Conditional Model Selection in Mixed-Effects Models with cAIC4

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Abstract

Model selection in mixed models based on the conditional distribution is appropriate for many practical applications and has been a focus of recent statistical research. In this paper we introduce the R-package cAIC4 that allows for the computation of the conditional Akaike Information Criterion (cAIC). Computation of the conditional AIC needs to take into account the uncertainty of the random effects variance and is therefore not straightforward. We introduce a fast and stable implementation for the calculation of the cAIC for linear mixed models estimated with lme4 and additive mixed models estimated with gamm4. Furthermore, cAIC4 offers a stepwise function that allows for a fully automated stepwise selection scheme for mixed models based on the conditional AIC. Examples of many possible applications are presented to illustrate the practical impact and easy handling of the package.

Keywords: conditional AIC, lme4, Mixed Effects Models, Penalized Splines.

1. Introduction

The linear mixed model is a flexible and broadly applicable statistical model. It is naturally used for analysing longitudinal or clustered data. Furthermore, any regularized regression model incorporating a quadratic penalty can be written in terms of a mixed model. This incorporates smoothing spline models, spatial models and more general additive models (Wood 2017). Thus efficient and reliable estimation of such models is of major interest for applied statisticians. The package lme4 for the statistical computing software R (R Core Team 2016) offers such an exceptionally fast and generic implementation for mixed models (see Bates, Mächler, Bolker, and Walker 2015). The package has a modular framework allowing for the profile restricted maximum likelihood (REML) criterion as a function of the model parameters to be optimized using any constrained optimization function in R and uses rapid techniques for solving penalized least squares problems based on sparse matrix methods. The fact that mixed models are widely used popular statistical tools make model selection an indispensable necessity. Consequently research regarding model choice, variable selection and hypothesis testing in mixed models has flourished in recent years. Hypothesis testing on random effects is well established, although for likelihood ratio tests...
boundary issues arise (Crainiceanu and Ruppert 2004; Greven, Crainiceanu, Küchenhoff, and Peters 2008; Wood 2013). In model selection for mixed models using the Akaike information criterion (AIC Akaike 1973), Vaida and Blanchard (2005) suggest to use different criteria depending on the focus of the underlying research question. They make a distinction between questions with a focus on the population and on clusters, respectively. For the latter, they introduce a conditional AIC accounting for the shrinkage in the random effects. Based on this conditional AIC, Liang, Wu, and Zou (2008) propose a criterion that corrects for the estimation uncertainty of the random effects variance parameters based on a numerical approximation. Greven and Kneib (2010) show that ignoring this estimation uncertainty induces a bias and derive an analytical representation for the conditional AIC. For certain generalized mixed models, analytical representations of the conditional AIC exist, for instance for Poisson responses (see Lian 2012). Although there is no general unbiased criterion in analytical form for all exponential family distributions as argued in Säfken, Kneib, van Waveren, and Greven (2014), bootstrap-based methods can often be applied as we will show for those in presented in Efron (2004). An asymptotic criterion for a wider class of distributions is described in Wood, Pya, and Säfken (2016).

In this paper, we describe an add-on package to lme4 that facilitates model selection based on the conditional AIC and illustrates it with several examples. For the conditional AIC proposed by Greven and Kneib (2010) for linear mixed models, the computation of the criterion is not as simple as it is for other common AIC criteria. This article focuses on techniques for fast and stable computation of the conditional AIC in mixed models estimated with lme4, as they are implemented in the R-package cAIC4. The amount of possible models increases substantially with the R-package gamm4 (see Wood and Scheipl 2016) allowing for the estimation of a wide class of models with quadratic penalty such as spline smoothing and additive models. The presented conditional AIC applies to any of these models. In addition to translating the findings of Greven and Kneib (2010) to the model formulations used in Bates et al. (2015), we present the implementation of conditional AICs proposed for non-Gaussian settings in Säfken et al. (2014) and as we propose based on Efron (2004). With these results, a new scheme for stepwise conditional variable selection in mixed models is introduced. This allows for fully automatic choice of fixed and random effects based on the optimal conditional AIC. All methods are accompanied by examples, mainly taken from lme4, see Bates et al. (2015). The rest of this paper is structured as follows:

In Section 2 the mixed model formulations are introduced based on one example with random intercepts and random slopes and a second example on penalised spline smoothing. The conditional AIC for Gaussian, Poisson and Bernoulli responses is introduced in Section 3. Section 4 gives a hands-on introduction to cAIC4 with specific examples for the sleepstudy and the grouseticks data from lme4. The new scheme for stepwise conditional variable selection in mixed models is presented in Section 5 and applied to the Pastes data set. After the conclusion in Section 6, part A of the appendix describes how cAIC4 automatically deals with boundary issues. Furthermore the underlying code for the rapid computation of the conditional AIC is presented in part B of the appendix.

2. The mixed model

In a linear mixed model, the conditional distribution of the response $y$ given the random
effects $u$ has the form

$$ y \mid u \sim \mathcal{N}(X\beta + Zu, \sigma^2 I_n), \quad (1) $$

where $y$ is the $n$-dimensional vector of responses, $\beta$ is the $p$-dimensional vector of fixed effects and $u$ is the $q$-dimensional vector of random effects. The matrices $X$ and $Z$ are the $(n \times p)$ and $(n \times q)$ design matrices for fixed and random effects, respectively, and $\sigma^2$ refers to the variance of the error terms.

The unconditional distribution of the random effects $u$ is assumed to be a multivariate Gaussian with mean $0$ and positive semidefinite $(q \times q)$ covariance matrix $D_\theta$, i.e.,

$$ u \sim \mathcal{N}(0, D_\theta). $$

The symmetric covariance matrix $D_\theta$ depends on the covariance parameters $\theta$ and may be decomposed as

$$ D_\theta = \sigma^2 \Lambda_\theta \Lambda^t_\theta, \quad (2) $$

with the lower triangular covariance factor $\Lambda_\theta$ and the variance parameter $\sigma^2$ of the conditional response distribution. In analogy to generalized linear models, the generalized linear mixed model extends the distributional assumption in (1) to a distribution $\mathcal{F}$ from the exponential family,

$$ y \mid u \sim \mathcal{F}(\mu, \phi) $$

where $\phi$ is a scale parameter and the mean has the form

$$ \mu = \mathbb{E}(y \mid u) = h(X\beta + Z u), \quad (3) $$

with $h$ being the response function applied componentwise and natural parameter $\eta = h^{-1}(\mu)$. As the hereinafter presented results are limited to the Poisson and binomial distributions we can assume $\phi = 1$. The symmetric covariance matrix in (2) then is the same as for Gaussian responses except that $\sigma^2$ is omitted, i.e., $D_\theta = \Lambda_\theta \Lambda^t_\theta$.

The given conditional formulations of (generalized) linear mixed models imply marginal models, which can (conceptually) be obtained by integrating the random effects out of the joint distribution of $y$ and $u$, i.e.,

$$ f(y) = \int f(y \mid u) f(u) du. $$

However, there is typically no closed form solution for this integral. While the marginal model formulation is usually used for estimation, an analytic representation of $f(y)$ is only available for the linear mixed model (1). The marginal distribution $f(y)$ for Gaussian responses $y$ is given by

$$ y \sim \mathcal{N}(X\beta, \sigma^2 \left( I_n + Z \Lambda_\theta \Lambda^t_\theta Z^t \right)). $$
Further extensions of linear mixed models can be obtained by, for example, relaxing the assumption $\text{Cov}(\mathbf{y}|\mathbf{u}) = \sigma^2 \mathbf{I}_n$.

**Example I: Random intercepts and random slopes**

Some special cases of mixed models are commonly used in applications, including the random intercept model and the random slope model. In the random intercept model, the responses differ in an individual- or cluster-specific intercept for $m$ individuals or clusters. In this case the individual-specific intercept is modeled as random effect $\mathbf{u} = (u_{1,1}, u_{1,2}, \ldots, u_{1,m})$, yielding the (generalized) linear mixed model

$$\mathbb{E}(y_{ij}|u_{1,i}) = h(\mathbf{x}_{ij}\mathbf{\beta} + u_{1,i}), \quad u_{1,i} \overset{iid}{\sim} \mathcal{N}(0, \tau^2_0 \mathbf{I}_m)$$

for the $j$-th observation from an individual or cluster $i$.

