

Coefficients of Determination for Mixed-Effects Models

Dabao Zhang

Department of Statistics, Purdue University

May 4, 2022

Abstract

The coefficient of determination is well defined for linear models and its extension is long wanted for mixed-effects models in agricultural, biological, and ecological research. We revisit its extension to define measures for proportions of variation explained by the whole model, fixed effects only, and random effects only. We propose to calculate unexplained variations conditional on individual random and/or fixed effects so as to keep individual heterogeneity brought by available predictors. While naturally defined for linear mixed models, these measures can be defined for a generalized linear mixed model using a distance measured along its variance function, accounting for its heteroscedasticity. We demonstrate the promising performance and utility of our proposed methods via simulation studies as well as applications to real data sets in agricultural and ecological studies.

Keywords: Exponential family distribution; Generalized linear mixed model; Linear mixed model; Quasi-model; R^2 ; Variance function

1 Introduction

Mixed-effect models are widely used in agricultural, biological, and ecological research to understand the variation components of a response variable (Gbur et al., 2012; Zuur et al., 2009). The law of total variance provides a theoretical basis for defining the coefficient of determination, also known as R^2 , for linear models and sheds light on defining similar measures for mixed-effects models.

Suppose that a linear mixed model (McCulloch et al., 2008) is considered for observed response variable Y_{ij} from the j -th individual inside the i -th cluster, with $j = 1, \dots, n_i$ and $i = 1, \dots, m$. In general, we write the corresponding linear mixed model as,

$$Y_{ij} = \eta_{ij}^F + \eta_{ij}^R + \epsilon_{ij}, \quad \epsilon_{ij} \sim N(0, \sigma^2), \quad (1)$$

where η_{ij}^F and η_{ij}^R respectively summarize all fixed and random effects on the response variable with

$$\eta_{ij}^R | \tau_{ij}^2 \sim N(0, \tau_{ij}^2).$$

Note that $\{\epsilon_{ij}, j = 1, \dots, n_i\}$ may be an autocorrelated series in, for example, longitudinal studies (Laird and Ware, 1982). For construction simplicity, we will not emphasize such correlation as it does not affect the unbiasedness of estimated variances in the below although the estimation may not be optimal.

Similar to linear models, the law of total variance provides a clear path to extend R^2 for linear mixed models, measuring the proportion of variation in the dependent variable modeled by fixed effects, random effects, or both (Xu, 2003; Nakagawa and Schielzeth, 2013; Nakagawa et al., 2017; Jaeger et al., 2017, 2019). However, unlike usual calculation that heavily relies on estimated error variance σ^2 , we instead propose to calculate unexplained variations conditional on individual random and/or fixed effects so as to keep individual heterogeneity brought by available predictors which also shed lights on their extensions to more general models.

The inherent heteroscedasticity makes it difficult to properly define R^2 for generalized linear mixed models. Indeed, such heteroscedasticity also challenges the proper definition of R^2 for generalized linear models (McCullagh and Nelder, 1989). Therefore, many different measures have been proposed to define R^2 for generalized linear models from

different aspects of view (Cameron and Windmeijer, 1997; Cox and Snell, 1989; Maddala, 1983; Magee, 1990; Nagelkerke, 1991; Zhang, 2017). However, it is difficult to extend these measures to account for random effects involved in generalized linear mixed models.

A common strategy to define R^2 for generalized linear mixed models, adopted by Nakagawa and Schielzeth (2013) and Nakagawa et al. (2017), is to recognize the linear function presented by the link function $g(\cdot)$, i.e.,

$$g(E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R]) = \eta_{ij}^F + \eta_{ij}^R, \quad (2)$$

and instead construct R^2 for a transformed linear mixed model for $g(Y_{ij})$. However, such measures rely on the specified link function and even the approximation method used to calculate the error variance (Nakagawa et al., 2017). On the other hand, the link function does not necessarily provide homoscedastic variance on the error term, which is the primary challenge in extending classical R^2 from linear models to generalized linear models, although it may describe a linear relationship of all effects on $g(E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R])$, and present additive variance components in $g(Y_{ij})$.

A critical concern of defining R^2 based on a transformed linear model is that proportions of different variance components in $g(Y_{ij})$ may not represent the genuine proportions of different variance components in Y_{ij} . For example, it is well-known that the latent linear model of a probit model may present a much higher R^2 , but the binomial response still holds a lot of uncertainty, which is well recognized in the study of genetic heritability, see Dempster and Lerner (1950).

Recently Zhang (2017) showed that quantifying the variation change along the variance function can measure explained variation of a heteroscedastic response variable and hence proposed to define a variance-function-based R^2 . Unlike other likelihood-based measures, such a measure neither overstates the proportion of explained variation, nor demands the specification of likelihood functions. While it only requires specification of the link function and variance function, it reduces to classical R^2 for generalized linear models so it is conceptually consistent with classical R^2 . We thus use the variance-function-based measures to define R^2 for generalized linear mixed models.

In the next section, we revisit the definition of coefficients of determination to account for explained variation by fixed effects, random effects, or both in linear mixed models,

and propose our calculation emphasizing individual heterogeneity. In Section 3, we extend these measures for generalized linear mixed models by using the variance-function-based distance (Zhang, 2017). Our simulation studies to compare different measures are shown in Section 4. We also compare these measures in Section 5 by applying them to three sets of real data from agricultural and ecological studies, and conclude with a discussion in Section 6.

2 Linear Mixed Models

For the linear mixed model (1), we can follow the law of total variance and define the proportion of variation in Y_{ij} modeled by the fixed effects as

$$\rho_F^2 = 1 - \frac{E[\text{var}(Y_{ij} | \eta_{ij}^F)]}{\text{var}(Y_{ij})} = 1 - \frac{E[(Y_{ij} - E[Y_{ij} | \eta_{ij}^F])^2]}{E[(Y_{ij} - E[Y_{ij}])^2]}. \quad (3)$$

With η_{ij}^F estimated by $\hat{\eta}_{ij}^F$ and $E[Y_{ij}]$ estimated by the sample average $\bar{Y}_{..}$, we have the following estimate of ρ_F^2 ,

$$R_F^2 = 1 - \frac{\sum_{i,j} (Y_{ij} - \hat{\eta}_{ij}^F)^2}{\sum_{i,j} (Y_{ij} - \bar{Y}_{..})^2}. \quad (4)$$

Since

$$E[(Y_{ij} - E[Y_{ij} | \eta_{ij}^F])^2] = E[\tau_{ij}^2] + \sigma^2,$$

we may also take estimated variance components to construct R_F^2 to estimate ρ_F^2 , see, e.g., Xu (2003), Nakagawa and Schielzeth (2013), Nakagawa et al. (2017), and Jaeger et al. (2017). As our revisit to defining R^2 in linear mixed models also serves to shed light on their extensions to generalized linear mixed models (McCullagh and Nelder, 1989), we will not pursue this avenue as it cannot manage the heterogeneity in generalized linear mixed models.

