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

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Outline

- Akaike Information Criterion
- Linear Mixed Models
- Marginal Akaike Information Criterion
- Conditional Akaike Information Criterion
- Application: Childhood Malnutrition in Nigeria

Akaike Information Criterion

- Most commonly used model choice criterion for comparing parametric models.
- Definition:

$$\text{AIC} = -2l(\hat{\boldsymbol{\psi}}) + 2k.$$

  where $l(\hat{\boldsymbol{\psi}})$ is the log-likelihood evaluated at the maximum likelihood estimate $\hat{\boldsymbol{\psi}}$ for the unknown parameter vector $\boldsymbol{\psi}$ and $k = \dim(\boldsymbol{\psi})$ is the number of parameters.

- Properties:
  - Compromise between model fit and model complexity.
  - Allows to compare non-nested models.
  - Selects rather too many than too few variables in variable selection problems.

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

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

  where $\boldsymbol{z}$ is an independent replicate following the same distribution as $\boldsymbol{y}$.
- Decision rule: Out of a sequence of models, choose the one that minimises $K(f_{\boldsymbol{\psi}}, g)$.

- In practice, the parameter $\boldsymbol{\psi}$ will have to be estimated as $\hat{\boldsymbol{\psi}}(\boldsymbol{y})$ for the different models.
- To focus on average properties not depending on a specific data realisation, minimise the expected Kullback-Leibler distance

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

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

$$-2\,\mathrm{E}_{\boldsymbol{y}}[\mathrm{E}_{\boldsymbol{z}}[\log(f_{\hat{\boldsymbol{\psi}}(\boldsymbol{y})}(\boldsymbol{z}))]] \tag{1}$$

(the expected relative Kullback-Leibler distance).

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

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

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

  $\Rightarrow$ Introduce a correction term.

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

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

  is unbiased for (1).

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

$$\begin{aligned} 2\left[\log(f_{\hat{\boldsymbol{\psi}}(\boldsymbol{y})}(\boldsymbol{y})) - \log(f_{\tilde{\boldsymbol{\psi}}}(\boldsymbol{y}))\right] &\overset{a}{\sim} \chi^2_k, \\ 2\,\mathrm{E}_{\boldsymbol{z}}\left[\log(f_{\tilde{\boldsymbol{\psi}}}(\boldsymbol{z})) - \log(f_{\hat{\boldsymbol{\psi}}(\boldsymbol{y})}(\boldsymbol{z}))\right] &\overset{a}{\sim} \chi^2_k \end{aligned}$$

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

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

Linear Mixed Models

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

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

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

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

- In the following, we will concentrate on mixed models with only one variance component where

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

with $\boldsymbol{\Sigma}$ known.

- Special case I: Random intercept model for longitudinal data

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

  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.

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

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

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 $\kappa_1, \ldots, \kappa_K$ denotes a sequence of knots.

- Assume random effects distribution $\boldsymbol{b} \sim \mathrm{N}(\boldsymbol{0}, \tau^2 \boldsymbol{I})$ for the basis coefficients of truncated polynomials to enforce smoothness.

- 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:

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

with covariates

$csex$	gender of the child (1 = male, 0 = female)
$cfeed$	duration of breastfeeding (in months)
$cage$	age of the child (in months)
$mage$	age of the mother (at birth, in years)
$mheight$	height of the mother (in cm)
$mbmi$	body mass index of the mother
$medu$	education of the mother (1 = no education, 2 = primary school, 3 = elementary school, 4 = higher)
$mwork$	employment status of the mother (1 = employed, 0 = unemployed)
s	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:

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

where

$$\boldsymbol{V} = \sigma^2 \boldsymbol{I} + \boldsymbol{Z}\boldsymbol{D}\boldsymbol{Z}'$$

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

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

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

- Interest in the following is on the selection of random effects: Compare

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

  and

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

- Equivalent: Compare model with random effects ($\tau^2 > 0$) and without random effects ($\tau^2 = 0$).
- Random Intercept: $\tau^2 > 0$ versus $\tau^2 = 0$ corresponds to the inclusion and exclusion of the random intercept and therefore to the presence or absence of intra-individual correlations.
- Penalised splines: $\tau^2 > 0$ versus $\tau^2 = 0$ differentiates between a spline model and a simple polynomial model. In particular, we can compare linear versus nonlinear models.