Whereas for the random intercept model all covariates modeled with fixed effects are assumed to have the same influence on the response variable across individuals, the random slope model is suitable when an independent variable $x_s$ is assumed to have an individual-specific effect on the dependent variable. The random intercept model is extended to

$$\mathbb{E}(y_{ij}|\mathbf{u}_i) = h(\mathbf{x}_{ij}\mathbf{\beta} + u_{1,i} + x_{s,ij}u_{2,i}),$$

where $u_{2,i}$ is the individual-specific slope, which can be regarded as the deviation from the population slope $\beta_s$ corresponding to the $s$-th covariate $x_{s,ij}$ in $\mathbf{x}_{ij}$. In most cases, there is no reason to suppose $u_{1,i}$ and $u_{2,i}$ to be uncorrelated and the distributional assumption thus is

$$\begin{pmatrix} u_{1,i} \\ u_{2,i} \end{pmatrix} \sim \mathcal{N}\left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \tau^2_1 & \tau^{12} \\ \tau^{12} & \tau^2_2 \end{pmatrix} \right). \quad (4)$$

**Example II: Penalised spline smoothing**

In addition to many possibilities to extend these simple random effect models, linear mixed models can also be utilized to fit semi-parametric regression models (see, e.g., Ruppert, Wand, and Carroll 2003). For univariate smoothing, consider the model

$$\mathbb{E}(y_i) = f(x_i), \quad (5)$$

for $i = 1, \ldots, n$, where $f(\cdot)$ is a deterministic function of the covariate $x_i$, which shall be approximated using splines. For illustrative purposes, we consider the truncated polynomial basis representation

$$f(x) = \sum_{j=0}^{g} \beta_j x^j + \sum_{j=1}^{k} u_j (x - \kappa_j)^g_+,$$  

$$k, g,$$ 

(6)
in the following, where \( \kappa_1 < \ldots < \kappa_k \) are \( k \in \mathbb{N} \) knots, partitioning the domain of \( x, g \in \mathbb{N} \) and

\[
(z)^g_I = z^g \cdot I(z > 0) = \begin{cases} 
  z^g & \text{if } z > 0 \\
  0 & \text{if } z \leq 0
\end{cases}.
\] (7)

As the truncated part \( u_j(x - \kappa_j)^g_I \) is non-zero for \( x > \kappa_j \), \( u_j \) can be seen as a gradient change of the two consecutive function segments defined on \((\kappa_{j-1}, \kappa_j] \) and \((\kappa_j, \kappa_{j+1}] \). In order to estimate \( \beta_j, j = 0, \ldots, g \) and \( u_j, j = 1, \ldots, k \), the method of ordinary least squares (OLS) could in principle be applied. In most cases, however, this yields a rather rough estimate of \( f \) for suitably large \( k \) as the gradient changes of functions segments have a large impact. Therefore estimation methods for linear mixed models can be utilized in order to obtain a smooth function. Representing the untruncated polynomial part in (6) as the fixed effects and \( \sum_{j=1}^{k} u_j(x - \kappa_j)^g_I \) as the random effects part, the well known shrinkage effect of mixed models is transferred to the estimation of the \( u_j \)'s, shrinking the changes in the gradient of the fitted polynomials. The random effects assumption corresponds to a quadratic penalty on the \( u_j \), with the smoothing parameter estimated from the data.

This approach also works analogously for various other basis functions including the frequently used B-spline basis (see, e.g., Fahrmeir, Kneib, Lang, and Marx 2013). Moreover, a rich variety of models that can be represented as reduced rank basis smoothers with quadratic penalties allow for this kind of representation. The estimation via \texttt{lme4} can be employed by the use of \texttt{gamm4}. For an overview of possible model components see Wood (2017). An example is also given in Section 5.

3. The conditional AIC

The Akaike Information Criterion

Originally proposed by Hirotogu Akaike (Akaike 1973) as An Information Criterion (AIC), the AIC was one of the first model selection approaches to attract special attention among users of statistics. In some way, the AIC extends the maximum likelihood paradigm by making available a framework, in which both parameter estimation and model selection can be accomplished. The principle idea of the AIC can be traced back to the Kullback-Leibler distance (KLD Kullback and Leibler 1951), which can be used to measure the distance between a true (but normally unknown) density \( g(y) \) and a parametric model \( f(y \mid \nu) \). The unknown parameters \( \nu \) are commonly estimated by their maximum likelihood estimator \( \hat{\nu}(y) \). As minimizing the expected Kullback-Leibler distance is equivalent to minimizing the so called Akaike Information

\[
\text{AI} = -2 \mathbb{E}_{g(y)} \mathbb{E}_{g(\hat{y})} \log f(\hat{y} \mid \hat{\nu}(y)),
\] (8)

with \( \hat{y} \) a set of independent new observations from \( g \), minus twice the maximized log-likelihood \( \log f(y \mid \hat{\nu}(y)) \) as a natural measure of goodness-of-fit is an obvious estimator of the AI. However, this approach induces a bias as the maximized log-likelihood only depends on \( y \).
whereas (8) is defined as a predictive measure of two independent replications $\tilde{y}$ and $y$ from the same underlying distribution. Therefore the bias correction is defined by

$$BC = 2 \left( \mathbb{E}_{g(y)} \log f(y \mid \hat{\nu}(y)) - \mathbb{E}_{g(y)} \mathbb{E}_{g(\tilde{y})} \log f(\tilde{y} \mid \hat{\nu}(y)) \right).$$

(9)

Akaike derived the bias correction, which under certain regularity conditions can be estimated asymptotically by two times the dimension of $\nu$. This yields the well-known AI estimator

$$AIC(y) = -2 \log f(y \mid \hat{\nu}(y)) + 2 \text{dim}(\nu).$$

Hence, as the statistical model $f(\cdot \mid \nu)$ with the smallest AI aims at finding the model which is closest to the true model, the AIC can be seen as a relative measure of goodness-of-fit for different models of one model class. Notice that the bias correction is equivalent to the (effective) degrees of freedom and the covariance penalty, see Efron (2004).

The marginal and the conditional perspective on the AIC

Adopting this principle for the class of mixed models to select amongst different random effects is not straightforward. First of all, the question arises on the basis of which likelihood to define this AIC. For the class of mixed models, two common criteria exist, namely the marginal AIC (mAIC) based on the marginal log-likelihood and the conditional AIC (cAIC) based on the conditional log-likelihood. The justification of both approaches therefore corresponds to the purpose of the marginal and the conditional mixed model perspective, respectively. Depending on the question of interest, the intention of both perspectives differs, as for example described in Vaida and Blanchard (2005) or Greven and Kneib (2010).

The marginal perspective of mixed models is suitable when the main interest is to model fixed population effects with a reasonable correlation structure. The conditional perspective, by contrast, can be used to make statements based on the fit of the predicted random effects. In longitudinal studies, for example, the latter point of view seems to be more appropriate if the focus is on subject- or cluster-specific random effects. Another crucial difference in both approaches lies in the model’s use for prediction. On the one hand, the marginal model seems to be more plausible if the outcome for new observations comes from new individuals or clusters, i.e., observations having new random effects. The conditional model on the other hand is recommended if predictions are based on the same individuals or clusters, thereby predicting on the basis of already modeled random effects.

The corresponding AI criteria have closely related intentions. The conditional AIC estimates the optimism of the estimated log-likelihood for a new data set $\tilde{y}$ by leaving the random effects unchanged. This can be understood as a predictive measure based on a new data set originating from the same clusters or individuals as $y$. On the contrary, the marginal approach evaluates the log-likelihood using a new predictive data set $\tilde{y}$, which is not necessarily associated with the cluster(s) or individual(s) of $y$.

