Russian, 0=other.  
  
'AGE' age group (1=less than 20, 2=20+).  
  
'PRI' number of prior foreign language courses (1=none, 2=1-2,  
      3=3+).  
  
'SEX' 0=male, 1=female  
  
'MLAT' Modern Language Aptitude Test  
  
'FLAS' Foreign Language Attitude Scale  
  
'SATV' Scholastic Aptitude Test, verbal score  
  
'SATM' Scholastic Aptitude Test, math score  
  
'ENG' score on Penn State English placement exam  
  
'HGPA' high school grade point average  
  
'CGPA' current college grade point average  
  
'GRD' final grade in foreign language course (1=B or lower, 2=A)
```

Notice that the language variable, a nominal variable with four categories and no missing values, has been converted to three dummy codes. Including these dummy codes either as

responses or predictors allows the means of the other variables to vary without constraints across the four language groups.

## 8.2 Applying a ridge prior

When the EM algorithm is applied to the FLAS dataset, it converges quickly.

```
> data(flas)
> emResult <- emNorm(flas)
Note: Eigen power method failed to converge.
OCCURRED IN: estimate_worst_frac in MOD norm_engine
> summary(emResult, show.variables=F, show.patterns=F, show.params=F)

Method:                EM
Prior:                  "uniform"
Convergence criterion:  1e-05
Iterations:             17
Converged:              TRUE
Max. rel. difference:   6.0021e-06
-2 Loglikelihood:       7310.107
-2 Log-posterior density: 7310.107
Worst fraction missing information: NA
```

The quick convergence of EM suggests that the rates of missing information are low. However, the procedure for estimating the worst fraction of missing information failed, suggesting that something has gone awry. If we try to run MCMC using the default uniform prior, we encounter difficulty. The procedure does not abort, but the time-series and ACF plots for the mean of the variable GRD, which are shown in Figure 5, show that this parameter exhibits long-term drift. (In this example, the worst linear function of the parameters is not available, so we need to diagnose convergence by examine time-series and ACF plots for individual elements or other functions of  $\beta$  and  $\Sigma$ .)

```
> set.seed(765)
> mcmcResult <- mcmcNorm(emResult)
> par(mfrow=c(3,2))
> plot(mcmcResult$series.beta[,14])
> acf(mcmcResult$series.beta[,14])
```

Long-term drifts in a parameter series suggest that the parameter is poorly estimated or inestimable. Estimability problems may arise when missing values fall in a malicious pattern. In this example, the problem is that value of GRD happens to be missing for everyone who studied Russian.

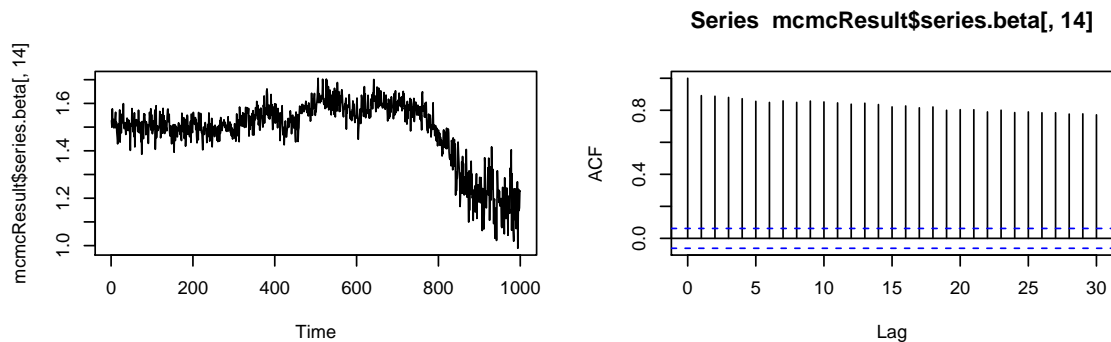


Figure 5: Time-series and ACF plots for the mean of variable GRD from 1,000 iterations of MCMC applied to the FLAS data under a uniform prior.

