

On the Behavior of Marginal and Conditional Akaike Information Criteria in Linear Mixed Models

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Overview

- Linear and additive mixed models.
- Akaike's information criterion (AIC).
- Marginal AIC
- Conditional AIC
- Application: Childhood malnutrition in Zambia

Linear and Additive Mixed Models

- Mixed models form a very useful class of regression models with general form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{b} + \boldsymbol{\varepsilon}$$

where $\boldsymbol{\beta}$ are usual regression coefficients while \mathbf{b} are **random effects** with distributional assumption

$$\begin{bmatrix} \boldsymbol{\varepsilon} \\ \mathbf{b} \end{bmatrix} \sim \text{N} \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \sigma^2 \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{D} \end{bmatrix} \right).$$

- Denote the vector of all **unknown variance parameters** as $\boldsymbol{\theta}$.
- In the following, we will concentrate on mixed models with **only one variance component** where

$$\mathbf{b} \sim \text{N}(\mathbf{0}, \tau^2 \mathbf{I}) \quad \text{or} \quad \mathbf{b} \sim \text{N}(\mathbf{0}, \tau^2 \boldsymbol{\Sigma})$$

with $\boldsymbol{\Sigma}$ known and therefore $\boldsymbol{\theta} = (\sigma^2, \tau^2)$.

- Special case I: Random intercept model for **longitudinal data**

$$y_{ij} = \mathbf{x}'_{ij}\boldsymbol{\beta} + b_i + \varepsilon_{ij}, \quad j = 1, \dots, J_i, \quad i = 1, \dots, I,$$

where i indexes individuals while j indexes **repeated observations** on the same individual.

- The random intercept b_i accounts for shifts in the individual level of response trajectories and therefore also for **intra-subject correlations**.
- Extended models include further random (covariate) effects, leading to random slopes.

- Special case II: **Penalised spline smoothing** for nonparametric function estimation

$$y_i = m(x_i) + \varepsilon_i, \quad i = 1, \dots, n,$$

where $m(x)$ is a **smooth, unspecified function**.

- Approximating $m(x)$ in terms of a **spline basis of degree d** leads (for example) to the truncated power series representation

$$m(x) = \sum_{j=0}^d \beta_j x^j + \sum_{j=1}^K b_j (x - \kappa_j)_+^d$$

where $\kappa_1, \dots, \kappa_K$ denotes a sequence of knots.

- The spline approximation leads to a **piecewise polynomial fit of degree d** on the intervals defined by the knots under appropriate smoothness restrictions.

- **Penalised estimation** to avoid overly wiggly function estimates:

$$(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\mathbf{b})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\mathbf{b}) + \lambda\mathbf{b}'\mathbf{b} \rightarrow \min_{\boldsymbol{\beta}, \mathbf{b}}$$

where \mathbf{X} and \mathbf{Z} correspond to design matrices obtained from the truncated power series representation.

- The smoothness of the curve is determined by the **smoothing parameter** λ .
- Equivalent to assuming the **random effect distribution** $\mathbf{b} \sim \mathbf{N}(\mathbf{0}, \tau^2\mathbf{I})$ and setting the smoothing parameter to

$$\lambda = \frac{\sigma^2}{\tau^2}.$$

- Works also for other basis choices (e.g. B-splines) and other types of flexible modelling components (varying coefficients, surfaces, spatial effects, etc.).

- Additive mixed models consist of a **combination of random effects and flexible modelling components** such as penalised splines.
- Example: Childhood malnutrition in Zambia.
- Determine the nutritional status of a child in terms of a Z-score.
- We consider chronic malnutrition measured in terms of **insufficient height for age (stunting)**, i.e.

$$zscore_i = \frac{cheight_i - med}{s},$$

where med and s are the median and standard deviation of (age-stratified) height in a reference population.

- Additive mixed model for stunting:

$$zscore_i = \mathbf{x}'_i \boldsymbol{\beta} + m_1(cage_i) + m_2(cfeed_i) + m_3(mage_i) + m_4(mbmi_i) \\ + m_5(mheight_i) + b_{s_i} + \varepsilon_i,$$

with covariates

| | |
|----------------|---|
| <i>csex</i> | gender of the child (1 = male, 0 = female) |
| <i>cfeed</i> | duration of breastfeeding (in months) |
| <i>cage</i> | age of the child (in months) |
| <i>mage</i> | age of the mother (at birth, in years) |
| <i>mheight</i> | height of the mother (in cm) |
| <i>mbmi</i> | body mass index of the mother |
| <i>medu</i> | education of the mother (1 = no education, 2 = primary school, 3 = elementary school, 4 = higher) |
| <i>mwork</i> | employment status of the mother (1 = employed, 0 = unemployed) |
| <i>s</i> | residential district (54 districts in total) |

- The random effect b_{s_i} captures **spatial variability** induced by unobserved spatially varying covariates.

- **Marginal perspective** on a mixed model:

$$\mathbf{y} \sim \text{N}(\mathbf{X}\boldsymbol{\beta}, \mathbf{V})$$

where

$$\mathbf{V} = \sigma^2 \mathbf{I} + \mathbf{ZDZ}'$$

- Interpretation: The random effects induce a **correlation structure** and therefore enable a proper statistical analysis of correlated data.
- **Conditional perspective** on a mixed model:

$$\mathbf{y}|\mathbf{b} \sim \text{N}(\mathbf{X}\boldsymbol{\beta} + \mathbf{Zb}, \sigma^2 \mathbf{I}).$$

- Interpretation: Random effects are **additional regression coefficients** (for example subject-specific effects in longitudinal data) that are estimated subject to a regularisation penalty.