In particular for the use of mixed models in penalized spline smoothing, the cAIC usually represents a more plausible choice. As demonstrated in Example II of Section 2, the representation of penalized spline smoothing via mixed models divides certain parts of the spline basis into fixed and random effects. Using the marginal perspective in Example II, predictions would therefore be based only on the polynomial coefficients of $f$. If the fitted non-linear
function is believed to represent a general relationship of $x$ and $y$, predictions as well as the predictive measure in terms of the Akaike Information, however, make more sense if the truncated parts of the basis are also taken into account.

Vaida and Blanchard (2005) proposed the cAIC, an estimator of the conditional Akaike Information

$$ c_{\text{AIC}} = -2 \mathbb{E}_{g(y,u)} \log f(\tilde{y} | \tilde{\nu}(y), \tilde{u}(y)) $$

as an alternative to the mAIC, where $\nu$ includes the fixed effects and covariance parameters $\theta$. The cAIC may be more appropriate when the AIC is used for the selection of random effects. In addition, Greven and Kneib (2010) investigated the difference of both criteria from a mathematical point of view. Since the mAIC is intended for the use in settings where the observations are independent and the $k$-dimensional parameter space $\mathcal{V}_k$ can be transformed to $\mathbb{R}^k$, the corresponding bias correction $2 \dim(\nu)$ is biased for mixed models for which these conditions do not apply. In particular, Greven and Kneib showed that the mAIC leads to a preference for the selection of smaller models without random effects.

Conditional AIC for Gaussian responses

Depending on the distribution of $y$, different bias corrections of the maximized conditional log-likelihood exist to obtain the cAIC. For the Gaussian case, Liang et al. (2008) derive a corrected version of the initially proposed cAIC by Vaida and Blanchard (2005) for known error variance, taking into account the estimation of the covariance parameters $\theta$:

$$ c_{\text{AIC}}(y) = -2 \log f(y | \tilde{\nu}(y), \tilde{u}(y)) + 2 \text{tr} \left( \frac{\partial \hat{y}}{\partial y} \right). $$

Evaluating the bias correction $BC = 2 \text{tr} \left( \frac{\partial \hat{y}}{\partial y} \right)$ in expression (11) via numerical approximation, or a similar formula for unknown error variance, is however computationally expensive. Greven and Kneib (2010) develop an analytic version of the corrected cAIC making the calculation of the corrected cAIC feasible. We adapt their efficient implementation originally written for lme-objects (returned by the nlme package) and reimplement their algorithm for lmerMod-objects (returned by lme4). A more detailed description on the calculation of several terms in the proposed formula of Greven and Kneib (2010) is given in Appendix B. Furthermore, a partition of the parameter space is needed in order to account for potential parameters on the boundary of the parameter space, as presented in Theorem 3 in Greven and Kneib (2010). This process can be very unwieldy. Therefore, a fully automated correction algorithm is implemented in cAIC4 and presented in Appendix A.

Conditional AIC for Poisson responses

As for the Gaussian case, note that for the Poisson and the binomial distribution the bias
correction (9) can be rewritten as twice the sum of the covariances between $\hat{\eta}_i$ and $y_i$,

$$BC = 2 \sum_{i=1}^{n} \mathbb{E}(\hat{\eta}_i (y_i - \mu_i)), \quad (12)$$

with true but unobserved mean $\mu_i$ and the estimator of the natural parameter $\hat{\eta}$ depending on $y$. For the Poisson distribution an analytic reformulation of the bias correction term (12) has to be utilized to make it analytically accessible as in Säfken et al. (2014). Using results from Hudson (1978) and an identity due to Chen (1975), the bias correction (12) for Poisson distributed responses can be reformulated to

$$BC = 2 \sum_{i=1}^{n} \mathbb{E}(y_i (\log \hat{\mu}_i - \log \hat{\mu}_i(y_i - 1, y_i - 1))), \quad (13)$$

for observations $i = 1, \ldots, n$ and mean estimator $\hat{\mu}_i$. The $i$-th component of $y$ in $(y_{-i}, y_i - 1)$ is substituted by $y_i - 1$ along with the convention $y_i \log \hat{\mu}_i(y_{-i}, y_i - 1) = 0$ if $y_i = 0$. The computational implementation of the cAIC in this case requires $n - d$ model fits, where $d$ corresponds to the number of Poisson responses being equal to zero (see Section 4 for details). The resulting cAIC was first derived by Lian (2012).

**Conditional AIC for Bernoulli responses**

For binary responses there is no analytical representation for the bias correction (12), see Säfken et al. (2014). Nevertheless a bootstrap estimate for the bias correction can be based on Efron (2004). The bias correction is equal to the sum over the covariances of the estimators of the natural parameter $\hat{\eta}_i$ and the data $y_i$. To estimate this quantity, we could in principle draw a parametric bootstrap sample $z_i$ of size $B$ for the $i$-th data point - keeping all other observations fixed at their observed values - to estimate the $i$-th component $\mathbb{E}(\hat{\eta}_i (y_i - \mu_i))$ of the bias correction (12) for binary responses by

$$\frac{1}{B-1} \sum_{j=1}^{B} \hat{\eta}_i(z_{ij}) (z_{ij} - \bar{z}_i) = \frac{B_1}{B-1} \hat{\eta}_i(1) (1 - \bar{z}_i) + \frac{B_0}{B-1} \hat{\eta}_i(0) (-\bar{z}_i),$$

where $B_0$ is the number of zeros in the bootstrap sample, $B_1$ is the number of ones in the bootstrap sample, $\hat{\eta}_i(1) = \log \left( \frac{\hat{\mu}_i(1)}{1 - \hat{\mu}_i(1)} \right)$ is the estimated logit (the natural parameter) with $z_{ij} = 1$, $\hat{\eta}_i(0) = \log \left( \frac{\hat{\mu}_i(0)}{1 - \hat{\mu}_i(0)} \right)$ is the estimated logit with $z_{ij} = 0$ and $\bar{z}_i$ is the mean of the bootstrap sample $z_i$. Letting the number of bootstrap samples tend to infinity, i.e., $B \to \infty$ the mean of the bootstrap sample $\bar{z}_i = \frac{1}{B} \sum_{j=1}^{B} z_{ij} = B_1/B$ (as well as $B_1/(B-1)$ ) converges to the estimate from the data, which corresponds to the true mean in the bootstrap, $\hat{\mu}_i$ and therefore

$$\frac{B_1}{B-1} \hat{\eta}_i(1) (1 - \bar{z}_i) - \frac{B_0}{B-1} \hat{\eta}_i(0) (\bar{z}_i) \to \hat{\mu}_i \hat{\eta}_i(1) (1 - \hat{\mu}_i) - (1 - \hat{\mu}_i) \hat{\eta}_i(0) (\hat{\mu}_i) = \hat{\mu}_i (1 - \hat{\mu}_i) (\hat{\eta}_i(1) - \hat{\eta}_i(0)) \text{ for } B \to \infty.$$
Since the bootstrap estimates are optimal if the number of bootstrap samples \( B \) tends to infinity, this estimator can be seen as the optimal bootstrap estimator. The resulting estimator of the bias correction

\[
\hat{BC} = 2 \sum_{i=1}^{n} \hat{\mu}_i (1 - \hat{\mu}_i) (\hat{\eta}_i(1) - \hat{\eta}_i(0)) \tag{14}
\]

, which we use in the following, avoids a full bootstrap but requires \( n \) model refits.

4. Introduction to cAIC4

Example for linear mixed models

An example that is often used in connection with the \texttt{R}-package \texttt{lme4} is the \texttt{sleepstudy} data from a study on the daytime performance changes of the reaction time during chronic sleep restriction, see Belenky, Wesensten, Thorne, Thomas, Sing, Redmond, Russo, and Balkin (2003). Eighteen volunteers were only allowed to spend three hours of their daily time in bed for one week. The speed (mean and fastest 10% of responses) and lapses (reaction times greater than 500 ms) on a psychomotor vigilance task where measured several times. The averages of the reaction times are saved as response variable \texttt{Reaction} in the data set. Each volunteer has an identifier \texttt{Subject}. Additionally the number of days of sleep restriction at each measurement is listed in the covariate \texttt{Days}.