The proportion of variation in Y_{ij} modeled by both fixed and random effects can be similarly defined as

$$\rho_M^2 = 1 - \frac{E[\text{var}(Y_{ij} | \eta_{ij}^F, \eta_{ij}^R)]}{\text{var}(Y_{ij})} = 1 - \frac{E[(Y_{ij} - E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R])^2]}{E[(Y_{ij} - E[Y_{ij}])^2]}. \quad (5)$$

With $\text{var}(Y_{ij} | \eta_{ij}^F, \eta_{ij}^R) = \sigma^2$, it is tempting to estimate ρ_M^2 on the basis of $\rho_M^2 = 1 - \sigma^2/\text{var}(Y_{ij})$ as in Xu (2003), Nakagawa and Schielzeth (2013), Nakagawa et al. (2017),

Jaeger et al. (2017), and Ives (2019). However, the total variation in the response variable is described by $SST = \sum_{i,j} (Y_{ij} - \bar{Y}_{..})^2$, and we thus would rather to calculate the total unexplained variation by emphasizing individual heterogeneity of τ_{ij} and the contribution of individual observation, which also help the extension to generalized linear models.

Note that,

$$E [(Y_{ij} - E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R])^2] = E [E[(Y_{ij} - E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R])^2 | Y_{ij}, \eta_{ij}^F, \tau_{ij}^2, \sigma^2]],$$

implying that each observation contributes $E [(Y_{ij} - E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R])^2 | Y_{ij}, \eta_{ij}^F, \tau_{ij}^2, \sigma^2]$ with observed value Y_{ij} and estimable parameters in η_{ij}^F, τ_{ij}^2 , and σ^2 . That is, the expectation is on the random variable η_{ij}^R conditional on the observed values and these estimable parameters. With the conditional distribution

$$\eta_{ij}^R | Y_{ij}, \eta_{ij}^F, \tau_{ij}^2, \sigma^2 \sim N \left(\frac{\tau_{ij}^2}{\sigma^2 + \tau_{ij}^2} (Y_{ij} - \eta_{ij}^F), \frac{\sigma^2 \tau_{ij}^2}{\sigma^2 + \tau_{ij}^2} \right),$$

we have

$$E[(Y_{ij} - E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R])^2 | Y_{ij}, \eta_{ij}^F, \tau_{ij}^2, \sigma^2] = \left(\frac{\sigma^2}{\sigma^2 + \tau_{ij}^2} \right)^2 (Y_{ij} - \eta_{ij}^F)^2 + \frac{\sigma^2 \tau_{ij}^2}{\sigma^2 + \tau_{ij}^2}.$$

Therefore, ρ_M^2 will be estimated by

$$R_M^2 = 1 - \frac{\sum_{i,j} \frac{\hat{\sigma}^2}{\hat{\sigma}^2 + \hat{\tau}_{ij}^2} \left\{ \hat{\tau}_{ij}^2 + \frac{\hat{\sigma}^2}{\hat{\sigma}^2 + \hat{\tau}_{ij}^2} (Y_{ij} - \hat{\eta}_{ij}^F)^2 \right\}}{\sum_{i,j} (Y_{ij} - \bar{Y}_{..})^2}. \quad (6)$$

The proportion of variation in Y_{ij} modeled by random effects can be simply defined as

$$\rho_R^2 = \rho_M^2 - \rho_F^2 = \frac{E[(Y_{ij} - E[Y_{ij} | \eta_{ij}^F, \tau_{ij}^2])^2] - E[(Y_{ij} - E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R])^2]}{\text{var}(Y_{ij})}, \quad (7)$$

and can be estimated as

$$R_R^2 = R_M^2 - R_F^2. \quad (8)$$

Such a simple definition on ρ_R^2 assumes that ρ_F^2 has a priority over ρ_R^2 , that is, when fixed and random effects overlapped, we would rather know the proportion of variation explained by available fixed effects, and therefore use ρ_R^2 to measure the proportion of variable additionally explained by random effects.

3 Generalized Linear Mixed Models

For the generalized linear mixed model (2), the variance of Y_{ij} , given both fixed and random effects, can be specified via a dispersion parameter ϕ and a known variance function $V(\cdot)$, i.e.,

$$\text{var}(Y_{ij} \mid \eta_{ij}^F, \eta_{ij}^R) = \phi V(g^{-1}(\eta_{ij}^F + \eta_{ij}^R)).$$

In general, as long as the mean $g^{-1}(\eta_{ij}^F + \eta_{ij}^R)$ can be modeled well and linked appropriately to a set of predictors, a generalized linear model with known variance function $V(\cdot)$ can be investigated for the utility of the involved predictors.

The variance function describes the effect of the mean on the variation of the response variable besides the dispersion parameter. For a response variable with its mean moving from a to b , its variation changes accordingly along the variance function from $\phi V(a)$ to $\phi V(b)$. Taking advantage of relationship between mean and variance defined by the variance function, we measure the variation change along the variance function (Zhang, 2017). That is, the variation change of the response variable should be measured using, instead of $(a - b)^2$, the squared length of the variance function $V(\cdot)$ between $V(a)$ to $V(b)$,

$$d_V(a, b) = \left\{ \int_a^b \sqrt{1 + [V'(t)]^2} dt \right\}^2.$$

As show in Table 1, $d_V(\cdot, \cdot)$ may dramatically differ than the Euclidean distance when the variance function is nonlinear.

Table 1: Difference Between the Euclidean Distance and $d_V(\cdot, \cdot)$.

Distribution	$V(\mu)$	μ_1	μ_2	Y	$\frac{(Y-\mu_2)^2}{(Y-\mu_1)^2}$	$\frac{d_V(Y, \mu_2)}{d_V(Y, \mu_1)}$
Binomial	$\mu(1 - \mu)$.5	.75	1	.25	.2991
Poisson	μ	1	2	3	.25	.25
Gamma	μ^2	1	2	3	.25	.3805
Inverse Gaussian	$\mu^3/2$	0	1	2	.25	.6735

Our definition of R^2 for generalized linear mixed models will proceed by replacing the Euclidean distance by the above manifold distance along the variance function.