- Best linear unbiased estimates / predictions in the linear mixed model:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}, \quad \hat{\mathbf{b}} = \mathbf{D}\mathbf{Z}'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}).$$

- Unknown variance parameters $\boldsymbol{\theta}$ are estimated using maximum likelihood (ML) or **restricted maximum likelihood** (REML).
- Interest in the following is on **model choice** in linear mixed models with the special form

$$\mathbf{D} = \text{blockdiag}(\tau_1^2\boldsymbol{\Sigma}_1, \dots, \tau_q^2\boldsymbol{\Sigma}_q)$$

(q independent random effects) for known correlation matrices $\boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_q$ and in particular in models with only one variance component such as

$$\mathbf{D} = \tau^2\mathbf{I}.$$

- Without loss of generality, we consider the comparison of

$$M_1 : \mathbf{D} = \text{blockdiag}(\tau_1^2 \boldsymbol{\Sigma}_1, \dots, \tau_q^2 \boldsymbol{\Sigma}_q)$$

and

$$M_2 : \mathbf{D} = \text{blockdiag}(\tau_1^2 \boldsymbol{\Sigma}_1, \dots, \tau_{q-1}^2 \boldsymbol{\Sigma}_{q-1}).$$

- The two models are nested since M_1 reduces to M_2 when $\tau_q^2 = 0$.
- Random Intercept: $\tau_q^2 > 0$ versus $\tau_q^2 = 0$ corresponds to the **inclusion and exclusion of the random intercept** and therefore to the presence or absence of intra-individual correlations.
- Penalised splines: $\tau_q^2 > 0$ versus $\tau_q^2 = 0$ differentiates between a spline model and a simple polynomial model. In particular, we can compare **linear versus nonlinear models**.

Akaike's Information Criterion

- Data \mathbf{y} generated from a **true underlying model** described in terms of density $g(\cdot)$.
- Approximate the true model by a **parametric class of models** $f_\psi(\cdot) = f(\cdot; \psi)$.
- Measure the discrepancy between a model $f_\psi(\cdot)$ and the truth $g(\cdot)$ by the **Kullback-Leibler distance**

$$\begin{aligned} K(f_\psi, g) &= \int [\log(g(\mathbf{z})) - \log(f_\psi(\mathbf{z}))] g(\mathbf{z}) d\mathbf{z} \\ &= \mathbb{E}_{\mathbf{z}} [\log(g(\mathbf{z})) - \log(f_\psi(\mathbf{z}))]. \end{aligned}$$

where \mathbf{z} is an independent replicate following the same distribution as \mathbf{y} .

- Note that $K(f_\psi, g) \geq 0$ and $K(f_\psi, g) = 0$ iff $f_\psi = g$ almost everywhere.

- Decision rule: Out of a sequence of models, **choose the one that minimises $K(f_\psi, g)$** .
- In practice, the parameter ψ will have to be **estimated as $\hat{\psi}(\mathbf{y})$** for the different models.
- To focus on average properties not depending on a specific data realisation, minimise the **expected Kullback-Leibler distance**

$$\mathbf{E}_{\mathbf{y}}[K(f_{\hat{\psi}(\mathbf{y})}, g)] = \mathbf{E}_{\mathbf{y}}[\mathbf{E}_{\mathbf{z}} [\log(g(\mathbf{z})) - \log(f_{\hat{\psi}(\mathbf{y})}(\mathbf{z}))]]]$$

- Since $g(\cdot)$ does not depend on the data, this is equivalent to minimising

$$-2 \mathbf{E}_{\mathbf{y}}[\mathbf{E}_{\mathbf{z}}[\log(f_{\hat{\psi}(\mathbf{y})}(\mathbf{z}))]] \quad (1)$$

(the expected **relative** Kullback-Leibler distance).

- The best available estimate for (1) is given by

$$-2 \log(f_{\hat{\psi}(\mathbf{y})}(\mathbf{y})).$$

- While (1) is a **predictive quantity** depending on both the data \mathbf{y} and an independent replication \mathbf{z} , the density and the parameter estimate are **evaluated for the same data \mathbf{y}** .

⇒ Introduce a correction term.

- Let $\tilde{\psi}$ denote the parameter vector minimising the Kullback-Leibler distance.
- Then

$$\begin{aligned} AIC &= -2 \log(f_{\hat{\psi}(\mathbf{y})}(\mathbf{y})) + 2 \mathbf{E}_{\mathbf{y}}[\log(f_{\hat{\psi}(\mathbf{y})}(\mathbf{y})) - \log(f_{\tilde{\psi}}(\mathbf{y}))] \\ &\quad + 2 \mathbf{E}_{\mathbf{y}}[\mathbf{E}_{\mathbf{z}}[\log(f_{\tilde{\psi}}(\mathbf{z})) - \log(f_{\hat{\psi}(\mathbf{y})}(\mathbf{z}))]] \end{aligned}$$

is unbiased for (1).

- Consider the **regularity conditions**
 - ψ is a k -dimensional parameter with parameter space $\Psi = \mathbb{R}^k$ (possibly achieved by a change of coordinates).
 - \mathbf{y} consists of independent and identically distributed replications y_1, \dots, y_n .
- In this case, the AIC simplifies since

$$2 \mathbb{E}_{\mathbf{z}} \left[\log(f_{\tilde{\psi}}(\mathbf{z})) - \log(f_{\hat{\psi}(\mathbf{y})}(\mathbf{z})) \right] \stackrel{a}{\sim} \chi_k^2,$$
$$2 \left[\log(f_{\hat{\psi}(\mathbf{y})}(\mathbf{y})) - \log(f_{\tilde{\psi}}(\mathbf{y})) \right] \stackrel{a}{\sim} \chi_k^2$$

and therefore an (asymptotically) unbiased estimate for (1) is given by

$$AIC = -2 \log(f_{\hat{\psi}(\mathbf{y})}(\mathbf{y})) + 2k.$$

- In linear mixed models, **two variants of AIC** are conceivable based on either the marginal or the conditional distribution.

