DECOMPOSITION OF EXPLAINED VARIATION IN THE LINEAR MIXED MODEL

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This is a preprint and has not been peer reviewed yet.

ABSTRACT

In the linear mixed model (LMM), the simultaneous assessment and comparison of dispersion relevance of explanatory variables associated with fixed and random effects remains an important open practical problem. Based on the restricted maximum likelihood equations in the variance components form of the LMM, we prove a proper decomposition of the sum of squares of the dependent variable into unbiased estimators of interpretable estimands of explained variation. This result leads to a natural extension of the well-known adjusted coefficient of determination to the LMM. Further, we allocate the novel unbiased estimators of explained variation to specific contributions of covariates associated with fixed and random effects within a single model fit. These parameter-wise explained variations constitute easily interpretable quantities, assessing dispersion relevance of covariates associated with both fixed and random effects on a common scale, thus allowing for a covariate ranking.

For illustration, we contrast the variation explained by subjects and time in the longitudinal sleep deprivation study. By comparing the dispersion relevance of population characteristics and spatial levels, we determine literacy as a major driver of income inequality in Burkina Faso. Finally, we develop a novel relevance plot to visualize the dispersion relevance of high-dimensional genomic markers in Arabidopsis thaliana.

1 Introduction

Decomposition of observed sum of squares into contributions of explanatory factors and unexplained variation constitutes the basis of the analysis of variance (ANOVA). This concept is generalized in the linear model (LM), where the total sum of squares is decomposed into explained and residual sum of squares, leading to the well-known coefficient of determination, $R^2$. It measures the proportion of variance in the response explained by the covariates and is widely applied to assess absolute goodness of model fit. The relevance or usefulness of individual covariates in the LM could be assessed, for example, by the associated estimated effect sizes or $p$-values, which, however, depend heavily on scaling and sample size, respectively\cite{1}. Consequently, measures of dispersion relevance have come to the fore, such as the proportion of explained to observed variation. Partitioning the explained variance into contributions of specific covariates is straightforward and unambiguous in the uncorrelated case. In observational studies, however, covariates...
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are typically correlated, leading to a general debate about how to assess the usefulness or relevance of individual covariates in the LM\(^1\). On the one hand, the drop in model \(R^2\) when a predictor is removed has been utilized\(^2\). This approach, which is equivalent to the so-called semi-partial \(R^2\)\(^3\), assesses how well the remaining covariates compensate the omitted variable in terms of model \(R^2\) but does not lead to a proper partitioning of the model \(R^2\) (i.e. semi-partial \(R^2\)’s do not add up to the model \(R^2\)). Hence, they are only useful in relation to each other but do not lead to a meaningful interpretation in terms of individual explained variation with respect to the model. On the other hand, fractions of \(R^2\) from a single model fit can be properly allocated to the covariates in the model, for example resulting in Engelhart’s measure\(^4\) or the measure introduced by Hoffmann\(^5\) and formalized by Pratt\(^6\).

The variance components form of the linear mixed model (LMM) extends the LM to handle correlated observations\(^5\). Routine applications include modeling of hierarchical or multi-level data, e.g. in the presence of clustered, repeated or longitudinal measurements. Genome-wide association studies (GWAS) in which all genomic markers are fitted simultaneously as random slopes for regularization are another important application of the LMM in the variance components form\(^7\). In this context, the combined explained variation of the covariates, representing genomic markers, associated with random effects is termed genomic variance of a trait e.g.\(^8\).

Although arguably of equal importance as in the LM, it has not yet been agreed on a unified measure of explained variation in the LMM, amongst others, because the LMM specifies not only the mean but also the covariance structure via random effects\(^8\) which introduces additional uncertainty and heterogeneity. A general definition of a \(R^2\) for both model aspects has been called mathematically unresolvable, hence explained variations have often been treated distinctively for both model part\(^9\) and are inherently difficult to compare.