Replacing $(a - b)^2$ with $d_V(a, b)$ in (3), we can define the proportion of variation in Y_{ij} modeled by the fixed effects as

$$\rho_F^2 = 1 - \frac{E[d_V(Y_{ij}, E[Y_{ij} | \eta_{ij}^F])]}{E[d_V(Y_{ij}, E[Y_{ij}])]} \quad (9)$$

Note that $E[Y_{ij} | \eta_{ij}^F]$ is estimated via $\hat{\eta}_{ij}^F$ resulted from fitting the linear mixed model in (4). Suppose $\hat{\eta}_{ij}^F$ can also be obtained by fitting the generalized linear mixed model (2). However, unlike the linear mixed models, fitting a generalized linear model with only the fixed effect η_{ij}^F but ignoring the random effect η_{ij}^R in model (2) may result in an estimate $\tilde{\eta}_{ij}^F$ which is much different from $\hat{\eta}_{ij}^F$. Since $\tilde{\eta}_{ij}^F$, instead of $\hat{\eta}_{ij}^F$, represents better the contribution of fixed effects to explaining the variation in the response variable, we propose to estimate ρ_F^2 by

$$R_F^2 = 1 - \frac{\sum_{i,j} d_V(Y_{ij}, g^{-1}(\tilde{\eta}_{ij}^F))}{\sum_{i,j} d_V(Y_{ij}, \bar{Y}_{..})} \quad (10)$$

With (5), we can similarly define the proportion of variation in Y_{ij} modeled by both fixed and random effects as

$$\rho_M^2 = 1 - \frac{E[d_V(Y_{ij}, E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R])]}{E[d_V(Y_{ij}, E[Y_{ij}])]} = 1 - \frac{E[d_V(Y_{ij}, g^{-1}(\eta_{ij}^F + \eta_{ij}^R))]}{E[d_V(Y_{ij}, E[Y_{ij}])]} \quad (11)$$

We can simply plug in $\hat{\eta}_{ij}^F$ and $\hat{\eta}_{ij}^R$, estimates of η_{ij}^F and η_{ij}^R respectively from fitting (2), to estimate ρ_M^2 ,

$$R_M^2 = 1 - \frac{\sum_{i,j} d_V(Y_{ij}, g^{-1}(\hat{\eta}_{ij}^F + \hat{\eta}_{ij}^R))}{\sum_{i,j} d_V(Y_{ij}, \bar{Y}_{..})} \quad (12)$$

The proportion of variation in Y_{ij} modeled by random effects can be defined as

$$\rho_R^2 = \rho_M^2 - \rho_F^2 = \frac{E[d_V(Y_{ij}, E[Y_{ij} | \eta_{ij}^F])]}{\text{var}(Y_{ij})} - \frac{E[d_V(Y_{ij}, E[Y_{ij} | \eta_{ij}^F, \eta_{ij}^R])]}{\text{var}(Y_{ij})} \quad (13)$$

Accordingly, we can calculate the R^2 for random effects using $R_R^2 = R_M^2 - R_F^2$ with R_M^2 and R_F^2 calculated in (12) and (10), respectively. Such a calculation of R_R^2 based on the above definition of ρ_R^2 follows the fact that we usually want to evaluate the contribution due to random effects by removing those attributable to the fixed effects. However, in the case that we prioritize the contribution due to the random effects over the contribution due

to the fixed effects, we may parallel the definition of ρ_R^2 and R_R^2 , instead of ρ_F^2 and R_F^2 , to that of ρ_M^2 and R_M^2 .

Similar to classical R^2 defined for linear regression models, both R_F^2 and R_M^2 defined as above may increase as more predictors are included into the underlying model. We can define the adjusted R_F^2 and adjusted R_M^2 by dividing the numerators and denominators in (10) and (12) with proper degrees of freedom. The adjusted R_R^2 can be accordingly calculated via the adjusted R_F^2 and adjusted R_M^2 .

4 Simulation Studies

4.1 Linear Mixed Models

For linear mixed models, we compared the performance of our proposed R^2 to those proposed by Xu (2003) and Nakagawa et al. (2017), with a total of 1,000 data sets simulated from each model under investigation. Each data set has a total of 200 random samples, evenly clustered inside m groups with $m = 10$ and 50 , respectively. A binary covariate X_1 was generated for each observation, with half observations within the same group taking 1 and the other half taking -1. A second variable X_2 was generated from the standard normal distribution, independent of X_1 and the response variable. The j -th response value inside the i -th cluster, i.e., y_{ij} , was generated by

$$y_{ij} = \mu_i + x_{1ij}\beta + \epsilon_{ij},$$

where x_{1ij} is the corresponding value of the binary covariate X_1 , the random effect $\mu_i \stackrel{iid}{\sim} N(0, 1)$, and $\epsilon_{ij} \stackrel{iid}{\sim} N(0, 1)$.

For each data set, we fit different models, i.e., regressing against only X_1 or only X_2 , with the maximum likelihood method, and then estimate both ρ_M^2 and ρ_F^2 with different approaches as shown in Figure 1. Note that, when regressing against only X_1 , we have

$$\rho_M^2 = \frac{\beta^2 + 1}{\beta^2 + 2}, \quad \rho_F^2 = \frac{\beta^2}{\beta^2 + 2}.$$

While Xu (2003) only estimates ρ_M^2 but not ρ_F^2 , it may severely overestimate ρ_M^2 especially when the number of groups is large. Indeed, the bias can be more than 0.15 when

there are 100 groups (the results are not shown). Our proposed R_M^2 and the methods by Nakagawa et al. (2017) estimate ρ_M^2 and ρ_F^2 well, however, there are slight bias especially when the number of groups is small. When regressing against only X_2 , we have

$$\rho_M^2 = \frac{1}{\beta^2 + 2}, \quad \rho_F^2 = 0.$$

While our proposed R_F^2 and the method by Nakagawa et al. (2017) estimate ρ_F^2 very well, they both underestimate ρ_M^2 , which may be a desirable property for model selection.