- The **marginal AIC relies** on the marginal model

$$\mathbf{y} \sim \text{N}(\mathbf{X}\boldsymbol{\beta}, \mathbf{V})$$

and is defined as

$$mAIC = -2l(\mathbf{y}|\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\theta}}) + 2(p + q),$$

where the **marginal likelihood** is given by

$$l(\mathbf{y}|\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\theta}}) = -\frac{1}{2} \log(|\hat{\mathbf{V}}|) - \frac{1}{2}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})' \hat{\mathbf{V}}^{-1} (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})$$

and $p = \dim(\boldsymbol{\beta})$, $q = \dim(\boldsymbol{\theta})$.

- The **conditional AIC** relies on the conditional model

$$\mathbf{y}|\mathbf{b} \sim \text{N}(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{b}, \sigma^2\mathbf{I})$$

and is defined as

$$cAIC = -2l(\mathbf{y}|\hat{\boldsymbol{\beta}}, \hat{\mathbf{b}}, \hat{\boldsymbol{\theta}}) + 2(\rho + 1),$$

where

$$l(\mathbf{y}|\hat{\boldsymbol{\beta}}, \hat{\mathbf{b}}, \hat{\boldsymbol{\theta}}) = -\frac{n}{2} \log(\hat{\sigma}^2) - \frac{1}{2\hat{\sigma}^2} (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}} - \mathbf{Z}\hat{\mathbf{b}})' (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}} - \mathbf{Z}\hat{\mathbf{b}})$$

is the **conditional likelihood** and

$$\rho = \text{trace} \left(\left(\begin{pmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Z} \\ \mathbf{Z}'\mathbf{X} & \mathbf{Z}'\mathbf{Z} + \sigma^2\mathbf{D} \end{pmatrix} \right)^{-1} \begin{pmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Z} \\ \mathbf{Z}'\mathbf{X} & \mathbf{Z}'\mathbf{Z} \end{pmatrix} \right)$$

are the **effective degrees of freedom** (trace of the hat matrix).

- The conditional AIC seems to be recommended when the model shall be used for predictions with the **same set of random effects** (for example in penalised spline smoothing).
- The marginal AIC is more plausible when observations with **new random effects** shall be predicted (e.g. new individuals in longitudinal studies).
- Still, both variants have been considered in both situations and seem to work reasonably well (see for example Wager, Vaida & Kauermann, 2007).

Marginal AIC

- Consider the special case of comparing

$$M_1 : \mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{b} + \boldsymbol{\varepsilon}, \quad \mathbf{b} \sim \text{N}(\mathbf{0}, \tau^2 \mathbf{I})$$

versus

$$M_2 : \mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

i.e. decide on the inclusion of a random effect.

- Corresponds to the decision $\tau^2 > 0$ (M_1) versus $\tau^2 = 0$ (M_2).

- Model M_1 is preferred over M_2 when

$$\begin{aligned} mAIC_1 < mAIC_2 &\Leftrightarrow -2l(\mathbf{y}|\hat{\boldsymbol{\beta}}_1, \hat{\tau}^2, \hat{\sigma}_1^2) + 2(p+2) < -2l(\mathbf{y}|\hat{\boldsymbol{\beta}}_2, \mathbf{0}, \hat{\sigma}_2^2) + 2(p+1) \\ &\Leftrightarrow 2l(\mathbf{y}|\hat{\boldsymbol{\beta}}_1, \hat{\tau}^2, \hat{\sigma}_1^2) - 2l(\mathbf{y}|\hat{\boldsymbol{\beta}}_2, \mathbf{0}, \hat{\sigma}_2^2) > 2. \end{aligned}$$

- The left hand side is simply the test statistic for a **likelihood ratio test on $\tau^2 = 0$ versus $\tau^2 > 0$** .
- Under standard asymptotics, we would have

$$2l(\mathbf{y}|\hat{\boldsymbol{\beta}}_1, \hat{\tau}^2, \hat{\sigma}_1^2) - 2l(\mathbf{y}|\hat{\boldsymbol{\beta}}_2, \mathbf{0}, \hat{\sigma}_2^2) \stackrel{a, H_0}{\sim} \chi_1^2$$

and the marginal AIC would have a type 1 error of

$$P(\chi_1^2 > 2) \approx 0.1572992$$

- Common interpretation: AIC selects **rather too many than too few effects**.

- In contrast to the regularity conditions for likelihood ratio tests, we are testing on the **boundary of the parameter space!**
- The likelihood ratio test statistic is no longer χ^2 -distributed but (approximately) follows a mixture of a **point mass in zero and a scaled χ_1^2 variable.**
- The point mass in zero corresponds to the probability