Whereas Xu\(^10\) defines three measures for the overall proportion of explained variance via residuals (coefficients of alienation), Edwards et al.\(^11\) define an \(R^2\) statistic for the fixed effects part of the marginal LMM based on an approximate \(F\) statistic while keeping the random effect structure constant. Complementary to that, Demidenko et al.\(^12\) investigate explained variation of random effects by treating them, conditionally, as fixed effects and then applying \(F\)-test statistics. Nakagawa and Schielzeth\(^13\) propose the calculation of a marginal (variance explained by mean structure) and a conditional (variance explained by mean and covariance structure) \(R^2\) which has been extended to random slope and generalized LMMs by Johnson\(^14\) and Nakagawa et al.\(^15\). Finally, generalized variance approaches projecting the (generalized) LMM covariance matrix to a single number, e.g. by determinant or semi-variance, have been used to calculate \(R^2\) for the mean structure only, e.g. by Jaeger et al.\(^16\) and Piepho\(^17\)\(^18\). For a detailed review of \(R^2\)’s for mixed models we refer to Cantoni et al.\(^19\).

The usual results of a LMM fit include effect size estimates and \(t\)-statistics for the fixed effects and estimates of the variance components corresponding to the random effects. These results do not enable a parameter-wise comparison of the relevance of covariates associated with fixed and random effects. The relevance of individual covariates associated with fixed effects has been judged using (semi-)partial \(F\)-statistics either in the marginal LMM\(^2\) or using standardized general variance adjustments\(^2\). For LMM’s with identical covariance structure, Stoffel et al.\(^20\) propose sequential comparisons of the variance of the fixed effects part of the linear predictor in the full model versus nested models in which covariates associated with fixed effects are iteratively dropped. These approaches effectively lead to semi-partial \(R^2\)’s for the fixed part of the LMM. They require multiple model fits, do not add up to the model \(R^2\) and do not constitute interpretable quantities in terms of model \(R^2\) but only in relation to each other. Similar semi-partial approaches for the covariates associated with random effects are not advisable, because dropping these coefficients implies an alteration of the covariance structure of the models to be compared. On the other hand, the intra-class correlation coefficient (ICC) e.g.\(^2\) and variance partition coefficients e.g.\(^2\) have been used to determine the level-specific variations explained in random intercept and multi-level models, respectively. In this context, computation of the explained variation accounted for by covariates associated with fixed effects is not intended. Further, an addition of covariates changes the magnitude of variance component estimates and possibly leads to negative level-specific explained variances. Moreover, whereas the relevance of clusters in a random intercept model without fixed effects might be approximated by the ratio of
variance components (ICC), this assessment fails when fixed effects and higher order random effects such as random slopes are introduced.

Hence, to the best of our knowledge, there is no method available which properly partitions the model explained variation for covariates associated with fixed and random effects at the same time. We believe that such an approach is the only viable option for parameter-wise and interpretable assessments of the simultaneous relevance of covariates associated with fixed and random effects in the LMM.

Our contribution is two-fold. Firstly, we prove a novel and proper decomposition of the observed variance in the LMM into unbiased estimators of meaningful and interpretable estimands of explained variation. We utilize our decomposition to derive an extension of the adjusted coefficient of determination to the LMM, and to attribute the total explained variation to the contributions of covariates associated with fixed and random effects. We emphasize that the concept of explained variation in the LMM is a combination of the variance of the data-generating process of covariates and the variance of the associated effects (zero for fixed but non-zero for random effects). Our decomposition is proper because it includes the estimates of realizations of the random effects (empirical best linear unbiased prediction), the use of which has been advocated before such that the analysis is not solely based on population averages.

Secondly, we partition the estimators of explained variation further and attribute components to individual parameters. This enables an unbiased, model-consistent and unified parameter-wise attribution of explained variation to single covariates associated with fixed and random effects on the same scale within a single model fit. These contributions are conditional on the other variables in the model, i.e., we do not aim at selecting or removing model coefficients but to describe their dispersion relevance within the model at hand.