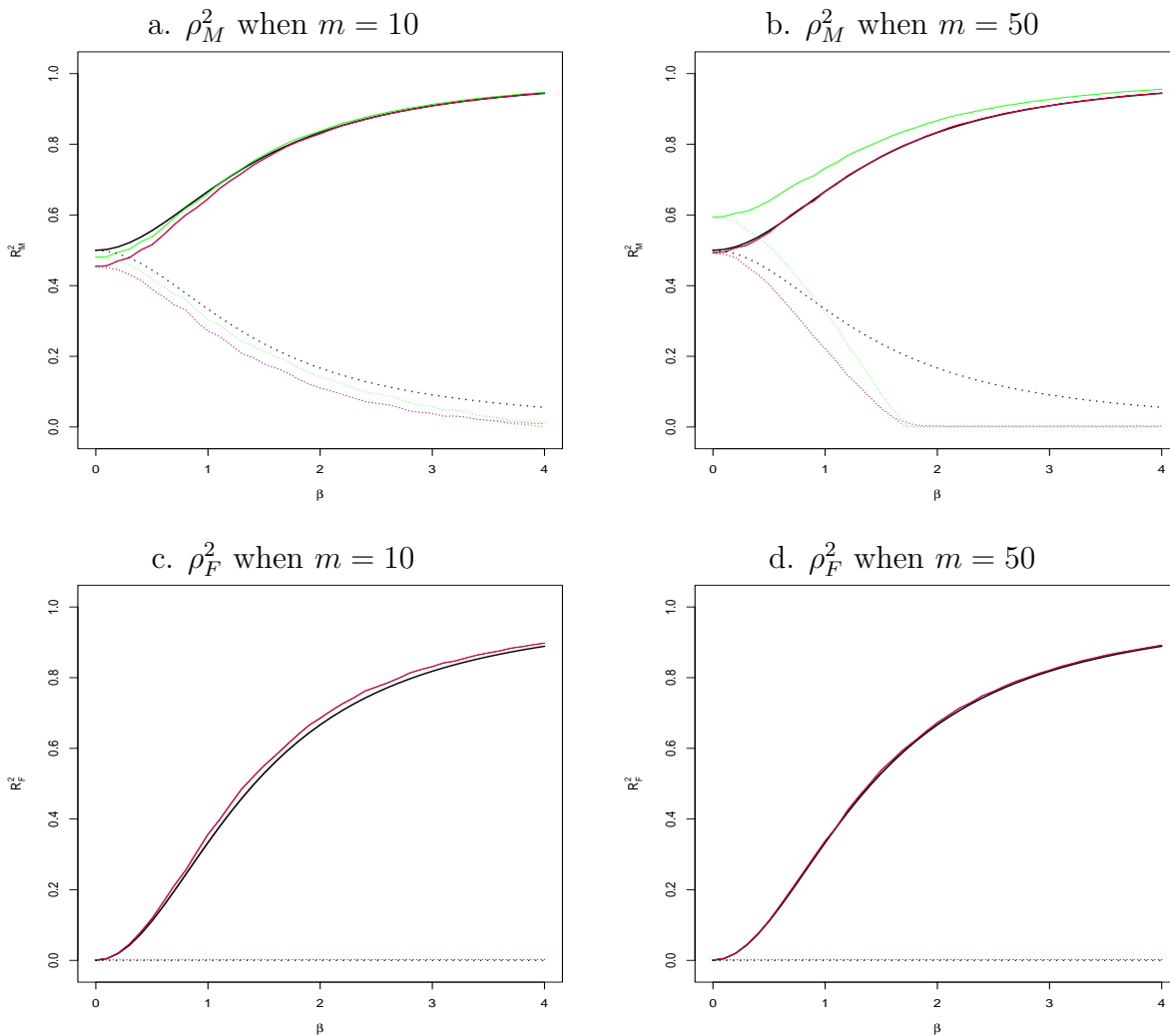


Figure 1: Medians of estimated ρ_M^2 and ρ_F^2 in linear mixed models (with ρ_M^2 and ρ_F^2 shown in black). Shown in the plot are R_M^2 and R_F^2 (blue), the method by Nakagawa et al. (2017) (red), and the method by Xu (2003) (green). The solid lines are for the models including X_1 , and the dashed lines are for the models including X_2 instead.

We also fitted all models using the restricted maximum likelihood method and resultant coefficients of determinations are in general very close to the corresponding values calculated from the maximum likelihood estimators (the results are not shown). In particular, the method by Xu (2003) is rarely affected by the choice of the restricted maximum likelihood or maximum likelihood method estimator because the difference between restricted maximum likelihood and maximum likelihood estimators lies only in the estimated variances of the random effects, i.e., τ_{ij}^2 .

4.2 Logistic Mixed Models

For logistic models, we compared the performance of our proposed R^2 to those proposed by Nakagawa et al. (2017), with a total of 1,000 data sets simulated from each model under investigation. Each data set has a total of 400 random samples, evenly clustered inside m groups with $m = 10$ and 50 , respectively. The binary X_1 and continuous X_2 were generated similarly to those in the previous section. The j -th response value inside the i -th cluster, i.e., y_{ij} , was generated from a Bernoulli distribution with

$$E[y_{ij} | \mu_i, x_{1ij}] = \{1 + \exp(-\mu_i - x_{1ij}\beta)\}^{-1},$$

where x_{1ij} is the corresponding value of the binary covariate X_1 , and the random effect $\mu_i \stackrel{iid}{\sim} N(0, 1)$.

For each data set, we fit different models with the maximum likelihood method, and then estimate both ρ_M^2 and ρ_F^2 with our approach and the method by Nakagawa et al. (2017) as shown in Figure 2. With true values unknown, we fit a generalized linear model for each mixed-effects model by including fixed, instead of random, group effects, and calculated R_{KL}^2 by Cameron and Windmeijer (1997) and R_V^2 by Zhang (2017). Note that R_V^2 may conceptually favor our proposed R^2 . However, R_{KL}^2 can serve well as a benchmark although R_{KL}^2 takes into account of whole distributional diffusion including quadratic variation. Figure 2 indeed shows that both R_V^2 and R_{KL}^2 have similar increasing patterns with the discrepancies due to their conceptual difference.

When the true predictor X_1 is included in the model, the estimated ρ_M^2 and ρ_F^2 by Nakagawa et al. (2017) are in general flatter than other estimates. All estimates of ρ_M^2 and