An example of how the \texttt{sleepstudy} data looks can be derived by the first 13 of the 180 measurements it contains:

```r
R> sleepstudy[1:13,]

       Reaction Days Subject
1  249.56000   0   308
2  258.70471   1   308
3  250.80062   2   308
4  321.43978   3   308
5  356.85189   4   308
6  414.69015   5   308
7  382.20378   6   308
8  290.14859   7   308
9  430.58530   8   308
10 466.35350    9   308
11 222.73370   0   309
12 205.26581   1   309
13 202.97778   2   309
```

Further insight into the data can be gained by a lattice plot, as presented in Bates et al. (2015). The average reaction times of each volunteer are plotted against the days of sleep restriction with the corresponding linear regression line. Such a plot can be found in Figure 1.
Figure 1: Lattice plot of the sleepstudy data. For each volunteer there is one panel. The identification number of each volunteer is in the heading of the panels. In the panels the reaction time is plotted against the days of sleep restriction and a regression line is added for each volunteer/panel.
The conditional AIC can be used to find the model that best predicts future observations, assuming that future observations share the same random effects as the ones used for the model fitting. In case of this data set, using the cAIC for model choice corresponds to finding the model that best predicts future reaction times of the volunteers that took part in the study.

After looking at the lattice plot, a first model that could be applied is a model with a random intercept and a random slope for Days within each volunteer (Subject):

\[ y_{ij} = \beta_0 + \beta_1 \cdot \text{day}_{ij} + u_{j0} + u_{j1} \cdot \text{day}_{ij} + \epsilon_{ij} \]  

(15)

for \( i = 1, \ldots, 18 \) and \( j = 1, \ldots, 10 \), with

\[
\begin{pmatrix}
u_{j0} \\
u_{j1}
\end{pmatrix} \sim \mathcal{N} \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \tau^2_{12} & \tau^2_{21} \\ \tau^2_{21} & \tau^2_2 \end{pmatrix} \right).
\]

In the preceding notation \( \tau^2_1 = \theta_1, \tau^2_2 = \theta_2 \) and \( \tau^2_{12} = \theta_3 \). That \( \tau^2_{12} \) is not necessarily zero indicates that the random intercept and the random slope are allowed to be correlated.

R> (m1 <- lmer(Reaction ~ 1 + Days + (1 + Days|Subject), sleepstudy))

Linear mixed model fit by REML ['lmerMod']
Formula: Reaction ~ 1 + Days + (1 + Days | Subject)
Data: sleepstudy
REML criterion at convergence: 1743.628
Random effects:
| Groups     | Name      | Std.Dev. | Corr |
|------------|-----------|----------|------|
| Subject    | (Intercept) | 24.740   |      |
|            | Days      | 5.922    | 0.07 |
| Residual   |           | 25.592   |      |
Number of obs: 180, groups: Subject, 18
Fixed Effects:
| (Intercept) | Days |
|-------------|------|
| 251.41      | 10.47|

The output shows that the within-subject correlation between the random intercepts \( u_{j0} \) and the random slopes \( u_{j1} \) is low, being estimated as 0.07. Hence there seems to be no evidence that the initial reaction time of the volunteers has systematic impact on the pace of increasing reaction time following the sleep restriction. Consequently a suitable model might be one in which the correlation structure between both is omitted. The model for the response therefore stays the same as in (15), but the random effects covariance structure is predefined as

\[
\begin{pmatrix}
u_{j0} \\
u_{j1}
\end{pmatrix} \sim \mathcal{N} \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \tau^2_{0} & 0 \\ 0 & \tau^2_2 \end{pmatrix} \right).
\]

Such a model without within-subject correlation is called by
\begin{verbatim}
R> (m2 <- lmer(Reaction ~ 1 + Days + (1|Subject) + (0 + Days|Subject),
+ sleepstudy))

Linear mixed model fit by REML ['lmerMod']
Formula: Reaction ~ 1 + Days + (1 | Subject) + (0 + Days | Subject)
Data: sleepstudy
REML criterion at convergence: 1743.669
Random effects:
Groups     Name        Std.Dev.
Subject    (Intercept) 25.051
Subject.1  Days         5.988
Residual     25.565
Number of obs: 180, groups: Subject, 18
Fixed Effects:
             (Intercept)   Days
            251.41        10.47

Notice that the estimates of standard deviations of the random effects do not differ much
between the first and the second model. To decide which model is more appropriate in terms
of subject specific prediction the conditional AIC can be used. Calling the \texttt{cAIC}-function from
the \texttt{cAIC4}-package gives the output:

\begin{verbatim}
R> cAIC(m1)

$loglikelihood
[1] -824.507

$df
[1] 31.30192

$reducedModel
NULL

$new
[1] FALSE

$caic
[1] 1711.618
\end{verbatim}

The conditional log-likelihood and the corrected degrees of freedom, i.e., the bias correction,
are the first two elements of the resulting list. The third element is called \texttt{reducedModel} and
is the model without the random effects covariance parameters that were estimated to lie on
the boundary of the parameter space, see Appendix A and Greven and Kneib (2010), and
\texttt{NULL} if there were none on the boundary. The fourth element says if such a new model was
fitted because of the boundary issue, which was not the case here. The last element is the
conditional AIC as proposed in Greven and Kneib (2010).

The \texttt{cAIC} of the second model \texttt{m2} is:
\end{verbatim}
\end{verbatim}
From a conditional perspective, the second model is thus preferred to the first one. This confirms the assertion that the within-subject correlation can be omitted in the model. There are several further possible models for these data. For instance the random slope could be excluded from the model. In this model the pace of increasing reaction time does not systematically vary between the volunteers. This model is estimated by

\[
R> m3 \leftarrow \text{lmer}(\text{Reaction} \sim 1 + \text{Days} + (1|\text{Subject}), \text{sleepstudy})
\]

The conditional AIC of this model is

\[
R> \text{cAIC}(m3)\$caic
\]

\[1767.118\]

This is by far larger than the cAIC for the two preceding models. The lattice plot in Figure 1 already indicated that there is strong evidence of subject-specific (random) slopes. This is also reflected by the cAIC.

The conditional AIC is also appropriate for choosing between a simple null model without any random effects and a complex model incorporating random effects, as has been noticed by Greven and Kneib (2010). Thus it is possible to compare the cAIC of the three previous mixed models with the standard AIC for a linear model, here including three parameters (intercept, linear effect for Days and error variance)

\[
R> -2 \cdot \text{logLik(lm(Reaction} \sim 1 + \text{Days, sleepstudy), \text{REML = TRUE})[1] + 2 \times 3
\]

\[1899.664\]

In this case, however, the mixed model structure is evident, reflected by the large AIC for the linear model.

**Example for generalized linear mixed models**

The cAIC4-package additionally offers a conditional AIC for conditionally Poisson distributed responses and an approximate conditional AIC for binary data. The Poisson cAIC uses the bias correction (13) and the bias correction term for the binary data is (14).

Making use of the fast refit() function of the lme4-package, both cAICs can be computed moderately fast, since \(n - d\) and \(n\) model refits are required, respectively, with \(n\) being the number of observations and \(d\) the number of responses that are zero for the Poisson responses. In the following, the cAIC for Poisson response is computed for the grouseticks data set from the lme4-package as an illustration.

The grouseticks data set was originally published in Elston, Moss, Boulinier, Arrowsmith, and Lambin (2001). It contains information about the aggregation of parasites, so-called
sheep ticks, on red grouse chicks. The variables in the data set are given in Table 1. Every chick, identified by **INDEX**, is of a certain **BROOD** and every **BROOD**, in turn, corresponds to a specific **YEAR**.