$$P(\hat{\tau}^2 = 0)$$

that is typically **larger than 50%.**

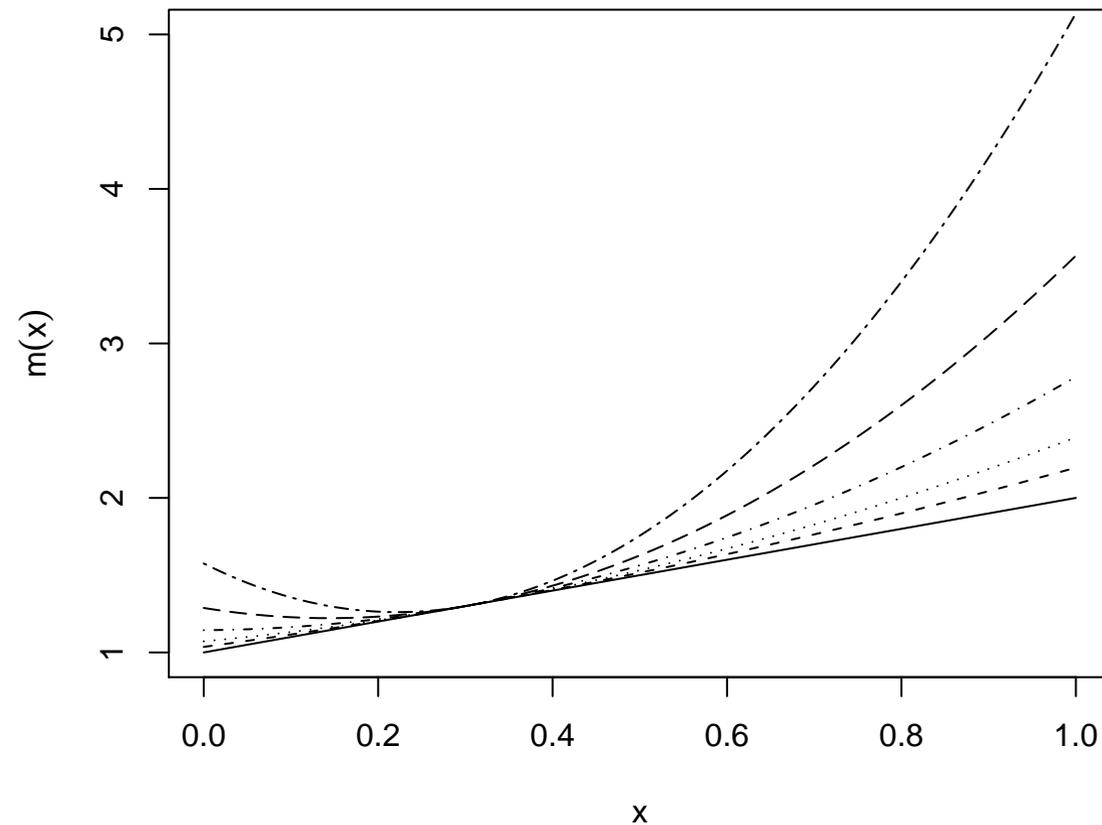
- Similar difficulties appear in more complex models with several variance components when deciding on zero variances.

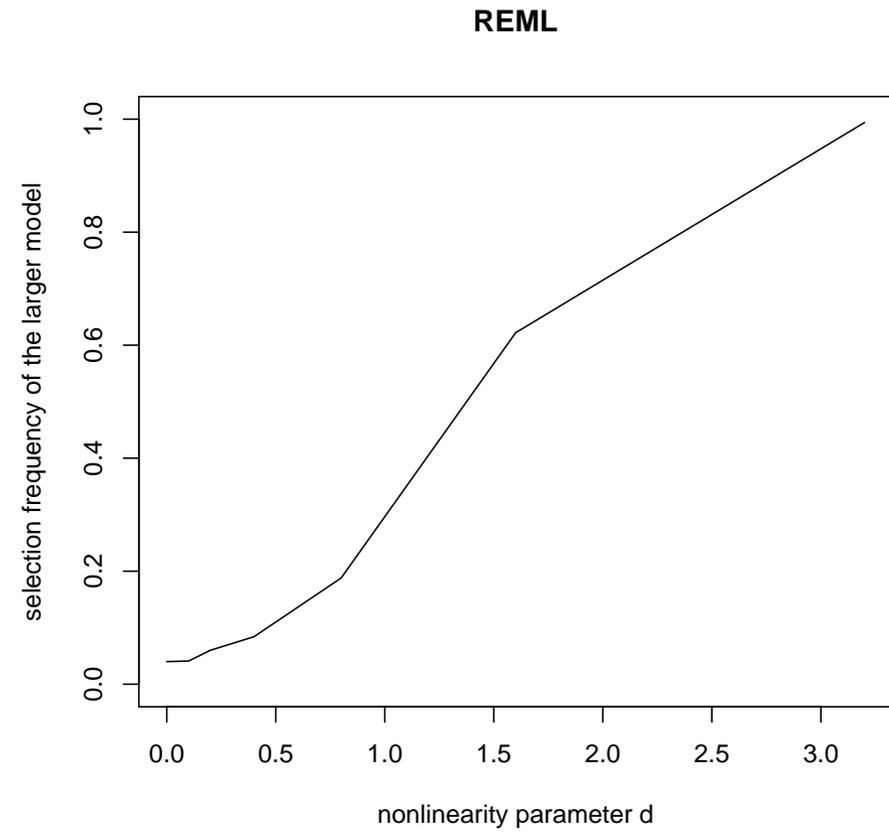
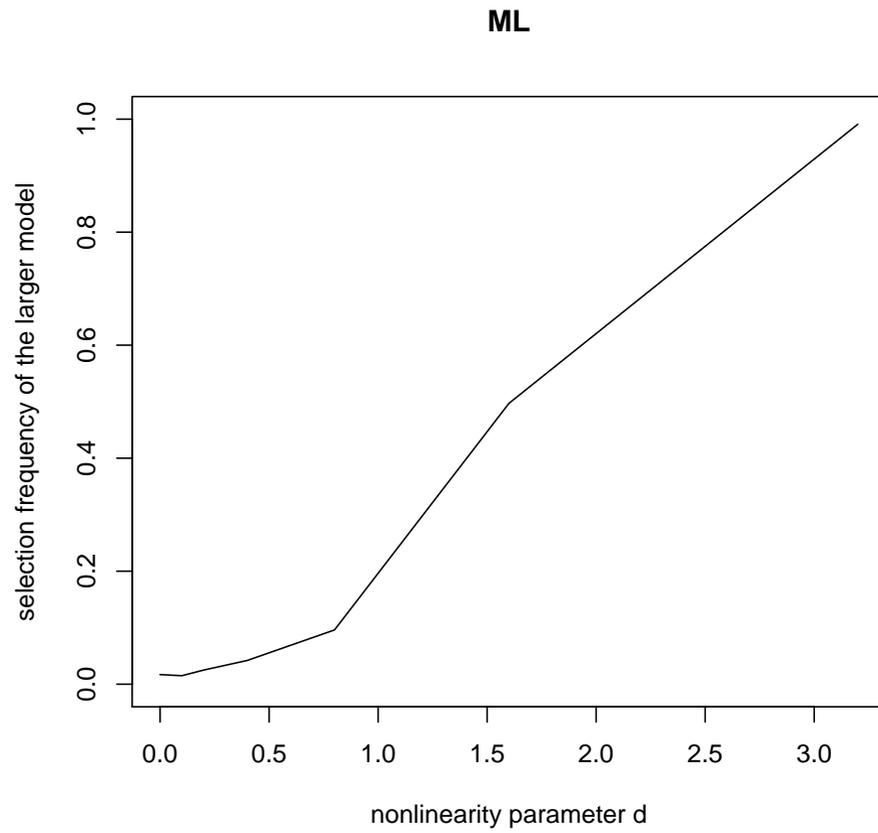
- The classical assumptions underlying the derivation of AIC are also not fulfilled.
- The high probability of estimating a zero variance yields a **bias towards simpler models**:
 - The marginal AIC is positively biased for twice the expected relative Kullback-Leibler-Distance.
 - The bias is dependent on the true unknown parameters in the random effects covariance matrix D and this dependence does not vanish asymptotically.
 - Compared to an unbiased criterion, the marginal AIC favors smaller models excluding random effects.
- This contradicts the usual intuition that the AIC picks rather too many than too few effects.