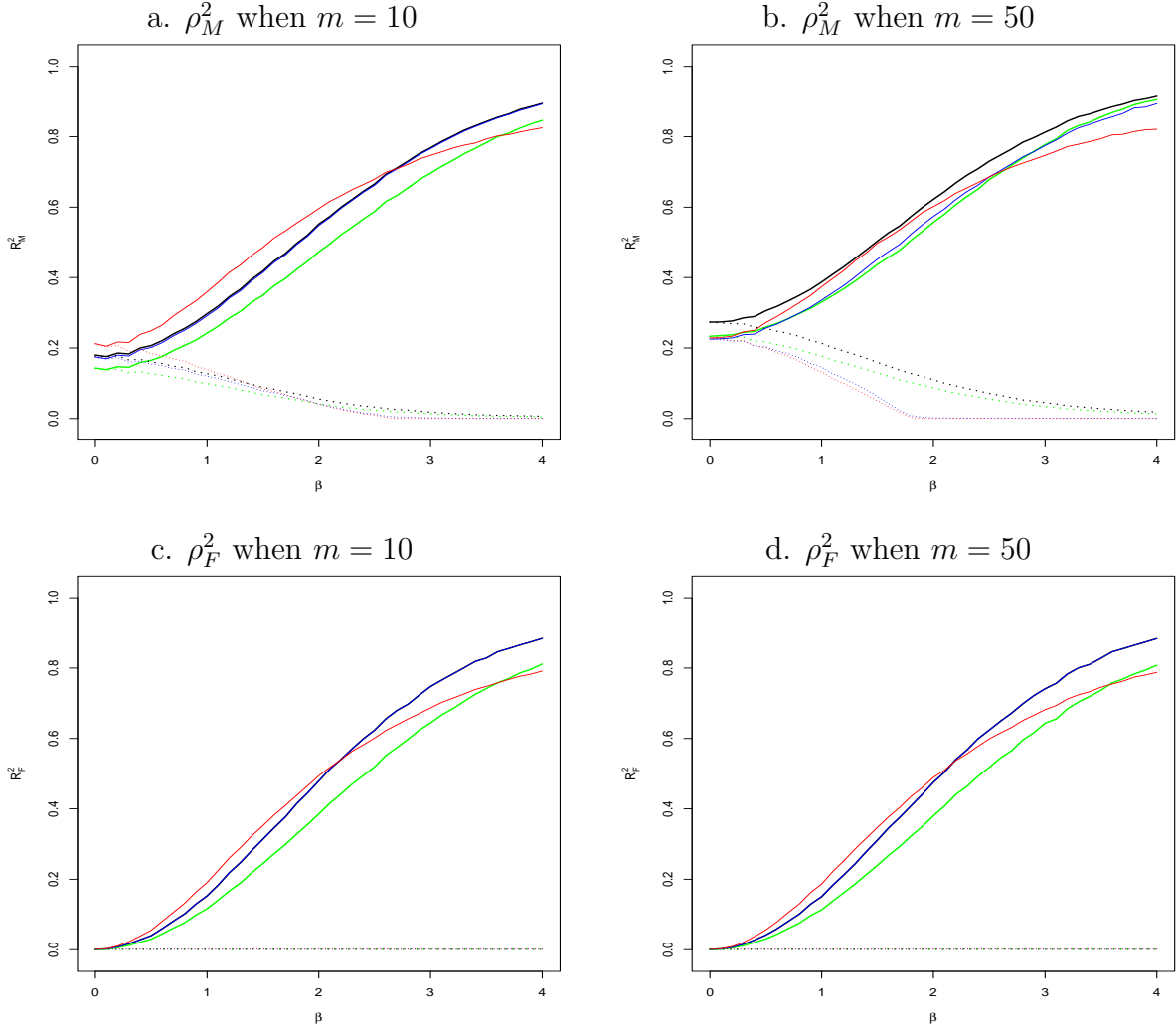


Figure 2: Medians of estimated ρ_M^2 and ρ_F^2 in logistic mixed models. Shown in the plot are R_M^2 and R_F^2 (blue), and the method by Nakagawa et al. (2017) (red). For reference, we also plot R_{KL}^2 (green) and R_V^2 (black) for corresponding generalized linear models. The solid lines are for the models including X_1 , and the dotted lines are for the models including X_2 instead.

ρ_F^2 are slightly affected by the number of groups. It is not surprising that, in Figures 2.a and 2.b, both R_{KL}^2 and R_V^2 are significantly affected by the number of groups as including more fixed group effects in the model may inflate the corresponding R^2 . Both R_{KL}^2 and R_V^2 perform consistently between Figures 2.c and 2.d as the group effects are excluded from the models. Note that R_F^2 and R_V^2 are overlapped in Figures 2.c and 2.d due to their identity by definition. When regressing Y vs. X_2 by excluding the true predictor X_1 , our proposed measures and the measures by Nakagawa et al. (2017) perform consistently with $m = 10$ and $m = 50$. In general, R_M^2 and R_F^2 capture well the increasing proportion of explained variation in a binary response variable, and perform better than the method by Nakagawa et al. (2017).

4.3 Loglinear Mixed Models

For loglinear models, we compared the performance of our proposed R^2 to those proposed by Nakagawa et al. (2017), with a total of 1,000 data sets simulated from each model under investigation. Each data set has a total of 400 random samples, evenly clustered inside $m = 50$ groups. The binary X_1 and continuous X_2 were generated similarly to those in the previous sections. The j -th response value inside the i -th cluster, i.e., y_{ij} , was generated from a Poisson distribution with

$$E[y_{ij} \mid \mu_i, x_{1ij}] = \exp(\mu_i + x_{1ij}\beta),$$

where x_{1ij} is the corresponding value of the binary covariate X_1 , and the random effect $\mu_i \stackrel{iid}{\sim} N(0, .25)$. We also simulated overdispersed counts from a negative binomial distribution with the success probability

$$p_{ij} = 1 / \{1 + \exp(-\mu_i - x_{1ij}\beta)\}.$$

For each data set, we fit the different models with the maximum likelihood method, and then estimate both ρ_M^2 and ρ_F^2 with our approach and the method by Nakagawa et al. (2017) as shown in Figure 3. For each model, we also fit a generalized linear model by including fixed, instead of random, group effects, and calculated R_{KL}^2 by Cameron and Windmeijer (1997) and R_V^2 by Zhang (2017) as benchmarks.