The number of ticks is the response variable. Following the authors in a first model the expected number of ticks $\lambda_I$ with **INDEX** ($l$) is modelled depending on the year and the height as fixed effects and for each of the grouping variables **BROOD** ($i$), **INDEX** ($j$) and **LOCATION** ($k$) a random intercept is incorporated. The full model is

$$
\log (E(\text{TICKS}_l)) = \log (\lambda_l) = \beta_0 + \beta_1 \cdot \text{YEAR}_l + \beta_2 \cdot \text{HEIGHT}_l + u_{1,i} + u_{2,j} + u_{3,k}
$$

(16)

with random effects distribution

$$
\begin{pmatrix}
  u_{1,i} \\
  u_{2,j} \\
  u_{3,k}
\end{pmatrix}
\sim \mathcal{N}
\left(\begin{pmatrix}
  0 \\
  0 \\
  0
\end{pmatrix},
\begin{pmatrix}
  \tau^2_1 & 0 & 0 \\
  0 & \tau^2_2 & 0 \\
  0 & 0 & \tau^2_3
\end{pmatrix}
\right).
$$

Before fitting the model the covariates **HEIGHT** and **YEAR** are centred for numerical reasons and stored in the data set `grouseticks_cen`.

R> formula <- TICKS ~ YEAR + HEIGHT + (1|BROOD) + (1|INDEX) + (1|LOCATION)
R> p1 <- glmer(formula, family = "poisson", data = grouseticks_cen)

A summary of the estimated model is given below. Notice that the reported AIC in the automated summary of `lme4` is not appropriate for conditional model selection.

**Generalized linear mixed model fit by maximum likelihood**

*(Laplace Approximation) ['glmerMod']*

**Family**: poisson  ( log )

**Formula**: `TICKS ~ YEAR + HEIGHT + (1 | BROOD) + (1 | INDEX) + (1 | LOCATION)`

**Data**: `grouseticks_cen`

| AIC  | BIC  | logLik | deviance | df.resid |
|------|------|--------|----------|----------|
| 1845.5 | 1869.5 | -916.7 | 1833.5 | 397 |

**Scaled residuals:**

| Min | 1Q  | Median | 3Q | Max |
|-----|-----|--------|----|-----|
|     |     |        |    |     |
Random effects:

| Groups  | Name       | Variance  | Std.Dev. |
|---------|------------|-----------|----------|
| INDEX   | (Intercept)| 2.979e-01 | 5.458e-01|
| BROOD   | (Intercept)| 1.466e+00 | 1.211e+00|
| LOCATION| (Intercept)| 5.411e-10 | 2.326e-05|

Number of obs: 403, groups: INDEX, 403; BROOD, 118; LOCATION, 63

Fixed effects:

|                  | Estimate | Std. Error | z value | Pr(>|z|) |
|------------------|----------|------------|---------|----------|
| (Intercept)      | 0.472353 | 0.134712   | 3.506   | 0.000454 *** |
| YEAR             | -0.480261| 0.166128   | -2.891  | 0.003841 **  |
| HEIGHT           | -0.025715| 0.003772   | -6.817  | 9.32e-12 *** |

Correlation of Fixed Effects:

|        | (Intr) | YEAR |
|--------|--------|------|
| YEAR   | 0.089  |      |
| HEIGHT | 0.096  | 0.061|

The conditional log-likelihood and the degrees of freedom for the conditional AIC with conditionally Poisson distributed responses as in (13) for model (16) are obtained by the call of the `cAIC`-function:

```r
R> set.seed(42)
R> cAIC(p1)
```

$\loglikelihood

```
[1] -572.0133
```

$df

```
[1] 205.5786
```

$reducedModel

NULL

$new

```
[1] FALSE
```

$caic

```
[1] 1555.184
```

The output is the same as for Gaussian linear mixed models. It becomes apparent that there is a substantial difference between the conditional and the marginal AIC: In the output of the model the marginal AIC is reported to be 1845.48. Note that the marginal AIC is biased,
see Greven and Kneib (2010), and based on a different likelihood. In the full model, the standard deviations of the random effects are rather low. It thus may be possible to exclude one of the grouping variables from the model, only maintaining two random effects. There are three possible models with one of the random effects terms excluded.

If the random intercept associated with LOCATION is excluded the model is

```r
R> formel <- TICKS ~ YEAR + HEIGHT + (1|BROOD) + (1|INDEX)
R> p2 <- glmer(formel, family = "poisson", data = grouseticks_cen)
R> cAIC(p2)$caic
```

[1] 1555.214

The conditional AIC is almost the same as for the full model. It may thus make sense to choose the reduced model and for the prediction of the number of ticks not to make use of the random intercept associated with the LOCATION grouping.

Another possible model can be obtained by omitting the random intercepts for the INDEX grouping structure instead of those associated with LOCATION. This would make the model considerably simpler, since each chick has an INDEX and hence a random intercept is estimated for each observation in order to deal with overdispersion in the data.

```r
R> formel <- TICKS ~ YEAR + HEIGHT + (1|BROOD) + (1|LOCATION)
R> p3 <- glmer(formel, family = "poisson", data = grouseticks_cen)
R> cAIC(p3)$caic
```

[1] 1842.205

The large cAIC in comparison with the two preceding models documents that the subject-specific random intercept for each observation should be included.

The final model for the comparison omits random intercepts associated with the BROOD grouping. This is equivalent to setting the associated random intercepts variance to zero, i.e., \( \tau^2 = 0 \).

```r
R> formel <- TICKS ~ YEAR + HEIGHT + (1|INDEX) + (1|LOCATION)
R> p4 <- glmer(formel, family = "poisson", data = grouseticks_cen)
R> cAIC(p4)$caic
```

[1] 1594.424

The cAIC is higher than the cAICs for the full model and the model without the LOCATION grouping structure. Consequently either the full model or the model without the LOCATION grouping structure is favoured by the cAIC. The authors favour the latter.

### 5. A scheme for stepwise conditional variable selection

Now having the possibility to compare different (generalized) linear mixed models via the conditional AIC, we introduce a model selection procedure in this section, searching the
space of possible model candidates in a stepwise manner. Inspired by commonly used step-
functions as for example given by the stepAIC function in the MASS-package (Venables and
Ripley 2002), our stepcAIC-function provides an automatic model selection applicable to all
models of the class merMod (produced by [g]lmer) or objects resulting from a gamm4-call.
For example, consider the sleepstudy model

\[
R> fm1 <- lmer(Reaction ~ Days + (Days | Subject), sleepstudy)
\]

which implicitly fits the random effects structure \((1 + Days \mid Subject)\) (correlated random
intercept and slope). In order to perform a data-driven search for the best model, a backward
step procedure needs to fit and evaluate the following three nested models (uncorrelated
random intercept and slope, only random slope, only random intercept).

\[
R> fm1a <- lmer(Reaction ~ Days + (1 | Subject) + (0 + Days | Subject), sleepstudy)
R> fm1b <- lmer(Reaction ~ Days + (0 + Days | Subject), sleepstudy)
R> fm1c <- lmer(Reaction ~ Days + (1 | Subject), sleepstudy)
\]

Choosing the model \(fm1a\) in the first step, further model comparisons may be performed by for
example reducing the model once again or adding another random effect. For this purpose, the
stepcAIC-function provides the argument direction, having the options backward, forward
and both. Whereas the backward- and forward-direction procedures fit and evaluate all
nested or extended models step-by-step, the both-direction procedure alternates between
forward- and backward-steps as long as any of both steps lead to an improvement in the cAIC.
During model modifications in each step, the function allows to search through different types
of model classes.

For fixed effects selection, the step procedure furthermore can be used to successively extend
or reduce the model in order to check whether a fixed effect has a constant, linear or non-linear
impact. For example, we specify a generalized additive mixed model (GAMM) as follows (cf.
Gu and Wahba 1991)

\[
y_{ij} = \beta_0 + x_{1,i,j}\beta_1 + f(x_{3,i,j}) + b_i + \epsilon_{ij}, \quad i = 1, \ldots, 20, j = 1, \ldots, J_i,
\]

with metric variables \(x_1\) and \(x_3\) in the guWahbaData supplied in the cAIC4 package with
continuous covariates \(x_0, x_1, x_2\) and \(x_3\). .

The corresponding model fit in R using gamm4 is given by

\[
R> set.seed(42)
R> guWahbaData$fac <- fac <- as.factor(sample(1:20, 400, replace =TRUE))
R> guWahbaData$y <- guWahbaData$y + model.matrix(~ fac - 1) %*% rnorm(20) * 0.5
R> br <- gamm4(y ~ x1 + s(x3, bs = "ps"), data = guWahbaData, random = ~ (1 | fac))
\]

resulting in the following non-linear estimate of \(f(x_{3,i,j})\) (Figure 2).