Akaike Information Criteria in Linear Mixed Models

- 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

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

and is defined as

$$\mathrm{mAIC} = -2l(\boldsymbol{y}|\hat{\boldsymbol{\beta}}, \hat{\tau}^2, \hat{\sigma}^2) + 2(p+2),$$

where the marginal likelihood is given by

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

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

- The conditional AIC relies on the conditional model

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

and is defined as

$$\mathrm{cAIC} = -2l(\boldsymbol{y}|\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{b}}, \hat{\tau}^2, \sigma^2) + 2(\rho + 1),$$

where

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

is the conditional likelihood and

$$\rho = \mathrm{tr}\left(\begin{pmatrix} \boldsymbol{X}'\boldsymbol{X} & \boldsymbol{X}'\boldsymbol{Z} \\ \boldsymbol{Z}'\boldsymbol{X} & \boldsymbol{Z}'\boldsymbol{Z} + \sigma^2/\tau^2\boldsymbol{\Sigma} \end{pmatrix}^{-1} \begin{pmatrix} \boldsymbol{X}'\boldsymbol{X} & \boldsymbol{X}'\boldsymbol{Z} \\ \boldsymbol{Z}'\boldsymbol{X} & \boldsymbol{Z}'\boldsymbol{Z} \end{pmatrix}\right)$$

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).

Marginal AIC

- Model M_1 ($\tau^2 > 0$) is preferred over M_2 ($\tau^2 = 0$) when

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

- 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

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

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, τ^2 is on the boundary of the parameter space for model M_2.
- 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^2_1 variable.
- The point mass in zero corresponds to the probability

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

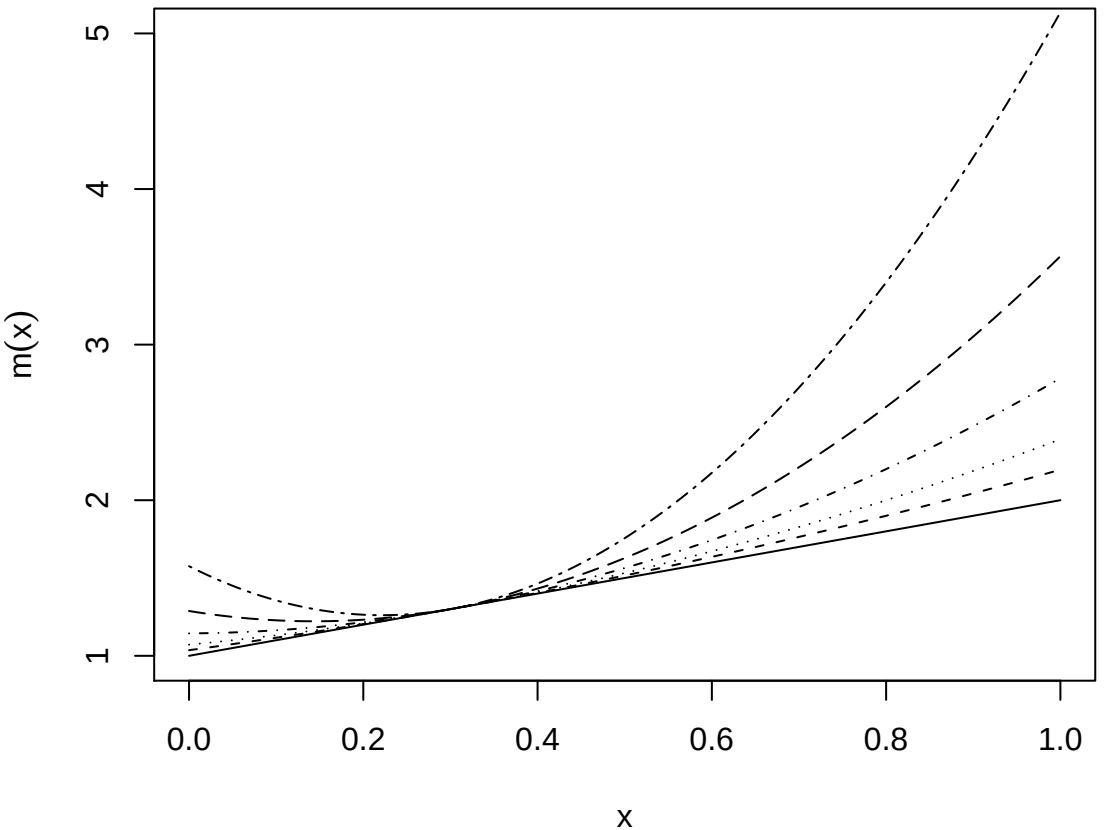
  that is typically larger than 50%.
- Similar difficulties appear in more complex models with several variance components when deciding on zero variances.