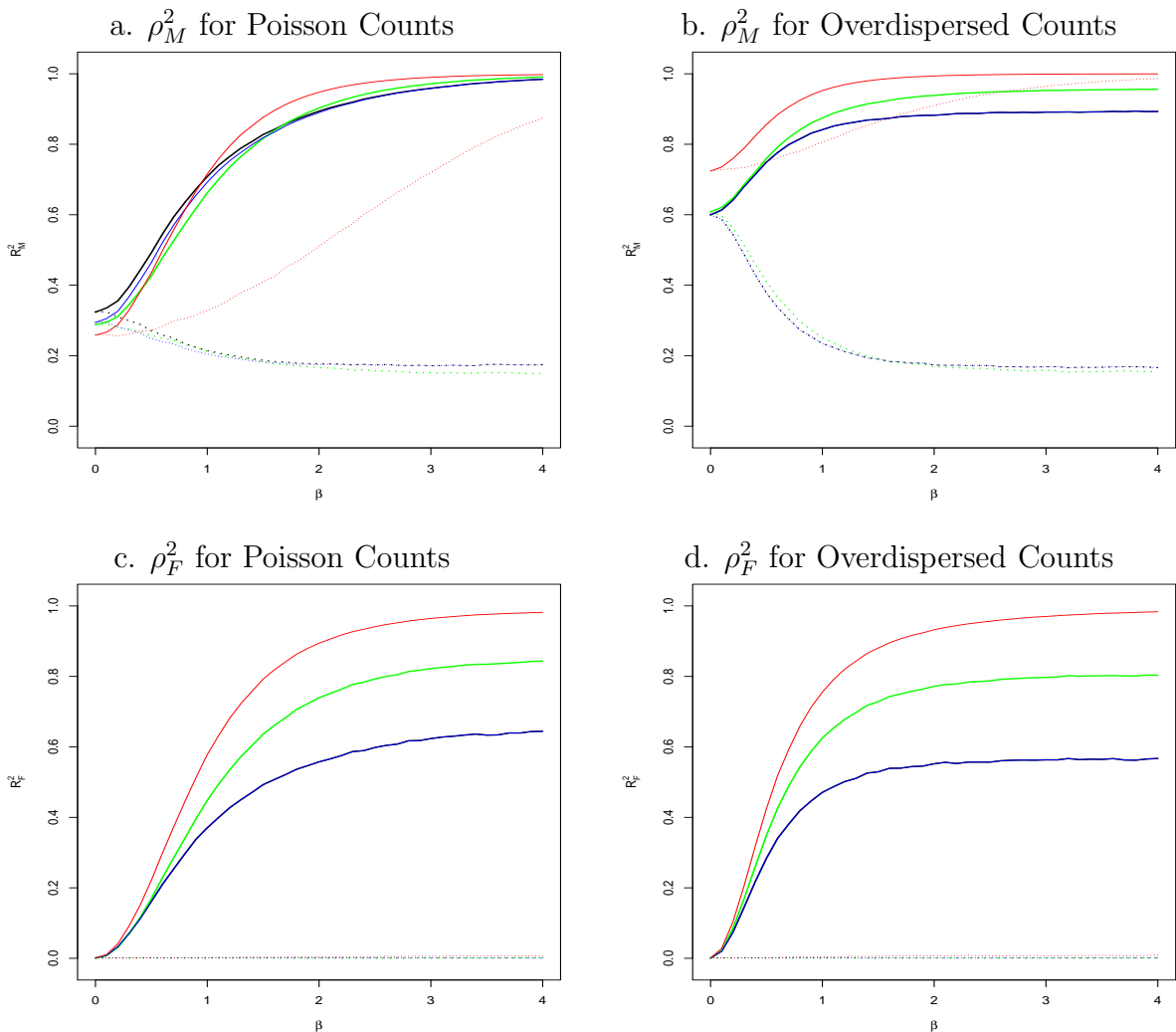


Figure 3: Medians of estimated ρ_M^2 and ρ_F^2 in loglinear mixed models. Shown in the plot are R_M^2 and R_F^2 (blue), and the method by Nakagawa et al. (2017) (red). For reference, we also plot R_{KL}^2 (green) and R_V^2 (black) for corresponding generalized linear models. The solid lines are for the models including X_1 , and the dotted lines are for the models including X_2 instead.

When the true predictor X_1 is included in the model, as shown in Figures 3.a and 3.b, R_M^2 overlays its reference R_V^2 for the Poisson counts data but is slightly smaller than R_V^2 for the overdispersed counts data. As conceptually identical, it is not surprising to observe overlaid R_V^2 and R_V^2 in Figures 3.c and 3.d. While R_{KL}^2 measures overall distributional diffusion including quadratic variation, it reports slightly larger values than R_M^2 in Figures 3.a and 3.b but much larger values than R_F^2 in Figures 3.c and 3.d, in particular when β is large. On the other hand, the method by Nakagawa et al. (2017) reports slightly larger estimate of ρ_M^2 than R_{KL}^2 in Figures 3.a and 3.b, but much larger estimate of ρ_F^2 than R_{KL}^2 in Figures 3.c and 3.d.

When X_2 , instead of the true predictor X_1 , is included in the model, ρ_M^2 only measures the proportion of variation due to the random effects so it should decrease when β increases. While R_M^2 as well as R_V^2 and R_{KL}^2 decreases, the estimate by Nakagawa et al. (2017) increases and approach to one as β increases, as shown in Figures 3.a and 3.b. Therefore, the method by Nakagawa et al. (2017) falsely evaluates the proportion of variation explained by X_2 . On the other hand, all methods perform well in estimating ρ_F^2 in this scenario as shown in Figures 3.c and 3.d. In general, the method proposed by Nakagawa et al. (2017) tends to overstate the proportion of explained variation in a count response while R_M^2 and R_F^2 capture well the increasing pattern as benchmarked by R_{KL}^2 .

5 Real Data Analysis

5.1 Corn Yield with Variable Nitrogen

A total of 1,705 observations were collected in 2001 from four different topographic regions on corn yield with five different nitrogen treatments in Argentina (Edmondson, 2014; Lambert et al., 2004). Recorded with each observation is a brightness value, proxy for low organic matter content, which varies across different topographic regions. With possible fixed-effects predictors nitrogen treatments (N) and brightness value (B), we consider different linear mixed models, all having the topographic region as a factor with random effects. Since there is high association between brightness value and topographic region, we also regressed brightness value against topographic region and include its residual (B_r),

instead of itself, in the models, see Table 2. As references, classical and adjusted coefficients of determination (R^2) are also calculated for the corresponding models but including the topographic region with fixed effects.

Table 2: Coefficients of Determination in Analysis of the Corn Yield Data*

Fixed Effects	ρ_M^2			ρ_F^2		AIC	BIC	R^2
	R_M^2	NJS ^a	Xu ^b	R_F^2	NJS ^a			
N, B, B ²	.779(. .778)	.754	.768	.303	.089	13444	13499	.769 (.767)
N, B	.778 (.778)	.758	.768	.284	.082	13446	13494	.768 (.767)
N	.730 (.729)	.774	.719	.005	.005	13770	13814	.719 (.717)
B, B ²	.774 (.774)	.748	.763	.297	.083	13460	13498	.763 (.762)
B	.774 (.773)	.753	.762	.279	.076	13485	13507	.762 (.762)
N, B _r , B _r ²	.778 (.777)	.813	.770	.069	.047	13433	13488	.770 (.769)
N, B _r	.776 (.775)	.813	.768	.054	.044	13447	13496	.768 (.767)
B _r , B _r ²	.773 (.773)	.809	.764	.063	.042	13473	13501	.764 (.764)
B _r	.771 (.771)	.809	.762	.048	.040	13486	13508	.762 (.762)

*With adjusted values in parentheses; ^a The method by Nakagawa et al. (2017);

^b The method by Xu (2003).