- Simulated example: $y_i = m(x) + \varepsilon$ where

$$m(x) = 1 + x + 2d(0.3 - x)^2.$$

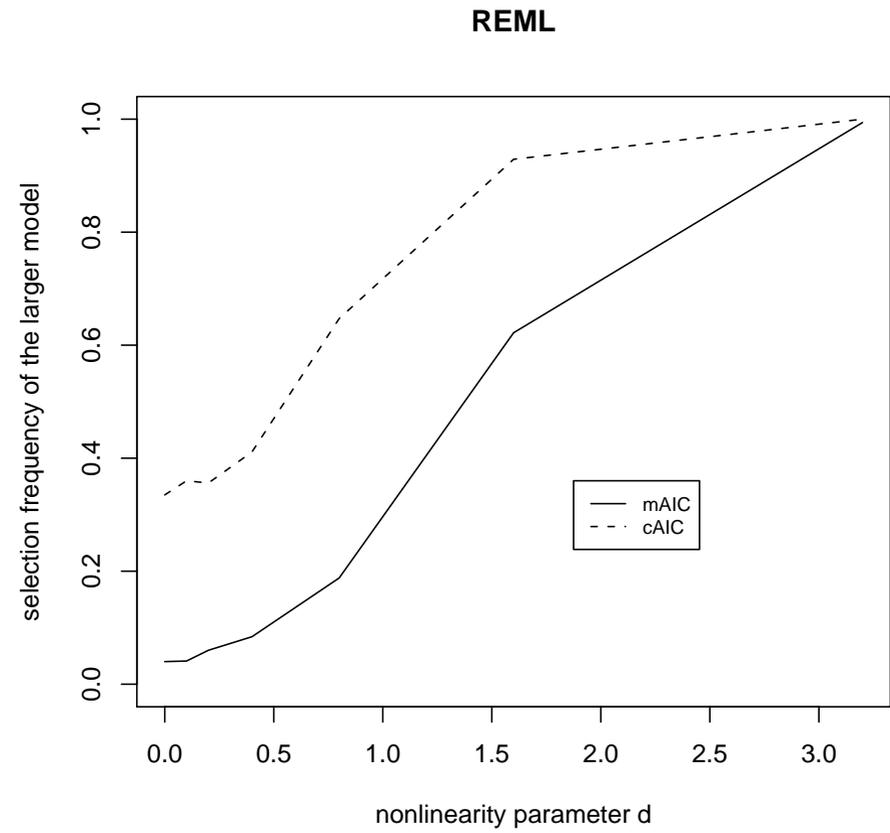
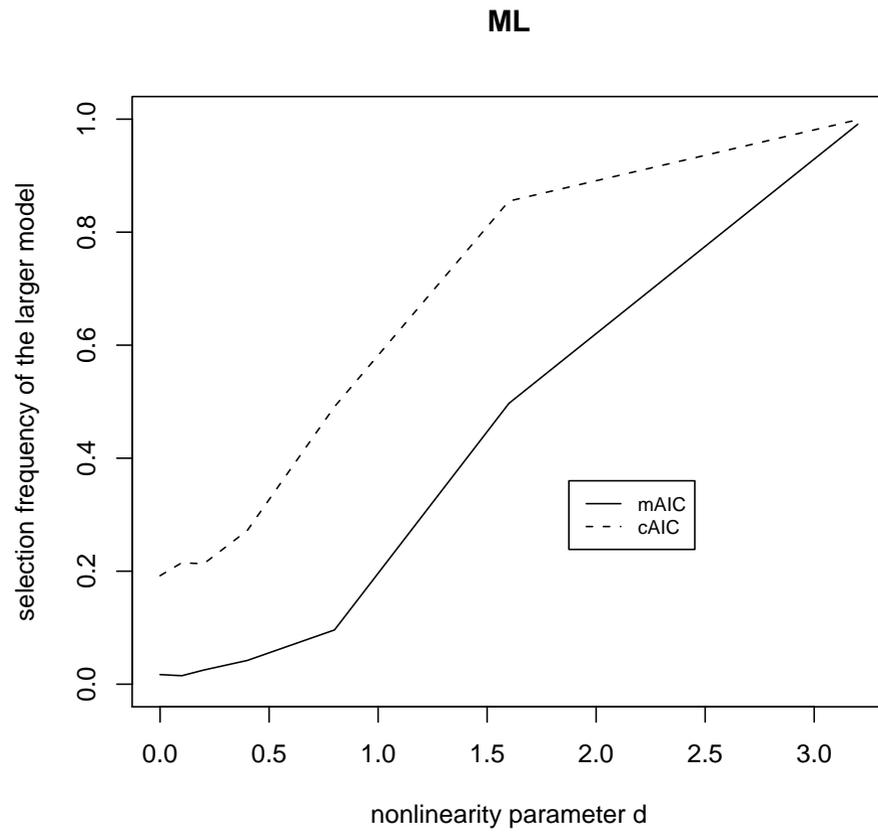
- The parameter d determines the **amount of nonlinearity**.