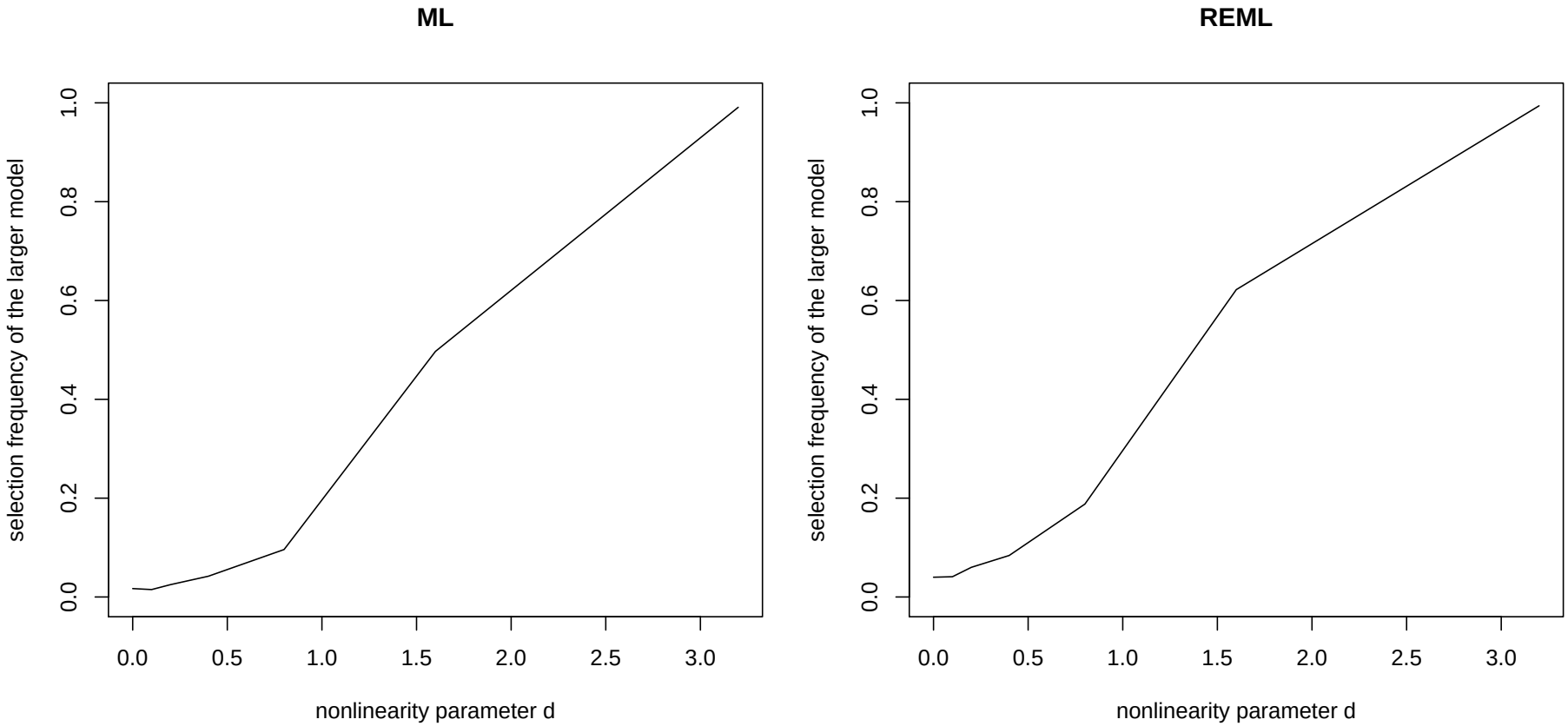
- The classical assumptions underlying the derivation of AIC are also not fulfilled.
- The high probability of estimating a zero variance yields a bias towards simpler models:
  - The marginal AIC is positively biased for twice the expected relative Kullback-Leibler-Distance.
  - The bias is dependent on the true unknown parameters in the random effects covariance matrix 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