```
> table( flas$LAN4, is.na(flas$GRD))
```

	FALSE	TRUE
0	232	27
1	0	20

This pattern of missing values makes it impossible to estimate the mean of GRD among those who study Russian. With an improper prior distribution and a malicious pattern of missing values, it is possible to have a situation where, even though the I- and P-steps are well defined at each iteration, the posterior distribution does not exist, and the MCMC algorithm cannot converge (Schafer, 1997, Sec. 3.5).

When some parameters are inestimable, different starting values for EM may lead to different parameter estimates with exactly the same loglikelihood. We can diagnose inestimability using a combination of EM and MCMC. In the code example below, we use MCMC to generate random starting values for the parameters and then run EM from these random starts. The three EM runs converge to different solutions (note the different estimates for the mean of GRD), but the loglikelihood at the three solutions looks exactly the same.

```
> data(flas)
> emResult <- emNorm(flas)
Note: Eigen power method failed to converge.
OCCURRED IN: estimate_worst_frac in MOD norm_engine
> summary(emResult, show.variables=F,
+   show.patterns=F, show.params=F)

Method:                EM
Prior:                  "uniform"
```

```

Convergence criterion:          1e-05
Iterations:                     17
Converged:                      TRUE
Max. rel. difference:          6.0021e-06
-2 Loglikelihood:               7310.107
-2 Log-posterior density:       7310.107
Worst fraction missing information: NA

```

Eigen power method failed to converge.

OCCURRED IN: estimate\_worst\_frac in MOD norm\_engine

```

> set.seed(765)
> mcmcResult <- mcmcNorm(emResult)
> par(mfrow=c(3,2))
> plot(mcmcResult$series.beta[,14])
> acf( mcmcResult$series.beta[,14])

> # generate three random starts by running MCMC
> # from the EM estimates
> set.seed(321)
> random.start.1 <- mcmcNorm(emResult,iter=100)
> random.start.2 <- mcmcNorm(emResult,iter=100)
> random.start.3 <- mcmcNorm(emResult,iter=100)

> # now run EM from the random starts
> emResult.1 <- emNorm( random.start.1 )
> emResult.2 <- emNorm( random.start.2 )
> emResult.3 <- emNorm( random.start.3 )

> # compare the loglikelihoods at the three EM solutions
> loglikNorm( emResult.1 )
[1] -3655.054
> loglikNorm( emResult.2 )
[1] -3655.054
> loglikNorm( emResult.3 )
[1] -3655.054

> # compare the estimates of beta
> emResult.1$param$beta
      LAN2      LAN3      LAN4      AGE      PRI
CONST 0.2795699 0.4086022 0.07168459 1.530772 2.196905
      SEX      MLAT      FLAS      SATV      SATM
CONST 0.4527892 82.48746 24.11213 498.3939 560.6742
      ENG      HGPA      CGPA      GRD
CONST 52.85448 2.749734 3.265421 1.39928

```

```

> emResult.2$param$beta
      LAN2      LAN3      LAN4      AGE      PRI
CONST 0.2795699 0.4086022 0.07168459 1.530772 2.196905
      SEX      MLAT      FLAS      SATV      SATM
CONST 0.4527892 82.48746 24.11213 498.3939 560.6742
      ENG      HGPA      CGPA      GRD
CONST 52.85448 2.749734 3.265421 1.537627

> emResult.3$param$beta
      LAN2      LAN3      LAN4      AGE      PRI
CONST 0.2795699 0.4086022 0.07168459 1.530772 2.196905
      SEX      MLAT      FLAS      SATV      SATM
CONST 0.4527892 82.48746 24.11213 498.3939 560.6742
      ENG      HGPA      CGPA      GRD
CONST 52.85448 2.749734 3.265421 1.728877

```

### 8.3 Applying a ridge prior

To overcome the problem of inestimability, we apply a ridge prior with  $\xi = 3$  prior degrees of freedom. This small amount of information, which corresponds to about 1% of the sample size, is enough to identify the inestimable parameters. With this prior, MCMC does converge, but very slowly. Here we run MCMC from 100,000 iterations beginning from the posterior mode, and then we plot the time series and ACF for the mean of GRD. The plots are shown in Figure 6.