Conditional AIC

- Vaida & Blanchard (2005) have shown that the conditional AIC is asymptotically unbiased for the expected relative Kullback Leibler distance for **given random effects covariance matrix D** .
- If D is estimated consistently, one would hope that their result carries over to the case of estimated \hat{D} .
- Simulation results seem to indicate that this is not the case.



- Surprising result of the simulation study: The complex model including the random effect is chosen **whenever $\hat{\tau}^2 > 0$** .
- If $\hat{\tau}^2 = 0$, the conditional AICs of the simple and the complex model coincide (despite the additional parameters included in the complex model).
- The observed phenomenon could be shown to be a general property of the conditional AIC:

$$\hat{\tau}^2 > 0 \quad \Leftrightarrow \quad cAIC(\hat{\tau}^2) < cAIC(0)$$

$$\hat{\tau}^2 = 0 \quad \Leftrightarrow \quad cAIC(\hat{\tau}^2) = cAIC(0).$$

- Principal difficulty: The degrees of freedom in the cAIC are **estimated from the same data as the model parameters**.

- Liang et al. (2008) propose a **corrected conditional AIC**, where the degrees of freedom ρ are replaced by

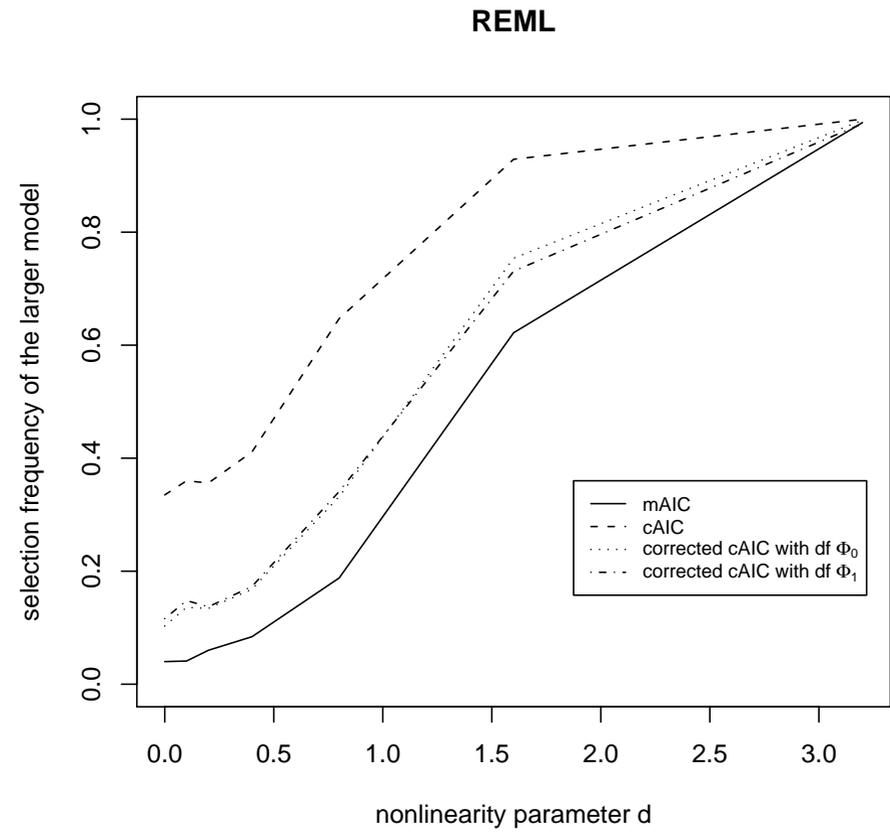
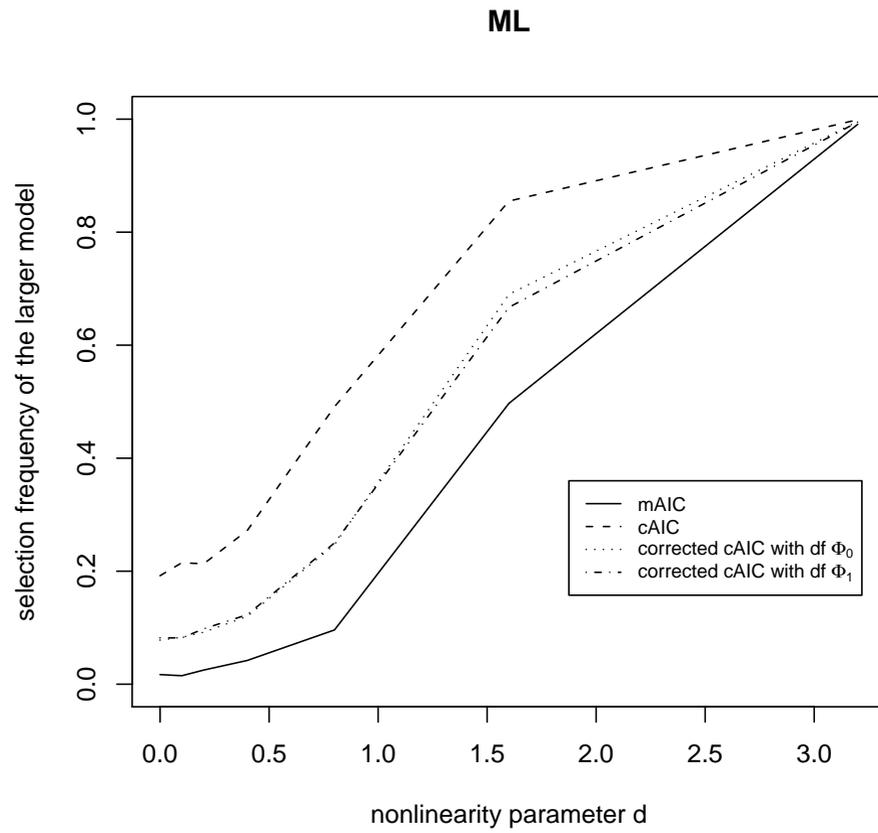
$$\Phi_0 = \sum_{i=1}^n \frac{\partial \hat{y}_i}{\partial y_i} = \text{trace} \left(\frac{\partial \hat{\mathbf{y}}}{\mathbf{y}} \right)$$