Our approach is made readily available in a user-friendly R-package and its usefulness is illustrated in several real data sets to emphasize the broad applicability. For instance, in the sleep deprivation study analysed by Bates et al, we show that about 60% of the variation in the reaction time of subjects is explained by the time of sleep deprivation, with approximately equal contributions of time associated with fixed and random slopes, while 20% are explained by the subjects themselves. Gräb and Grimm investigate inequality in Burkina Faso by using the ICC to decompose the variability of household expenditure in a multilevel spatial model. We illustrate that the dispersion relevance of spatial levels, such as communities, provinces and regions can be simultaneously assessed together with the dispersion relevance of household and community characteristics. Amongst others, we conclude that covariates related to literacy explain about 23% of the variance of household expenditure (proxying income inequality), while the spatial levels explain about 10% in total. Finally, in the context of GWAS data on Arabidopsis thaliana, we introduce a novel relevance plot for the genomic markers on the whole genome complementing the well-known Manhattan plot which neglects confounding and assesses significance but not relevance.

### 2 Preliminaries

#### 2.1 Linear Mixed Model and Notation

We consider the linear mixed model

\[ y = \mu 1_n + X\beta + \sum_{i=1}^{m} Z_i u_i + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2_\varepsilon I_n), \quad u_i \sim \mathcal{N}(0, \sigma^2_{u_i} I_p), \]  

in the traditional variance components form where \( y \) is the vector of quantitative observations, \( \mu \in \mathbb{R} \) is an intercept, \( 1_n \) is the column vector of ones of length \( n \), \( I_n \) denotes the \( n \)-dimensional identity matrix, and \( \sigma^2_\varepsilon > 0 \) and \( \sigma^2_{u_i} \geq 0, i = 1, \ldots, m \). The design matrix for the \( k \) fixed effects \( \beta \) is given by \( X \in \mathbb{R}^{n \times k} \). The matrices \( Z_i \in \mathbb{R}^{n \times p_i} \) code covariates corresponding to the random effect vectors \( u_i \). The random effects (including the residuals) are pairwise uncorrelated. By specifying \( Z_i \), model typically allows to model hierarchical data (clustered data, repeated measurements, longitudinal data) as well as high-dimensional GWAS data. Let the random vector
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\[ u = (u_1^T, \ldots, u_m^T)^T \sim \mathcal{N}(0, D) \] be of dimension \( p \), \( D = \text{diag}(\sigma_{u_1}^2, I_{p_1}, \ldots, \sigma_{u_m}^2, I_{p_m}) \), and \( Z = (Z_1, \ldots, Z_m) \) denote an \( n \times p \) design matrix. Model (i) has variance-covariance structure \( V = \text{cov}(y) = ZDZ^\top + \sigma_u^2 I_n = \sum_{i=1}^m \sigma_u^2 Z_i Z_i^\top + \sigma_u^2 I_n \), such that \( y \sim \mathcal{N}(1_n \mu + X \beta, V) \). Similar to Searle et al.\textsuperscript{[6]}, \( \sigma_u^2 \) is used. \( G = D/\sigma_u^2 \). Let \( H = V/\sigma_u^2 = I_n + ZGZ^\top \) and \( H_C = I_n + CZGZ^\top \), which originates from centring the columns of \( Z \) by the centering matrix \( C = I_n - \frac{1}{n} 1_n 1_n^\top \). We assume that \( \dot{X} = (1_n, X) \) has full column rank and that the inverses of \( H, X^\top H^{-1} X, H_C \) and \( X^\top C^{-1} C X \) exist. The following lemma introduces alternative expressions for the well-known best linear unbiased estimator (BLUE) \( \hat{\beta} \) and predictor (BLUP) \( \hat{u} \). The invariance property is important for explained variations and in particular striking because centring \( Z \) automatically changes the covariance structure \( V \) of the outcome. The proof can be found in the Supplemental Material.