```

> emResult <- emNorm(flas, prior="ridge", prior.df=3)
> set.seed(765)
> # relax, this may take a little while
> mcmcResult <- mcmcNorm(emResult, iter=100000)
> par(mfrow=c(2,2))
> # plot first tenth of the series
> plot(mcmcResult$series.beta[1:10000,14],type="l")
> # estimate the acf from the whole series
> acf(mcmcResult$series.beta[,14], lag.max=600, col="grey")

```

(If you are unable to run this example because of the memory limitations of your system, try reducing the number of iterations to `iter=1000` and use the option `multicycle=100`. MCMC will still run for 100,000 cycles, but `mcmcNorm` will save the simulated parameters only at every 100th cycle, and the ACF will die down by lag 6 rather than lag 600.)

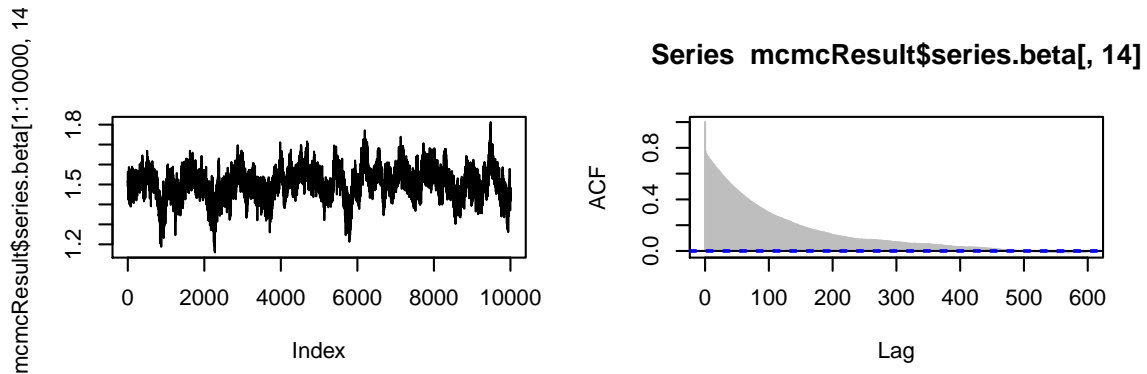


Figure 6: Time-series and ACF plots for the mean of variable GRD from MCMC applied to the FLAS data under a ridge prior.

## 8.4 Analysis by multiple imputation

In earlier analyses of these data, Schafer (1997, Sec. 6.3) imputed missing values under the joint normal model and then analyzed the imputed data by fitting logistic regressions with GRD as a binary response. Now we will try to replicate those results. First, we run MCMC for 50,000 iterations using a ridge prior with  $\xi = 3$ . We save the imputed values at every 1,000th iteration, producing  $M = 50$  multiple imputations. Because we no longer need to save the parameter series, we now call `mcmcNorm` with the argument `save.all.series=FALSE`.

```
> emResult <- emNorm(flas, prior="ridge", prior.df=3)
> set.seed(765)
> mcmcResult <- mcmcNorm(emResult, iter=50000,
+   save.all.series=FALSE, impute.every=1000)
```

After imputation, we round off the imputed values for the discrete variables AGE, PRI, SEX and GRD to the nearest categories. Then we recode AGE to a dummy indicator for age  $\geq 20$  and characterize the effect of PRI with linear and quadratic terms. Finally, we regress an indicator for GRD=2 on the entire set of recoded covariates, saving the coefficients and standard errors, and combine the results by Rubin's (1987) rules for scalar estimands.