When including original brightness value in the model, the method by Nakagawa et al. (2017) estimated ρ_M^2 with slightly lower values than R_M^2 except that, for the model with only N having fixed effects, the method by Nakagawa et al. (2017) reported its largest value at .774. Note that the method by Nakagawa et al. (2017) reported larger value for the model with B only then the model with B and B², and also decreasing values for the three increasing models: (i) the model with N only; (ii) the model with N and B; and (iii) the model with N, B, and B². Therefore, the method by Nakagawa et al. (2017) may not necessarily report larger values for larger models, unlike other unadjusted coefficients of determinations which usually report larger values for larger models. The method by Nakagawa et al. (2017) also estimated ρ_F^2 with much smaller values than R_F^2 except for the model with N only.

When the brightness values were replaced by their residuals, the method by Nakagawa et al. (2017) estimated ρ_M^2 with larger values than R_M^2 , and reported slightly smaller estimates of ρ_F^2 than R_F^2 . While the method by Nakagawa et al. (2017) reported the largest estimate of ρ_M^2 at .813 for two sets of models including N and B_r . Note that the model with N, B_r , and B_r^2 is selected by AIC, BIC, adjusted R^2 , the methods by Xu (2003) and Nakagawa et al. (2017), while adjusted R_M^2 reported this model with the highest value among all models replacing the brightness value with its residual. However, when selecting models by considering the original brightness values, the method by Nakagawa et al. (2017) selected the model with N only, while BIC selected the model with N and B, and all other methods selected the model with N, B, and B^2 .

5.2 Distribution of *Elaphostrongylus cervi* in Red Deers

Vicente et al. (2006) studied the distribution of the first-stage larvae of *Elaphostrongylus cervi* in the red deer across Spain. A total of 826 deers across 24 farms were surveyed for the incidence (Zuur et al., 2009). We considered different logistic mixed models to investigate how the length of a deer affected its chance to get the first-stage larvae of *Elaphostrongylus cervi*, and therefore include both the standardized length (L) and its quadratic term (L^2 , as well as deer sex (S), as possible predictors. All mixed-effect models included farm as a factor with random effects, see Table 3. As references, R_V^2 proposed by Zhang (2017) and R_{KL}^2 proposed by Cameron and Windmeijer (1997) were calculated for corresponding models but including farm as a factor with fixed effects instead.

In general, the method by Nakagawa et al. (2017) provided slightly larger estimates of ρ_F^2 than R_F^2 (except two models with similar values), but much larger estimates of ρ_M^2 than R_M^2 in all models. On the other hand, R_M^2 reported very similar values to R_V^2 while R_{KL}^2 reported slightly smaller values than both of them. However, adjusted versions of R_M^2 , R_V^2 , and R_{KL}^2 all selected the largest model as the best, while both AIC and BIC selected the model with L and L^2 , and the method by Nakagawa et al. (2017) selected the model with S, L, and L^2 instead.

Table 3: Coefficients of Determination in Analysis of the Red Deers Data*

Fixed Effects	ρ_M^2		ρ_F^2		AIC	BIC	R_V^2	R_{KL}^2
	R_M^2	NJS ^a	R_F^2	NJS ^a				
S*L, S*L ²	.352 (.347)	.507	.103	.156	832	865	.357 (.334)	.308 (.284)
S*L	.348 (.345)	.504	.087	.143	833	856	.354 (.333)	.305 (.283)
S, L, L ²	.349 (.346)	.509	.102	.099	831	854	.354 (.333)	.306 (.283)
S, L	.340 (.337)	.501	.083	.131	841	860	.345 (.324)	.296 (.274)
L, L ²	.347 (.345)	.507	.102	.159	830	849	.353 (.332)	.304 (.282)
L	.334 (.333)	.495	.083	.128	844	858	.340 (.320)	.291 (.270)
S	.239 (.237)	.344	.012	.005	931	945	.247 (.225)	.207 (.184)

*With adjusted values in parentheses; ^a The method by Nakagawa et al. (2017).

While all of R_M^2 , R_V^2 , and R_{KL}^2 reported larger values for larger models, the method by Nakagawa et al. (2017) also reported larger values for larger models except the model with S, L, and L² for which it reported the largest value at .509, higher than the value for the largest model. However, both R_F^2 and the method by Nakagawa et al. (2017) estimated ρ_F^2 with larger values for larger models.

5.3 The Begging Behavior of Nestling Barn Owls

Roulin and Bersier (2007) studied vocal begging behaviour of nestling barn owls when the parents brought prey across 27 nests, with 2 to 7 nestlings per nest. A total of 599 observations collected with the response variable sibling negotiation, which is defined as the number of calls just before arrival of a parent at a nest, as well as the number of siblings per nest, the parent's sex (S), arrival time at the nest (T), and whether the nestlings were food satiated or deprived (F) (Zuur et al., 2009). We considered loglinear mixed models with the number of calls offset by the number of siblings per nest. All models included nest as a factor with random effects, see Table 4. As references, R_V^2 proposed by Zhang (2017) and R_{KL}^2 proposed by Cameron and Windmeijer (1997) were calculated for corresponding models but including nest as a factor with fixed effects instead.

Table 4: Coefficients of Determination in Analysis of the Owl Data*

Fixed Effects	ρ_M^2		ρ_F^2		AIC	BIC	R_V^2	R_{KL}^2
	R_M^2	NJS ^a	R_F^2	NJS ^a				
S*F,S*T	.277 (.269)	.684	.174	.278	5009	5040	.276 (.237)	.226 (.184)
S*F, T	.275 (.269)	.684	.174	.279	5008	5034	.275 (.237)	.226 (.185)
S, F, T	.275 (.270)	.682	.174	.277	5010	5032	.275 (.238)	.225 (.186)
F, T	.275 (.271)	.682	.172	.276	5009	5027	.274 (.239)	.225 (.187)
T	.217 (.214)	.610	.096	.139	5288	5301	.218 (.181)	.157 (.117)
F	.201 (.199)	.639	.106	.184	5212	5226	.201 (.163)	.175 (.136)

*With adjusted values in parentheses; ^a The method by Nakagawa et al. (2017).