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

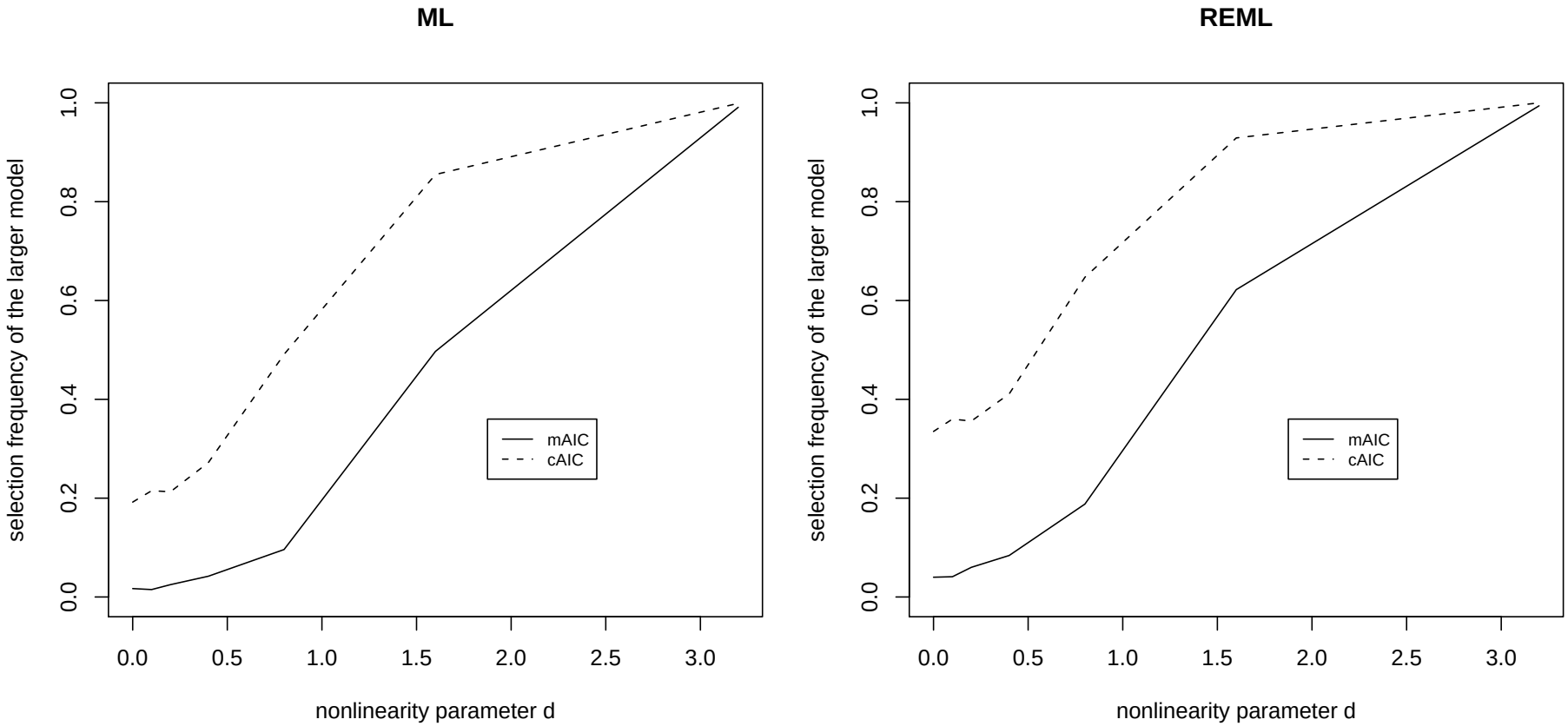
- The parameter d determines the amount of nonlinearity.