```
> est.list <- as.list(NULL) # to hold estimated coefficients
> std.err.list <- as.list(NULL) # to hold their standard errors
> for(m in 1:50){
+   imp <- mcmcResult$imp.list[[m]] # one imputed dataset
+   imp <- data.frame(imp) # convert into a data frame
+   # round AGE and change to dummy indicator for age=20+
+   imp$AGE.2 <- 1*(imp$AGE>1.5) # dummy indicator for age=20+
+   # round PRI and define linear, quadratic terms
```

```

+   imp$PRI <- round(imp$PRI)
+   imp$PRI[imp$PRI<1] <- 1
+   imp$PRI[imp$PRI>3] <- 3
+   imp$PRI.L <- -1*(imp$PRI==1) +0*(imp$PRI==2) + 1*(imp$PRI==3)
+   imp$PRI.Q <- 1*(imp$PRI==1) -2*(imp$PRI==2) + 1*(imp$PRI==3)
+   # round SEX and change to dummy indicator for female
+   imp$SEX <- 1*(imp$SEX>.5)
+   # round imputed GRD and recode to 1=A, 0=B or lower
+   imp$GRD <- 1*(imp$GRD > 1.5)
+   # fit logistic model
+   glmResult <- glm( GRD ~ LAN2 + LAN3 + LAN4 + AGE.2 + PRI.L +
+     PRI.Q + SEX + MLAT + FLAS + SATV + SATM + ENG + HGPA + CGPA,
+     data=imp, family=binomial)
+   # save estimates and SE's
+   est.list[[m]] <- glmResult$coefficients
+   std.err.list[[m]] <-
+     sqrt( diag( summary(glmResult)$cov.scaled ) ) }

> # combine the results by Rubin's (1987) rules
> miResult <- miInference(est.list, std.err.list)
> miResult

```

	Est	SE	Est/SE	df	p
(Intercept)	-1.5495e+01	2.9395e+00	-5.271	810.5	0.000
LAN2	3.6052e-01	5.0760e-01	0.710	2484.9	0.478
LAN3	1.1272e+00	4.4173e-01	2.552	7161.6	0.011
LAN4	-2.1253e-01	6.6213e+02	0.000	527837921.7	1.000
AGE.2	1.3719e+00	4.4020e-01	3.117	1014.3	0.002
PRI.L	2.9659e-01	2.4933e-01	1.190	1198.9	0.234
PRI.Q	-1.3100e-01	1.4701e-01	-0.891	1267.0	0.373
SEX	7.5617e-01	4.4557e-01	1.697	1272.6	0.090
MLAT	4.0815e-02	1.5886e-02	2.569	789.4	0.010
FLAS	1.0839e-01	5.0364e-02	2.152	366.9	0.032
SATV	-3.3027e-03	3.3211e-03	-0.994	1018.8	0.320
SATM	2.9059e-04	2.6788e-03	0.108	1975.8	0.914
ENG	9.5108e-03	2.2439e-02	0.424	919.0	0.672
HGPA	2.2366e+00	4.5447e-01	4.921	1678.3	0.000
CGPA	8.5284e-01	5.4255e-01	1.572	697.9	0.116

	Pct.mis
(Intercept)	24.6
LAN2	14.0
LAN3	8.3
LAN4	0.0
AGE.2	22.0
PRI.L	20.2
PRI.Q	19.7



SEX	19.6
MLAT	24.9
FLAS	36.5
SATV	21.9
SATM	15.7
ENG	23.1
HGPA	17.1
CGPA	26.5

The results from this analysis are quite similar to those reported by Schafer (1997, Table 6.8). The differences could plausibly be due to random noise, except for one discrepancy: the standard error for the coefficient of `LAN4` shown above is huge. This is the one parameter for which the observed data carry essentially no information. The logistic regression procedure converged for all  $M = 50$  imputed datasets, but for some of these, the estimated standard error was very large, suggesting that the Hessian of the loglikelihood was nearly singular. These large standard errors inflated the value of the within-imputation variance  $\bar{U}$  and caused the estimated rate of missing information for this parameter to be essentially zero.

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