**Lemma 2.1** The best linear unbiased estimator \( \hat{\beta} \) in model (i) can be represented by
\[
(X^\top C^{-1} C X)^{-1} X^\top C^{-1} C Y \text{ with covariance matrix } \Sigma_{\hat{\beta}} = \sigma_u^2 (X^\top C^{-1} C X)^{-1}.
\]
The best linear unbiased predictor \( \hat{u} \) of the random effects can be expressed as
\[
G Z^\top C^{-1} C (y - X \hat{\beta}) \text{ with covariance matrix } \Sigma_{\hat{u}} = \sigma_u^2 G Z^\top C^{-1} \left\{ H_C - C X (X^\top C^{-1} C X)^{-1} X^\top C \right\} H_C^{-1} C Z G.
\]

Typically, estimation of variance components is based on restricted maximum likelihood (REML). When we replace the variance components by their estimates we mark the resulting quantities by a dot. In case that the variable already has a superscript, we drop the first superscript for notational convenience.

### 2.2 Explained Variation and \( R^2 \) in the Linear Model

A special case of model (i) is the homoscedastic LM
\[
y = \mu 1_n + X \beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2 1_n).
\] (2)

The coefficient of determination \( R^2 = 1 - \frac{\text{TSS}}{\text{RSS}} = 1 - \frac{\sum_y (y - \hat{y})^2}{\sum_y (y - \bar{y})^2} \) is the most popular measure of goodness-of-fit in model (ii), where \( \text{TSS} = y^\top Cy \) is the centred total sum of squares, \( \text{RSS} = \hat{\varepsilon}^\top \hat{\varepsilon} \) is the residual sum of squares, and \( \hat{\varepsilon} \) are the estimated residuals, respectively. The centred explained sum of squares is \( \text{ESS} = \hat{y}^\top Cy \) where \( \hat{y} \) are the fitted values. The intercept in model (ii) allows for the proper decomposition \( \text{TSS} = \text{ESS} + \text{RSS} \), which leads to \( R^2 = \frac{\text{ESS}}{\text{TSS}} \), i.e. the coefficient of determination measures the proportion of total variation that can be explained by the covariates after a least squares fit, see e.g. Kvalseth\textsuperscript{[3]}\textsuperscript{.} The \( R^2 \) tends to overestimate the proportion of the explained variation which is why the adjusted coefficient of determination 
\[
\hat{R}^2 = 1 - \frac{(1 - R^2)(n - 1)/(n - k - 1)}{1 - \sigma_\varepsilon^2/\sigma_y^2}
\]
has been introduced, adjusting for the degrees of freedom\textsuperscript{[25]}\textsuperscript{.} The expectation of the sample variability in the observations, \( \hat{\sigma}_y^2 = \frac{\text{TSS}}{n - 1} \), is given by
\[
\mathbb{E}[\hat{\sigma}_y^2] = \frac{1}{n - 1} \text{tr} \left( \Sigma_X \Sigma_X \beta \right), \quad \Sigma_X = \frac{1}{n - 1} X^\top C X.
\] (3)

It comprises residual variation and variation due to the covariates associated with the fixed effects, \( \beta^\top \hat{\Sigma}_X \beta \), which is induced by the empirical variation of the explanatory variables \( X \). An unbiased estimator for the estimand, the sample variance \( \hat{\beta}^\top \hat{\Sigma}_X \beta \) of \( X \beta \), is given by \( S_X^2 = \hat{\beta}^\top \hat{\Sigma}_X \hat{\beta} - \text{tr}(\hat{\Sigma}_X \hat{\Sigma}_\beta) \). The estimator \( \hat{S}_X^2 \) measures the adjusted empirical variation explained by the covariates and their empirical pairwise covariances. In combination with \( \hat{\sigma}_y^2 = \frac{\text{RSS}}{(n - k - 1)} \) and \( \text{TSS} = \text{ESS} + \text{RSS} \) we obtain the proper decomposition
\[
\hat{\sigma}_y^2 = \hat{S}_X^2 + \hat{\sigma}_\varepsilon^2
\]
of the centred TSS into the unbiased estimator of the variability of covariates associated with the fixed effects and an unbiased estimator for the residual variation. Thus, an alternative expression for \( \hat{R}^2 \) in model (ii) follows as
\[
\hat{R}^2 = \frac{\hat{S}_X^2}{\hat{S}_X^2 + \hat{\sigma}_\varepsilon^2}.
\]