As shown in Table 4, the method by Nakagawa et al. (2017) provided much larger estimates of ρ_M^2 than R_M^2 as well as much larger estimates of ρ_F^2 than R_F^2 in all models. On the other hand, R_M^2 reported very similar values to R_V^2 as R_{KL}^2 reported slightly smaller values than both of them. However, adjusted versions of R_M^2 , R_V^2 , and R_{KL}^2 as well as BIC all selected the model with F and T as the best, while AIC selected the model with S*F and T. The method by Nakagawa et al. (2017) instead have two models including S*F and T with the highest estimate of ρ_M^2 at .684. In general, all coefficients of determination reported larger values for larger models.

6 Discussion

Unlike p -values that rely on sample sizes to signal the variable significance, the coefficient of determination, a.k.a. R^2 , measures the proportion of the variation in the response variable explained by a set of predictors. It plays an important role in agricultural, biological, and ecological research, for example, quantifying the heritability of a trait in molecular biology (Visscher et al., 2008). The popularly used mixed-effects models in such studies demand appropriate extension of R^2 . Our coefficients of determination are well-defined as long as the link and variance functions are specified, such as quasi-models that may rely on quasi-likelihood functions, other than likelihood functions, to obtain parameter estimates. When

the first-order derivative of the variance function is constant as for normal and Poisson distributions, our defined R^2 for generalized linear mixed models will be reduced to those defined for linear mixed models following the law of total variance. Together with Zhang (2017), our definitions unify linear models, generalized linear models, linear mixed models, and generalized linear mixed models.

Practice in science may demand further extension or improvement on the proposed measures. Firstly, it may be of interest to measure the utility of a set of predictors beyond others in modeling a response variable. We may define the coefficient of partial determination as shown in Zhang (2017) to measure the proportion of variation in the response variable unexplained by a set of predictors that can be explained by the additional set of predictors. Secondly, calculating aforementioned heritability may demand evaluation of the contribution due to certain random effects while controlling the fixed effects of other factors. In this case, we may directly define ρ_R^2 based on the law of total variance, though it may be a challenging task, in particular for generalized linear mixed models. Thirdly, our coefficients of determinations are defined for mixed-effects models assuming that observations are randomly sampled within groups and the groups are randomly sampled within the underlying population. However, a same number of observations may be collected within each group although the subpopulation may be of different size, and sometimes it is the other way around. Therefore the coefficients may be modified using different weights on individual variations from different groups.

All of our defined measures for linear mixed model and generalized linear mixed model are implemented in the R package `rsq`, which is publicly available via the Comprehensive R Archive Network (CRAN).

References

- CAMERON, A. C. AND WINDMEIJER, A. G. (1997). An R-squared measure of goodness of fit for some common nonlinear regression models. *Journal of Econometrics*, **77**, 329-342.
- COX, D. R. AND SNELL, E. J. (1989). *The Analysis of Binary Data*, 2nd ed. London: Chapman and Hall.

- DEMPSTER, E. R. AND LERNER, I. M. (1950). Heritability of threshold characters. *Genetics*, **35**, 212-236.
- EDMONDSON, R. N. (2014). Agridat. *Journal of Agricultural Science*, **152**, 2.
- GBUR, E. E., STROUP, W. W., MCCARTER, K. S., DURHAM, S., YONG, L. J., CHRISTMAN, M., WEST, M., AND KRAMER, M. (2012). *Analysis of Generalized Linear Mixed Models in the Agricultural and Natural Resources Sciences*. American Society of Agronomy.
- IVES, A. R. (2019). R^2 s for correlated data: phylogenetic models, LMMs, and GLMMs. *Systematic Biology*, **68**, 234-251.
- JAEGER, B. C., EDWARDS, L. J., DAS, K., AND SEN, P. K. (2017). An R^2 statistic for fixed effects in the generalized linear mixed model. *Journal of Applied Statistics*, **44**, 1086-1105.
- JAEGER, B. C., EDWARDS, L. J., AND GURKA, M. J. (2019). An R^2 statistic for covariance model selection in the linear mixed model. *Journal of Applied Statistics*, **46**, 164-184.
- LAIRD, N. M. AND WARE, J. H. (1982) Random-Effects Models for Longitudinal Data. *Biometrics*, **38**, 963-974
- LAMBERT, D. M., LOWENBERG-DEBOER, J., AND BONGIOVANNI, R. (2004) A Comparison of Four Spatial Regression Models for Yield Monitor Data: A Case Study from Argentina. *Precision Agriculture*, **5**, 579-600.
- MADDALA, G. S. (1983). *Limited-Dependent and Qualitative Variables in Econometrics*. Cambridge University.
- MAGEE, L. (1990). R^2 measures based on Wald and likelihood ratio joint significance tests. *The American Statistician*, **44**, 250-253.
- MCCULLAGH, P. (1983). Quasi-likelihood functions. *The Annals of Statistics*, **11**, 59-67.

- MCCULLAGH, P. AND NELDER, J. A. (1989). *Generalized Linear Models*. Chapman and Hall/CRC.
- MCCULLOCH, C. E., SEARLE, S. R., AND NEUHAUS, J. M. (2008). *Generalized, Linear, and Mixed Models*, 2nd Edition. New York: Wiley.
- NAGELKERKE, N. J. D. (1991). A note on a general definition of the coefficient of determination. *Biometrika*, **78**, 691-692.
- NAKAGAWA, S., JOHNSON, P. C. D., AND SCHIELZETH, H. (2017). The coefficient of determination R^2 and intra-class correlation coefficient from generalized linear mixed-effects models revisited and expanded. *Journal of the Royal Society Interface*, **14**, 20170213.
- NAKAGAWA, S. AND SCHIELZETH, H. (2013). A general and simple method for obtaining R^2 from generalized linear mixed models. *Methods in Ecology and Evolution*, **4**, 133-142.
- ROULIN A. AND BERSIER L. F. (1998). Nestling barn owls beg more intensely in the presence of their mother than their father. *Animal Behaviour*, **74**, 1099-1106.
- VICENTE, J., DE MERA, I. G. F., AND GORTAZAR, J. (2006). *Epidemiology and risk factors analysis of elaphostrongylosis in red deer (Cervus elaphus from Spain)*. *Parasitology Research*, **98**, 77-85.
- VISSCHER, P. M., HILL, W. G., AND WRAY, N. R. (2008). Heritability in the genomics era-concepts and misconceptions. *Nature Reviews Genetics*, **9**, 255-266.
- XU, X. (2003). Measuring explained variation in linear mixed effects models. *Statistics in Medicine*, **22**, 3527-3541.
- ZHANG, D. (2017). A coefficient of determination for generalized linear models. *The American Statistician*, **71**, 310-316.
- ZUUR, A. F., IENO, E. N., WALKER, N., SAVELIEV, A. A., AND SMITH, G. M. (2009). *Mixed Effects Models and Extensions in Ecology with R*. Springer.