ML
REML
selection frequency of the larger model
nonlinearity parameter d
0.0
0.2
0.4
0.6
0.8
1.0
0.5
1.5
2.0
2.5
3.0

Conditional AIC

- Vaida & Blanchard (2005) have shown that the conditional AIC from above is asymptotically unbiased for the expected relative Kullback Leibler distance for given random effects covariance matrix.
- Intuition: Result should carry over when using a consistent estimate.
- Simulation results indicate that this is not the case.


ML
REML
selection frequency of the larger model
nonlinearity parameter d
mAIC
cAIC
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0

- 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 can be shown to be a general property of the conditional AIC:

$$\begin{aligned} \hat{\tau}^2 > 0 \quad &\Leftrightarrow \quad \text{cAIC}(\hat{\tau}^2) < \text{cAIC}(0) \\ \hat{\tau}^2 = 0 \quad &\Leftrightarrow \quad \text{cAIC}(\hat{\tau}^2) = \text{cAIC}(0). \end{aligned}$$

- 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

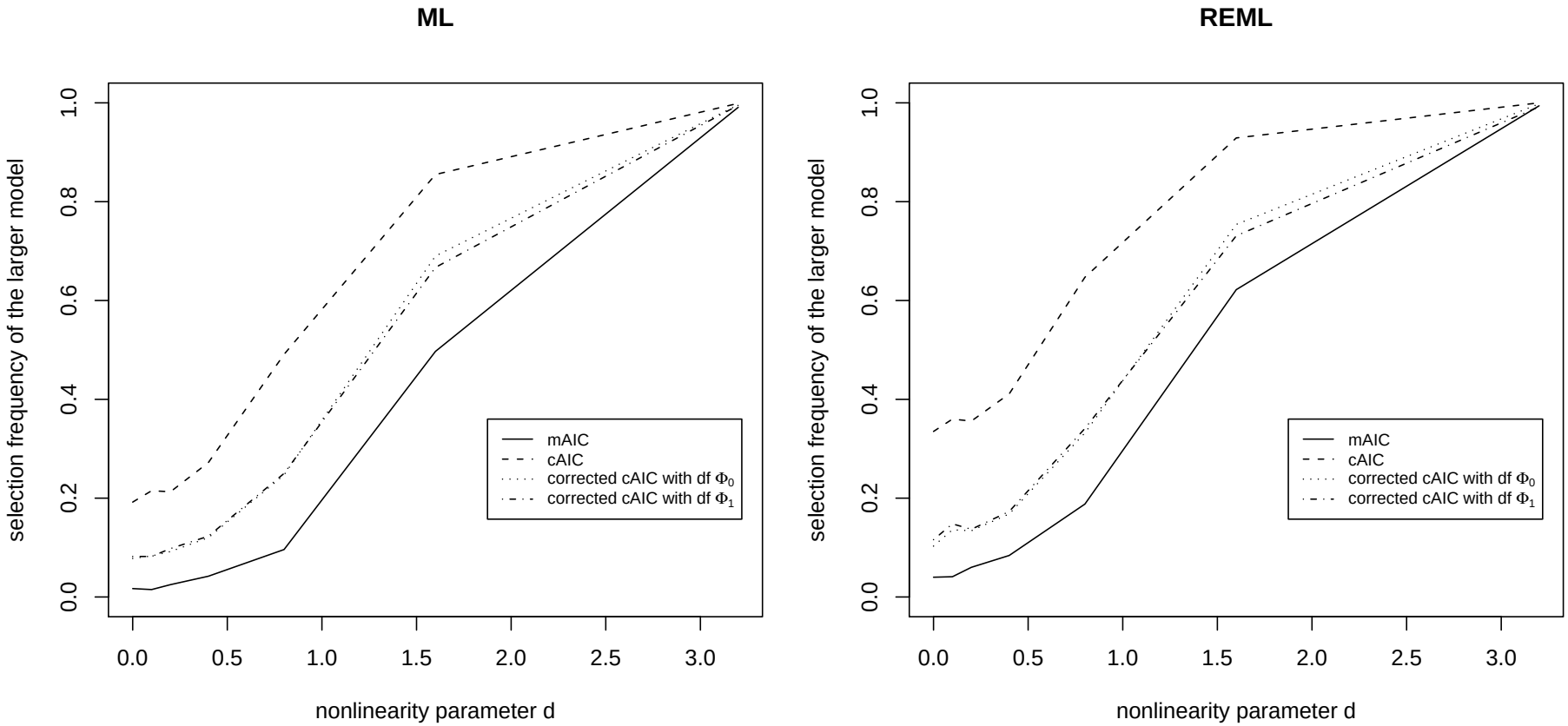
$$\Phi_0 = \sum_{i=1}^{n} \frac{\partial \hat{y}_i}{\partial y_i} = \operatorname{tr}\left(\frac{\partial \hat{\boldsymbol{y}}}{\boldsymbol{y}}\right)$$