Of note, \( \hat{S}_X^2 \) and with it \( \hat{R}^2 \) potentially produce negative estimates \((\hat{R}^2 \in [-k/(n - k - 1), 1])\). This can be the case, for instance, if \( R^2 = 0 \) and \( k > 0 \) and if \( \beta = 0 \) with \( \Sigma_{\beta} \neq 0 \), i.e. covariates have low/null explanatory potential but estimation uncertainty.
2.3 Components of Explained Variation in the Linear Model

A general partitioning of the variation of the (stochastic) LM is given by
\[ \text{var}(Y) = \sum_{j=1}^{k} \beta_j^2 \text{var}(X_j) + 2 \sum_{j=1}^{k} \sum_{i<j} \beta_i \beta_j \text{cov}(X_i, X_j) + \text{var}(\varepsilon), \]
see, e.g., Engelhart\cite{Engelhart2005}. The terms \( \beta_j^2 \text{var}(X_j), j = 1, \ldots, k, \) have been termed direct contributions of the respective variables, and the covariance terms have been called joint contributions of pairs of variables to the variance of the outcome. While the sum of all these contributions results in \( R^2, \) the highly debated issue is how to distribute the joint contributions to obtain total contributions of each parameter. Assigning parts of the joint distribution weighted by the proportion of the corresponding variables’ direct contributions possibly constitutes the first proposal to share the covariance terms\cite{Piepho2001}. One obvious, straightforward and data-independent approach is to assign each variable one part of its corresponding covariance terms implying equal shares as introduced by Hoffmann\cite{Hoffmann2001}. Pratt\cite{Pratt1991} justified the measure as the only one satisfying a set of desirable criteria. The so-obtained total contributions can become negative, which has been criticised\cite{Hoffmann2001}. However, variables might decrease the variance of the observations by a strong negative correlation with other variables, hence negative values are not necessarily unjustified\cite{Piepho2001}. More complicated assignments including sequential sum of squares in combination with iterative weighting (LMG) and data-dependent approaches such as the proportional marginal variance decomposition (PMVD) have been reviewed in Grömping\cite{Grömping2006}. Both LMG and PMVD derive from game theory and are often only heuristically discussed because the interpretation of the estimated quantities (estimand) is unclear\cite{Pratt1991}. Additionally, LMG depends on the ordering of the entering into the regression equation and is computationally challenging\cite{Grömping2006}. Contrary to that, the Hoffman-Pratt measure is argued to be the only theory-based measure with simple means of estimation and straightforward interpretation\cite{Piepho2001}.

3 Explained Variation in the Linear Mixed Model

3.1 Main Result - Decomposition

The lemma below introduces unbiased estimators and predictors for empirical explained variances which constitute the estimands of interest in this paper, see also Schreck\cite{Schreck2008} and an earlier preprint of this manuscript.