if σ^2 is known.

- For unknown σ^2 , they propose to replace $\rho + 1$ by

$$\Phi_1 = \frac{\tilde{\sigma}^2}{\hat{\sigma}^2} \text{trace} \left(\frac{\partial \hat{\mathbf{y}}}{\mathbf{y}} \right) + \tilde{\sigma}^2 (\hat{\mathbf{y}} - \mathbf{y})' \frac{\partial \hat{\sigma}^{-2}}{\partial \mathbf{y}} + \frac{1}{2} \tilde{\sigma}^4 \text{trace} \left(\frac{\partial^2 \hat{\sigma}^{-2}}{\partial \mathbf{y} \partial \mathbf{y}'} \right),$$

where $\tilde{\sigma}^2$ is an estimate for the true error variance.



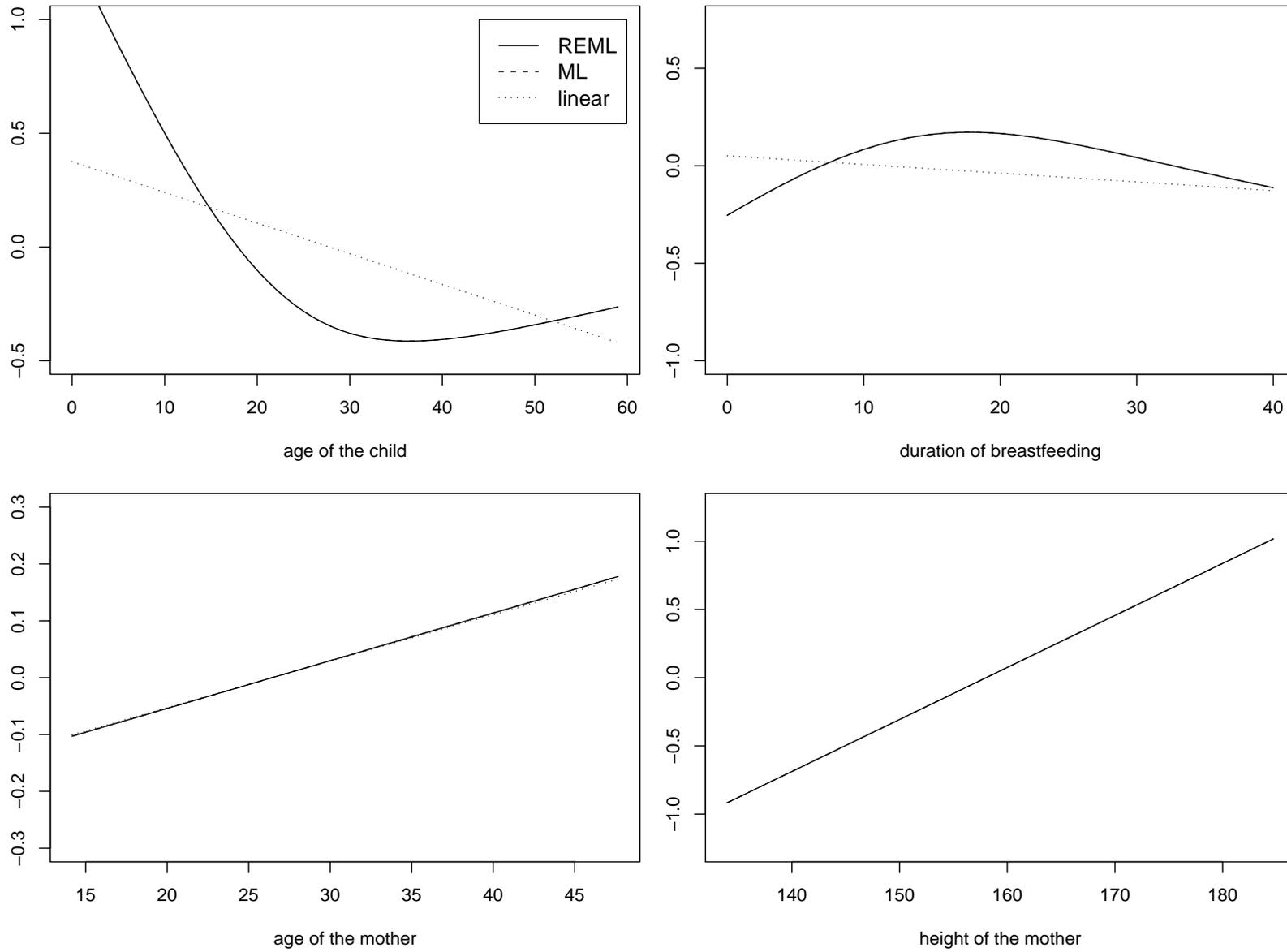
- The corrected conditional AIC shows **satisfactory theoretical properties**.
- However, it is **computationally cumbersome**:
 - The first and second derivative are not available in closed form and must be approximated numerically (by adding small perturbations to the data).
 - Numerical approximations require n and $2n$ model fits. In our example, computing the corrected conditional AICs would take about 110 days.
 - In addition, the numerical derivatives were found to be instable in some situations (for example the random intercept model with small cluster sizes).