  if σ^2 is known.

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

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

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


ML
REML
selection frequency of the larger model
nonlinearity parameter d
0.0
0.2
0.4
0.6
0.8
1.0
0.5
1.5
2.0
2.5
3.0
mAIC
cAIC
corrected cAIC with df Φ_0
corrected cAIC with df Φ_1

- The corrected conditional AIC shows satisfactory theoretical properties.
- However, it is computationally cumbersome:
  - Liang et al. suggested to approximate the derivatives numerically (by adding small perturbations to the data).
  - Numerical approximations require n and $2n$ model fits. In our application, 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).
- We have developed a closed form representation of Φ_0 that is available almost instantaneously.

Application: Childhood Malnutrition in Zambia

- Model equation:

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

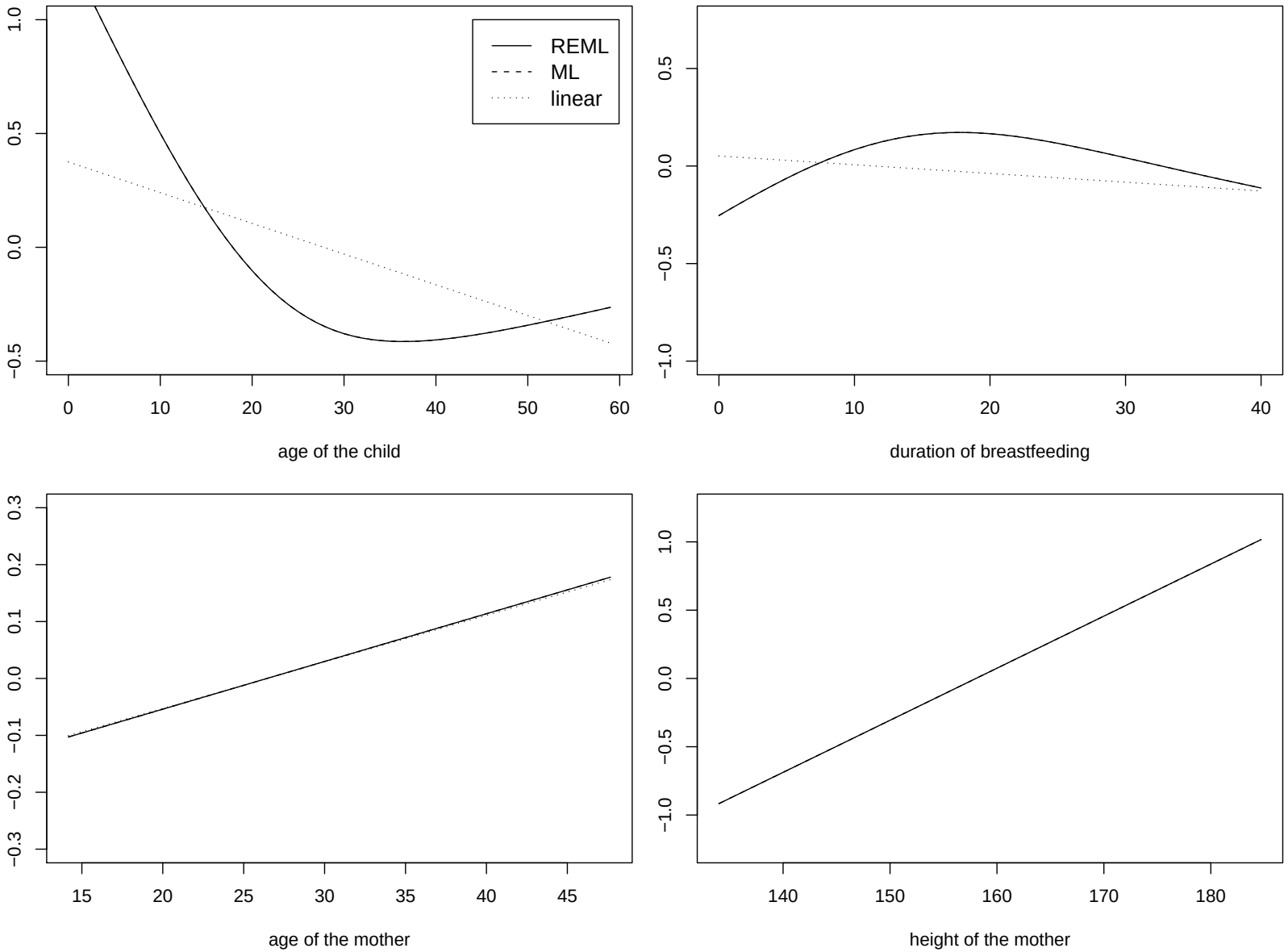
- Parametric effects in $\boldsymbol{x}'\boldsymbol{\beta}$ are not subject to model selection.

  $\Rightarrow 2^6 = 64$ models to consider in the model comparison.