**Lemma 3.1** Based on model (1) and the quantities introduced in Lemma 2.7, the estimator \( \hat{S}_X^2 = \hat{\beta}^\top \Sigma_X \hat{\beta} - \text{tr} (\hat{\Sigma}_X \Sigma_\beta) \) is unbiased for the estimand for the explained variation of the coefficients associated with fixed effects, the sample variance \( \sigma_f^2 = \hat{\beta}^\top \Sigma_X \beta \text{ of } (X \beta), (i = 1, \ldots, n). \) The predictor \( \hat{S}_Z^2 = \hat{u}^\top \hat{\Sigma}_Z \hat{u} - \text{tr} (\hat{\Sigma}_Z \Sigma_u) + \text{tr} (D \Sigma_Z) \) is unbiased for the estimand for the explained variation of the coefficients associated with random effects, the sample variance \( \sigma_r^2 = u^\top \Sigma_u \text{ of } (Z \mu), (i = 1, \ldots, n). \) The predictor \( \hat{S}_{X \times Z}^2 = 2 \hat{\beta}^\top \Sigma_{XZ} \hat{u} \) is unbiased for the estimand for the explained variation of the covariance induced by possible non-orthogonality of the columns of \( CX \) and \( CZ, \) the sample covariance \( 2 \hat{\beta}^\top \Sigma_{XZ} \). The quantities \( \hat{S}_X^2, \hat{S}_Z^2, \) and \( \hat{S}_{X \times Z}^2 \) are invariant to centring the data \( y, X, \) and \( Z. \)

Later, Piepho\cite{Piepho2001} derived an estimator for the average semisquared bias for the mean structure which equals \( \hat{S}_X^2 \) in the case of the variance components form of the LMM.

The following theorem states the decomposition of the centred total sum of squares.

**Theorem 3.2** Given restricted maximum likelihood estimators \( \hat{\sigma}_e^2 \) for the residual variance \( \sigma_e^2 \) and \( \hat{\sigma}_u^2, \) for the variance components \( \sigma_{u_i}^2, (i = 1, \ldots, m) \) in model (1), we find
\[
\hat{\sigma}_y^2 = \hat{S}_X^2 + \hat{S}_Z^2 + \hat{S}_{X \times Z}^2 + \hat{\sigma}_e^2.
\] (4)

Decomposition \( \hat{\sigma}_y^2 = \hat{S}_X^2 + \hat{\sigma}_e^2 \) and the deduction and interpretation of \( \hat{S}_X^2 \) follow in the special case of the LM as presented in Section 2.2. In the special case of a random effects model with only one random effect vector and no fixed effects but the intercept, decomposition (4) reduces to \( \hat{\sigma}_y^2 = \hat{S}_Z^2 + \hat{\sigma}_e^2, \) which has been observed, but not been proven, by Schreck et al.\cite{Schreck2008} in several genomic applications. In that context, \( \hat{S}_Z^2 \) has been termed empirical best predictor of the additive genomic variance\cite{Schreck2008}. 

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Due to the explicit nature of the estimand of the different variance contributions expressed in Lemma 3.1, their interpretation is intuitive. In particular, the explained variations (estimands) originate from sample variations of the covariate information, no matter whether their associated effects are fixed or random. This reflects that the data-generating processes of X and Z are vital drivers of the underlying variability. While for the mean structure variability is induced only through the data-generating process of the covariate corresponding to fixed effects, in the case of random effects both the associated data-generating process and the effects themselves induce variability, which is clearly reflected within \( \hat{S}_Z^2 \). The proper decomposition of the variability of the observations in (4) was made possible by the inclusion of the estimates of the realizations of the random effects. The latter are viewed as parameters to be estimated, reflecting an empirical best prediction approach (or parametric empirical Bayes, if the prior is Gaussian) as advocated, for instance, in Morris (1983), Robinson (2021), and Xu (2003). Consequently, the corresponding explained variation is not solely concerned with the contribution of population averages but also of data set specific realizations, as further discussed in the next section. Possible correlations between the data-generating processes of X and Z are captured by \( \hat{S}_{XZ}^2 \). Further interpretations follow in the next sections and in the applications.

3.2 Population and Data set Specific Explained Variation

The empirical predictor \( \hat{S}_Z^2 \) for the explained variation associated with the random effects, see Lemma 3.1 and Equation (4), can be further decomposed as

\[
\hat{S}_Z^2 = \hat{S}_Z^{2p} + \hat{S}_Z^{2d}, \quad \hat{S}_Z^{2p} = \text{tr}(D\hat{\Sigma}_Z), \quad \hat{S}_Z^{2d} = u^\top \hat{\Sigma}_Z \hat{u} - \text{tr}(\hat{\Sigma}_Z \hat{\Sigma}_u),
\]

into what we term population-specific (indexed by \( p \)) and data-specific (indexed by \( d \)) explained variation. The terminology and interpretation are based on the following reasoning.