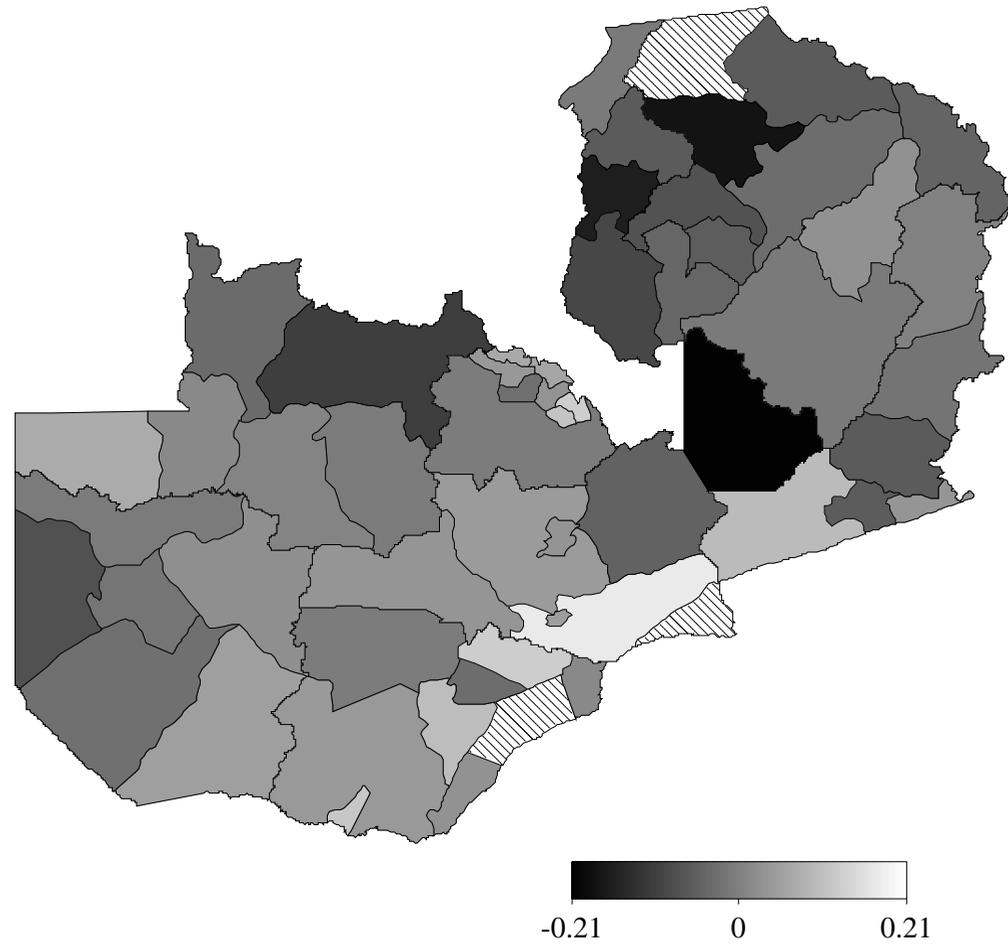
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- Model equation:

$$\begin{aligned} zscore_i = & \mathbf{x}'_i \boldsymbol{\beta} + m_1(cage_i) + m_2(cfeed_i) + m_3(mage_i) + m_4(mbmi_i) \\ & + m_5(mheight_i) + b_{s_i} + \varepsilon_i. \end{aligned}$$

- Parametric effects are not subject to model selection.
 $\Rightarrow 2^6 = 64$ models to consider in the model comparison.





- The six best fitting models:

| | cfeed | cage | mage | mheight | mbmi | district | <i>ML</i> | | <i>REML</i> | |
|----|-------|------|------|---------|------|----------|----------------|----------------|----------------|----------------|
| | | | | | | | <i>cAIC</i> | <i>mAIC</i> | <i>cAIC</i> | <i>mAIC</i> |
| 14 | + | + | - | - | - | + | 4125.78 | 4151.10 | 4125.78 | 4173.72 |
| 34 | + | + | + | - | - | + | 4125.78 | 4153.10 | 4125.78 | 4175.72 |
| 36 | + | + | - | + | - | + | 4125.78 | 4153.10 | 4125.78 | 4175.72 |
| 38 | + | + | - | - | + | + | 4125.78 | 4153.10 | 4125.78 | 4175.72 |
| 54 | + | + | + | + | - | + | 4125.78 | 4155.10 | 4125.78 | 4177.72 |
| 56 | + | + | + | - | + | + | 4125.78 | 4155.10 | 4125.78 | 4177.72 |
| 58 | + | + | - | + | + | + | 4125.78 | 4155.10 | 4125.78 | 4177.72 |
| 64 | + | + | + | + | + | + | 4125.78 | 4157.10 | 4125.78 | 4179.72 |

Summary

- The marginal AIC suffers from the same theoretical difficulties as likelihood ratio tests on the boundary of the parameter space.
- The marginal AIC is biased towards simpler models excluding random effects.
- The conventional conditional AIC tends to select too many variables.
- Whenever a random effects variance is estimated to be positive, the corresponding effect will be included.
- The corrected conditional AIC rectifies this difficulty but comes at a high computational price.

- Open questions:
 - Is there a computationally advantageous version / representation of the corrected conditional AIC?
 - Can the marginal AIC be corrected?
 - Is there a working likelihood ratio test based on the corrected conditional AIC?

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