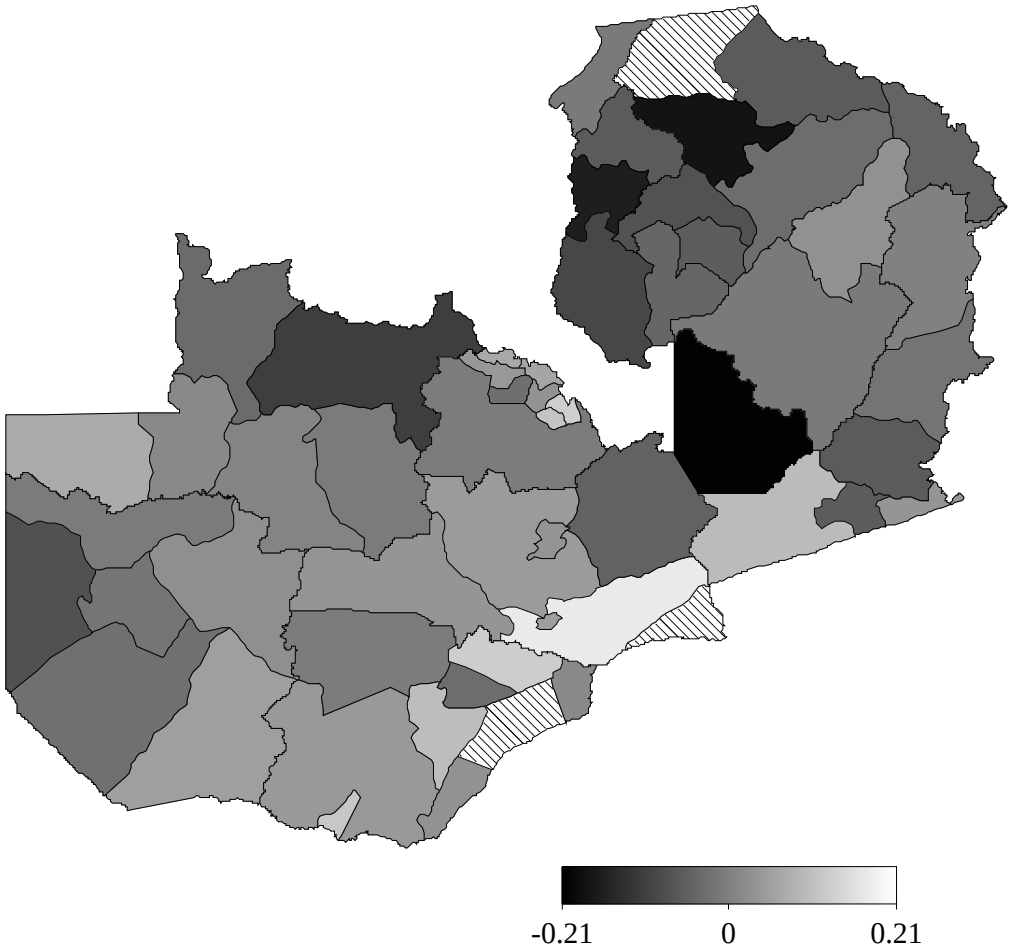
- The eight best fitting models:

						ML		$REML$	
cfeed	cage	mage	mheight	mbmi	s	$cAIC$	$mAIC$	$cAIC$	$mAIC$
+	+	−	−	−	+	**4125.78**	**4151.10**	**4125.78**	**4173.72**
+	+	+	−	−	+	**4125.78**	4153.10	**4125.78**	4175.72
+	+	−	+	−	+	**4125.78**	4153.10	**4125.78**	4175.72
+	+	−	−	+	+	**4125.78**	4153.10	**4125.78**	4175.72
+	+	+	+	−	+	**4125.78**	4155.10	**4125.78**	4177.72
+	+	+	−	+	+	**4125.78**	4155.10	**4125.78**	4177.72
+	+	−	+	+	+	**4125.78**	4155.10	**4125.78**	4177.72
+	+	+	+	+	+	**4125.78**	4157.10	**4125.78**	4179.72

- Linear effects are selected for age, height and body mass index of the mother.
- Some nonlinearity is detected for age of the child and duration of breastfeeding.


REML
ML
linear
1.0
0.5
0.0
−0.5
0
10
20
30
40
50
60
age of the child
0.5
0.0
−0.5
−1.0
0
10
20
30
40
duration of breastfeeding
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
15
20
25
30
35
40
45
age of the mother
1.0
0.5
0.0
−0.5
−1.0
140
150
160
170
180
height of the mother

- Inclusion of the region-specific random effect is required to capture spatial variation.



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 and is now available in closed form.

- References:
  - Greven, S. & Kneib, T. (2009): On the Behavior of Marginal and Conditional Akaike Information Criteria in Linear Mixed Models. Technical Report.
  - Liang, H., Wu, H. & Zou, G. (2008): A note on conditional AIC for linear mixed-effects models. Biometrika 95, 773–778.
  - Vaida, F. & Blanchard, S. (2005): Conditional Akaike information for mixed-effects models. Biometrika 92, 351–370.
- A place called home:

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