Applying the backward stepwise procedure to the model \(br\) via

\[
R> stepcAIC(br, trace = TRUE, direction = "backward", data = guWahbaData)
\]
the procedure stops after one step with a warning, saying that the model contains zero variance components and the corresponding terms must be removed manually. This is due to the fact that the \texttt{stepcAIC} function cannot reduce non-linear effects such as $f(x_{3,i,j})$ automatically, as the type of additive effect depends on the specification of the \texttt{s}-term and its arguments. Modifying the term manually, a GLMM is fitted and passed to the \texttt{stepcAIC} function.

\begin{verbatim}
R> br0 <- gamm4(y ~ x1 + x3, data = guWahbaData, random = ~ (1|fac))
R> stepcAIC(br0, trace = TRUE, direction = "backward", data = guWahbaData)
\end{verbatim}

In the next steps \texttt{stepcAIC} removes $x_3$ completely from the model and also checks whether a GLM with no random effects at all might be the best possible model, hence having searched for the smallest cAIC in three different model classes in the end.

Whereas the backward procedure has straightforward mechanism and does not need any further mandatory arguments as shown in the previous example, the \texttt{stepcAIC}-function provides several optional and obligatory arguments for the \texttt{forward} and \texttt{both} procedure in order to limit the possibly large number of model extensions. Regarding the required parameters, the user must specify the variables, which may be added with fixed or random effects as they are referred to in the \texttt{data.frame} given by the argument \texttt{data}. For the fixed effects, this is done by specifying the \texttt{fixEf} argument, which expects a character vector with the names of the covariates, e.g., \texttt{fixEf=c("x1","x2"). Variables listed in the \texttt{fixEf}-argument are firstly included in the model as linear terms and, if the linear effect leads to an improvement of the
cAIC, checked for their non-linearity by evaluating the cAIC of the corresponding model(s). Model extensions resulting from additional random effects are created in two different ways. A new model may, on the one hand, include a random intercept for a variable forming a grouping structure (in the sleepstudy example for Subject) or, on the other hand, a random slope for a variable (Days in this case). These two types are specified using the arguments `groupCandidates` for grouping variables candidates or `slopeCandidates` for candidates for variables with random slope, again by referring to the variable names in `data` as string.

Further optional arguments can determine the way random effects are treated in the step procedure:

- `allowUseAcross`: logical value whether slope variables, which are already in use with a grouping variable can also be used with other grouping variables,
- `maxSlopes`: maximum number of slopes for one grouping variable.

Following the `stepAIC`-function, the `stepCIC`-function also provides an argument for printing interim results (`trace`) and allows for the remaining terms of the initial model to be unaffected by the procedure (`keep`: list with entries `fixed` and `random`, each either `NULL` or a formula). In addition, the user may choose whether the cAIC is calculated for models, for which the fitting procedure in (generalized) linear models could not find an optimum (`calcNonOptimMod`, default = `FALSE`) and might choose the type of smoothing terms added in forward steps (`bsType`).

If the step-function is used for large datasets or in the presence of highly complex models the fitting procedures as well as the calculations of the cAIC can be parallelized by defining the number of cores (`numCores`) being used if more than one model has to be fitted and evaluated in any step (therefore passing the `numCores`-argument to a `mclapply`-function implemented in the `parallel`-package (R Core Team 2016)).

Due to the variety of additive model definitions in `gamm4`, the `stepCIC` is however limited in its generic step-functionality for GAMMs. On the one hand, extensions with non-linear effects are restricted to one smooth class given by `bsType`, on the other hand, the step-procedure is not able to deal with further arguments passed in smooth terms. The latter point is a current limitation, since the default basis dimension of the smooth term (i.e., the number of knots and the order of the penalty) is essentially arbitrary.

An additional current limitation of the `stepCIC`-function in its applications with GAMMs is the handling of zero variance components occurring during the function call. As a meaningful handling of zero variance smoothing terms would depend on the exact specification of the non-linear term, the stepwise procedure is stopped and returns the result of the previous step. After removing the zero variance term manually the user may call the step-function again.

**Examples**

In order to demonstrate some functionalities of the `stepCIC`-function, various examples are given in the following using the `Pastes` data set (Davies and Goldsmith 1972), which is available in the `lme4`-package. The data set consists of 60 observations including one metric variable `strength`, which is the strength of a chemical paste product and the categorical
variables batch (the delivery batch), the cask within the delivery batch and sample, which is an identifier from what cask in what batch the paste sample was taken. Starting with a random effects backward selection, the model fm3

\[ R> fm3 <- lmer(strength ~ 1 + (1|sample) + (1|batch), Pastes) \]

may be automatically reduced using

\[ R> fm3_step <- stepcAIC(fm3, direction = "backward", trace = TRUE, data = Pastes) \]

Starting stepwise procedure...

-----------------------------------------------
-----------------------------------------------
Step 1 (backward): cAIC=178.2809
Best model so far: ~ (1 | sample) + (1 | batch)
New Candidates:
Calculating cAIC for 2 model(s) ...

| models | loglikelihood | df  | caic   |
|--------|---------------|-----|--------|
| ~(1 | batch) | -141.49709    | 9.157892 | 301.3100 |
| ~(1 | sample) | -58.95458     | 30.144477 | 178.1981 |

-----------------------------------------------
-----------------------------------------------
Step 2 (backward): cAIC=178.1981
Best model so far: ~ (1 | sample)
New Candidates:
Calculating cAIC for 1 model(s) ...

| models | loglikelihood | df  | caic   |
|--------|---------------|-----|--------|
| ~1     | -155.1363     | 2   | 312.2727 |

-----------------------------------------------
-----------------------------------------------
Best model: ~ (1 | sample), cAIC: 178.1981

-----------------------------------------------

where in a first step, the random intercept of batch is dropped. Afterwards, the procedure compares the cAICs of the models \[ lmer(strength ~ 1 + (1|sample), Pastes) \] and \[ lm(strength ~ 1, Pastes) \], keeping the second random effect due to a smaller cAIC of the linear mixed model.
Using the step function the other way round, a forward stepwise selection can be initialized by a simple linear model

\[ R \text{> } \text{fm3\_min} \leftarrow \text{lm(strength} \sim 1, \text{data} = \text{Pastes}) \]

followed by a `stepcAIC`-call

\[ R \text{> fm3\_min\_step} \leftarrow \text{stepcAIC(fm3\_min}, + \text{ groupCandidates} = \text{c("batch", "sample")}, + \text{ direction} = \text{"forward", trace} = \text{TRUE}, + \text{ data} = \text{Pastes, analytic} = \text{TRUE}) \]

where possible new candidates for grouping variables are specified using the `groupCandidates`-argument. Again, the random intercept model with group `sample` is finally selected.

To illustrate the use of the `stepcAIC`-function in the context of GAMM selection, two examples are generated following the `gamm4`-help page on the basis of the `guWahbaData` data set. First, the GAMM

\[ y_{ij} = \beta_0 + f(x_{0,i,j}) + x_{1,i,j}\beta_1 + f(x_{2,i,j}) + b_i, \quad i = 1, \ldots, 20, j = 1, \ldots, J_i \]

is fitted to the `guWahbaData` including a nonlinear term for the covariate `x0` using a thin-plate regression spline, a P-spline (Eilers and Marx 1996) for the covariate `x2` as well as a random effect for the grouping variable `fac`.

\[ R \text{> br} \leftarrow \text{gamm4(y} \sim s(x0) + x1 + s(x2, bs = \text{"ps"}), + \text{ data} = \text{guWahbaData, random} = \text{\~(1/fac))} \]

In order to check for linear or non-linear effects of the two other covariates `x1` and `x3`, the `stepcAIC`-function is employed.

\[ R \text{> br\_step} \leftarrow \text{stepcAIC(br, fixEf} = \text{c("x1", "x3"), + \text{ direction} = \text{"both"}, + \text{ data} = \text{guWahbaData})} \]

After changing the linear effect `x1` to a non-linear effect, i.e., `s(x1, bs = "tp")`, and therefore improving the model’s cAIC in a first forward step, the function stops due to zero variance components.

The final model `br\_step` to this point is thus given by \( y \sim s(x0, bs = \text{"tp"}) + s(x2, bs = \text{"ps"}) + s(x1, bs = \text{"tp"}) + (1 \mid \text{fac}) \). In contrast to the effect of covariate `x2` modeled as P-spline, the effects of covariates `x0` and `x1` are modeled as thin plate regression splines (Wood 2017). For `x0`, this is due to the initial model definition, as `s(x0)` is internally equal to `s(x0, bs = \text{"tp"})`, whereas for `x1`, the definition of the spline is set by the argument `bsType` of the `stepcAIC`-function. As the `bsType`-argument is not specified in the call, the default "tp" is used.

Finally, a demonstration of the `keep`-statement is given for the model
\begin{verbatim}
R> br2 <- gamm4(y ~ s(x0, bs = "ps") + x2, data = guWahbaData,
+     random = ~(1|fac))

where the aim is to prevent the step procedure changing the linear effect of the covariate \textit{x2},
the non-linear effect of \textit{x0} as well as the random effect given by \textasciitilde~ (1|fac).

R> br2_step <- stepcAIC(br2, trace = TRUE, direction = "both",
+     fixEf = c("x1", "x3"), bsType = "cs",
+     keep = list(fixed = ~ s(x0, bs = "ps") + x2,
+     random= ~ (1|fac)), data = guWahbaData)

After successively adding a linear effect of \textit{x1} to the model, neither the following backward
step nor another forward step do improve the \textit{cAIC}. The final model is given by \textit{y} \sim \textit{s(x0, bs = "ps") + x1 + x2} and random effect \textit{(1|fac)}.

6. Conclusion

This paper gives a hands-on introduction to the R-package \textit{cAIC4} allowing for model selection
in mixed models based on the conditional AIC. The package and the paper offer a possibility
for users from the empirical sciences to use the conditional AIC without having to worry
about lengthy and complex calculations or mathematically sophisticated boundary issues of
the parameter space. The applications presented in this paper go far beyond model selection
for mixed models and extend to penalized spline smoothing and other structured additive re-
gression models. Furthermore a stepwise algorithm for these models is introduced that allows
for fast model selection.

Often statistical modelling is not about finding one ‘true model’. In such cases it is of in-
terest to define weighted sums of plausible models. This approach called model averaging is
presented in Zhang, Zou, and Liang (2014) for weights chosen by the \textit{cAIC}. We plan to imple-
ment this approach in \textit{cAIC4}. Another future research path is to implement an appropriate
version of the Bayesian information criterion (BIC) for conditional model selection.

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A. Dealing with the boundary issues

A major issue in obtaining the conditional AIC in linear mixed models is to account for
potential parameters of \textit{θ} on the boundary of the parameter space (see Greven and Kneib
2010). This needs to be done in order to ensure positive definiteness of the covariance matrix
\textit{D}_\textit{θ}.

The restructuring of the model in order to obtain the \textit{cAIC} is done automatically by \textit{cAIC4}.
To gain insight into the restructuring, an understanding of the mixed model formulas used in

**lme4** is essential. For an in depth explanation on how the formula module of **lme4** works, see Bates et al. (2015), Section 2.1.

Suppose we want to fit a mixed model with two grouping factors $g1$ and $g2$. Within the first grouping factor $g1$, there are three continuous variables $v1$, $v2$ and $v3$ and within the second grouping factor there is only one variable $x$. Thus there are not only random intercepts but also random slopes that are possibly correlated within the groups. Such a model with response $y$ would be called in **lme4** by

```
R> m <- lmer(y ~ (v1 + v2 + v3|g1) + (x|g2), exampledata)
```

In mixed models fitted with **lme4**, the random effects covariance matrix $D\theta$ always has block-diagonal structure. For instance in the example from above the Cholesky factorized blocks of the estimated $D\theta$ associated with each random effects term are

```
R> getME(m, "ST")
```


g2

```
[,1] [,2]  
[1,] 1.18830353 NaN  
[2,] -0.01488359 0
```


g1

```
[,1] [,2] [,3] [,4]  
[1,] 1.0184626697 0.00000000 NaN NaN  
[2,] -0.1438761295 0.05495809 NaN NaN  
[3,] -0.007341796 0.19904339 0 NaN  
[4,] -0.0883652598 -1.36463267 -Inf 0
```

If any of the diagonal elements of the blocks are zero the corresponding random effects terms are deleted from the formula. In **lme4** this is done conveniently by the component names list

```
R> m$cnms
```


g2

```
[1] "(Intercept)" "x"
```


g1

```
[1] "(Intercept)" "v1" "v2" "v3"
```

Thus a new model formula can be obtained by designing a new components names list:

```
R> varBlockMatrices <- getME(m, "ST")
R> cnms <- m$cnms
R> for(i in 1:length(varBlockMatrices)){
+    cnms[[i]] <- cnms[[i]][which(diag(varBlockMatrices[[i]]) != 0)]
+  }
R> cnms
```

23
The `cnms2formula` function from the `cAIC4`-package forms a new formula from the `cnms` object above. Hence the new formula can be computed by

```r
R> rhs <- cAIC4:::cnms2formula(cnms)
R> lhs <- formula(m)[[2]]
R> reformulate(rhs, lhs)
```

\[ y \sim (1 \mid g2) + (1 + v1 \mid g1) \]

This code is called from the `deleteZeroComponents` function in the `cAIC4`-package. This function automatically deletes all zero components from the model. The `deleteZeroComponents` function is called recursively, so the new model is checked again for zero components. In the example above only the random intercepts are non-zero. Hence the formula of the reduced model from which the conditional AIC is calculated is

```r
R> formula(cAIC4:::deleteZeroComponents(m))
```

\[ y \sim (1 \mid g2) + (1 \mid g1) \]

With the new model the conditional AIC is computed. If there are no random effect terms left in the formula, a linear model and the conventional AIC is returned. The `deleteZeroComponents` function additionally accounts for several special cases that may occur. Notice however that in case of using smoothing terms from `gam4` no automated check for boundary issues can be applied and zero components have to be manually deleted.

**B. Computational matters**

**Gaussian responses**

The corrected conditional AIC proposed in Greven and Kneib (2010) accounts for the uncertainty induced by the estimation of the random effects covariance parameters \( \theta \). In order to adapt the findings of Greven and Kneib (2010), a number of quantities from the `lmer` model fit need to be extracted and transformed. In the following these computations are presented. They are designed to minimize the computational burden and maximize the numerical stability. Parts of the calculations needed, for instance the Hessian of the ML/REML criterion, can also be found in Bates et al. (2015). Notice however, that `lme4` does not explicitly calculate these quantities but uses derivative free optimizers for the profile likelihoods.

A core ingredient of mixed models is the covariance matrix of the marginal responses \( y \). The inverse of the scaled covariance matrix \( V_0 \) will be used in the following calculations:
\[ V = \text{cov}(y) = \sigma^2 (I_n + Z \Lambda \Lambda^t Z^t) = \sigma^2 V_0. \]

Large parts of the computational methods in \texttt{lme4} rely on a sparse Cholesky factor that satisfies

\[ L_\theta L_\theta^t = \Lambda_\theta^t Z^t Z \Lambda_\theta + I_q. \quad (17) \]

From this equation and keeping in mind that \( I - V_0^{-1} = Z (Z^t Z + (\Lambda_\theta^t)^{-1} \Lambda_\theta^{-1})^{-1} Z^t \), see Greven and Kneib (2010), it follows that

\[ \Lambda_\theta (L_\theta^t)^{-1} L_\theta^{-1} \Lambda_\theta = (Z^t Z + (\Lambda_\theta^t)^{-1} \Lambda_\theta^{-1})^{-1} \Rightarrow I - V_0^{-1} = (L_\theta^{-1} \Lambda_\theta^t Z^t)^t (L_\theta^{-1} \Lambda_\theta Z^t). \]

Hence the inverse of the scaled variance matrix \( V_0^{-1} \) can be efficiently computed with the help of the R-package \texttt{Matrix} (see Bates and Maechler 2017) that provides methods specifically for sparse matrices:

\begin{verbatim}
R> Lambdat <- getME(m, "Lambdat")
R> V0inv <- diag(rep(1, n)) - + crossprod(solve(getME(m, "L"), system = "L")) %*% solve(getME(m, "L"), Lambdat, system = "P") %*% t(Z))
\end{verbatim}

Notice that \( \text{solve(getME(m, "L"), Lambdat, system = "P")} \) accounts for a fill-reducing permutation matrix \( P \) associated (and stored) with \( L_\theta \), see Bates \textit{et al.} (2015), and is thus equivalent to

\begin{verbatim}
R> P %*% Lambdat
\end{verbatim}

Another quantity needed for the calculation of the corrected degrees of freedom in the conditional AIC are the derivatives of the scaled covariance matrix of the responses \( V_0 \) with respect to the \( j \)-th element of the parameter vector \( \theta \):

\[ W_j = \frac{\partial}{\partial \theta_j} V_0 = Z D_\theta^{(j)} Z^t, \]

where the derivative of the scaled covariance matrix of the random effects with respect to the \( j \)-th variance parameter is defined by

\[ D_\theta^{(j)} = \frac{1}{\sigma^2} \frac{\partial}{\partial \theta_j} D_\theta. \]

Notice that \( D_\theta = [d_{st}]_{s,t=1,...,q} \) is symmetric and block-diagonal and its scaled elements are stored in \( \theta \), hence \( d_{st} = d_{ts} = \theta_j \sigma^2 \), for certain \( t, s \) and \( j \). Thus the matrix \( D_\theta^{(j)} = [d_{st}^{(j)}]_{s,t=1,...,q} \) is sparse with...
\( d_{st}^{(j)} = \begin{cases} 1 & \text{, if } d_{st} = d_{ts} = \theta_j \sigma^2 \\ 0 & \text{, else.} \end{cases} \)

The derivative matrices \( W_j \) can be derived as follows:

```r
R> Lambda <- getME(m, "Lambda")
R> ind <- getME(m, "Lind")
R> len <- rep(0, length(Lambda@x))
R>
R> for(j in 1:length(theta)) {
+ LambdaS <- Lambda
+ LambdaSt <- Lambdat
+ LambdaS@x <- LambdaSt@x <- len
+ LambdaS@x[which(ind == j)] <- LambdaSt@x[which(ind == j)] <- 1
+ diagonal <- diag(LambdaS)
+ diag(LambdaS) <- diag(LambdaSt) <- 0
+ Dj <- LambdaS + LambdaSt
+ diag(Dj) <- diagonal
+ Wlist[[j]] <- Z %*% Dj %*% t(Z)
+ }
```

The following matrix is essential to derive the corrected AIC of Theorem 3 in Greven and Kneib (2010). Adapting their notation, the matrix is

\[
A = V_0^{-1} - V_0^{-1} X \left( X^t V_0^{-1} X \right)^{-1} X^t V_0^{-1}.
\]

Considering that the cross-product of the fixed effects Cholesky factor is

\[
X^t V_0^{-1} X = R_X^t R_X,
\]

the matrix \( A \) can be rewritten

\[
A = V_0^{-1} - \left( X R_X^{-1} V_0^{-1} \right) \left( X R_X^{-1} V_0^{-1} \right)^t.
\]

Accordingly the computation in R can be done as follows:

```r
R> A <- V0inv - crossprod(crossprod(X %*% solve(getME(m, "RX")), V0inv))
```

With these components, the Hessian matrix

\[
B = \frac{\partial^2 \text{REML(} \theta \text{)}}{\partial \theta \partial \theta^t} \quad \text{or} \quad B = \frac{\partial^2 \text{ML(} \theta \text{)}}{\partial \theta \partial \theta^t}
\]

and the matrix

\[
G = \frac{\partial^2 \text{REML(} \theta \text{)}}{\partial \theta \partial y^t} \quad \text{or} \quad G = \frac{\partial^2 \text{ML(} \theta \text{)}}{\partial \theta \partial y^t},
\]
depending on whether the restricted or the marginal profile log-likelihood REML(θ) or ML(θ) is used, can be computed straightforward as in Greven and Kneib (2010). Depending on the optimization, it may not even be necessary to compute the matrix $B$. Considering that $B$ is the Hessian of the profile (restricted) log-likelihood, the matrix can also be taken from the model fit, although this is only a numerical approximation. If the Hessian is computed it is stored in:

```r
R> B <- m@optinfo$deriv$Hessian
```

The inverse of $B$ does not need to be calculated – instead, if $B$ is positive definite, a Cholesky decomposition and two backward solves are sufficient:

```r
R> Rchol <- chol(B)
R> L1 <- backsolve(Rchol, G, transpose = TRUE)
R> Gammay <- backsolve(Rchol, L1)
```

The trace of the hat matrix, the first part of the effective degrees of freedom needed for the cAIC, can also easily be computed with the help of the residual matrix $A$

```r
R> df <- n - sum(diag(A))
```

The correction needed to account for the uncertainty induced by the estimation of the variance parameters can be added for each random effects variance parameter separately by calculating

```r
R> for (j in 1:length(theta)) {
+   df <- df + sum(Gammay[,j] %*% A %*% Wlist[[j]] %*% A %*% y)
+ }
```

**Poisson responses**

The computation of the bias correction for Poisson distributed responses is obtained differently. In a first step the non-zero responses need to be identified and a matrix with the responses in each column is created. Consider the `grouseticks` example in Section 4 with the model `p1` fitted by `glmer`.

```r
R> y <- p1@resp$y
R> ind <- which(y != 0)
R> workingMatrix <- matrix(rep(y, length(y)), ncol = length(y))
```

The diagonal values of the matrix are reduced by one and only those columns of the matrix with non-zero responses are kept.

```r
R> diag(workingMatrix) <- diag(workingMatrix) - 1
R> workingMatrix <- workingMatrix[ind,]
```
Now the `refit()` function can be applied to the columns of the matrix in order to obtain the estimates $\log \hat{\mu}_i(y_{-i}, y_i - 1)$ in (13) from the reduced data.

```r
R> workingEta <- diag(apply(workingMatrix, 2, function(x) + refit(p1, newresp = x)@resp$eta)[ind,])
```

The computation of the bias correction is then straightforward:

```r
R> sum(y[ind] * (p1@resp$eta[ind] - workingEta))
[1] 205.5785
```

and corresponds to the bias correction obtained in Section 4.

**Bernoulli**

The computation of an estimator of the bias correction for Bernoulli distributed responses as in Equation (14) is similar to the implementation for Poisson distributed responses above. Therefore consider any Bernoulli model `b1` fitted by the `glmer` function in `lme4`. For the calculation of the bias correction for each observed response variable the model needs to be refitted with corresponding other value, i.e., 0 for 1 and vice versa. This is done best by use of the `refit()` function from `lme4`.

```r
R> muHat <- b1@resp$mu
R> workingEta <- numeric(length(muHat))
R> for(i in 1:length(muHat)){ +   workingData <- b1$y +   workingData[i] <- 1 - workingData[i] +   workingModel <- refit(b1, nresp = workingData) +   workingEta[i] <- log(workingModel@resp$mu[i] / (1 - workingModel@resp$mu[i])) - log(muHat[i] / (1 - muHat[i])) + }
```

The sign of the re-estimated logit (the natural parameter) in (14) which is stored in the vector `workingEta` needs to be taken into account, i.e., $\hat{\eta}_i(1)$ is positive and $\hat{\eta}_i(0)$ negative. With a simple sign correction

```r
R> signCor <- - 2 * b1@resp$y + 1
```

the following returns the bias correction:

```r
R> sum(muHat * (1 - muHat) * signCor * workingEta)
```

It should be pointed out that for the conditional AIC it is essential to use the conditional log-likelihood with the appropriate bias correction. Notice that the log-likelihood that by
default is calculated by the S3-method \texttt{logLik} for class \texttt{merMod} (the class of a mixed model fitted by a \texttt{lmer} call) is the marginal log-likelihood.

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