Similar to equation (3), the expectation of the quadratic form of the observations is

\[
\mathbb{E}[\hat{\beta}_y^2] = \frac{1}{n - 1} \text{tr}
\left(
C(\text{cov}(y) - \mathbb{E}[y]\mathbb{E}[y]^\top)
\right) = \sigma_y^2 + \beta^\top \hat{\Sigma}_X \beta + \text{tr}(D\hat{\Sigma}_Z). \tag{5}
\]

Whereas bias-reduced estimators for \( \sigma_y^2 \) and \( \beta^\top \hat{\Sigma}_X \beta \) are directly reflected by \( \hat{S}_Z^{2p} \) and \( \hat{S}_X^2 \) in decomposition (4), the relationship of \( \hat{S}_Z^2 \) and \( \hat{S}_{XZ}^2 \) with Equation (5) might not be obvious. From Lemma 3.1 recall that the sample variance \( \sigma_y^2 = u^\top Z^\top CZu/(n - 1) \) of the random vector \( Z \) is itself a random variable in the context of model (1). The unconditional expectation \( \mathbb{E}[\sigma_y^2] = \text{tr}(D\hat{\Sigma}_Z) \) represents the last term in Equation (5). Similar to the best linear unbiased predictor \( \mathbb{E}[u \mid y] \) of the random effects \( u \), the conditional expectation is

\[
\mathbb{E}[\sigma_y^2 \mid y] = \text{tr}(\mathbb{E}[uu^\top \mid y] \hat{\Sigma}_Z) = \mathbb{E}[u^\top \mid y] \hat{\Sigma}_Z \mathbb{E}[u \mid y] + \text{tr}(D\hat{\Sigma}_Z) - \text{tr}(\Sigma_u \hat{\Sigma}_Z),
\]

where the last equality holds because of the variance components form of model (1).

The empirical predictor \( \hat{S}_Z^2 \) directly estimates \( \mathbb{E}[\sigma_y^2 \mid y] \). This conditional expectation includes the unconditional expectation \( \text{tr}(D\hat{\Sigma}_Z) \) and the BLUP’s of the random effects as a measure of realized effect size, similarly to the fixed effects estimates in the variance explained by covariates associated with fixed effects. Conditioning on the data, it utilizes the information provided by the data \( y \). From a Bayesian perspective, \( \hat{S}_Z^2 \) can be interpreted as the posterior expectation of explained variation of covariates associated with random effects, also called parametric empirical Bayes estimator. Compared to the unconditional expectation (or the prior expectation \( \text{tr}(D\hat{\Sigma}_Z) \)), the conditional expectation has superior properties as an estimator of the realizations of a random variable, e.g., Consequently, we prefer \( \hat{S}_Z^2 \) to \( \text{tr}(D\hat{\Sigma}_Z) \) as an estimator of the realization of \( \sigma_y^2 \). The terminology population-specific explained variation for \( \hat{S}_Z^{2p} \) originates from the derivation as the unconditional expectation of \( \sigma_y^2 \) and the implied interpretation as the mean of the hypothetical population. The deviation of the conditional from the unconditional expectation, \( \hat{S}_Z^{2d} \), has expectation 0 with respect to the population. Hence, we call \( \hat{S}_Z^{2d} \) data-specific explained variation.

For instance in longitudinal studies with fixed and random time effect, \( \hat{S}_X^2 \) can be viewed as the explained variation associated with the covariates associated with the mean effect of time. The corresponding explained variation associated
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with random slopes can be split into $\hat{S}_Z^2$ which resembles the average of the individual variation around the fixed slope in the hypothetical population. The additional deviations of the variation in the underlying data set given the information of the sampling population are accounted for by $\hat{S}_d^2$.

In Section 2.2, we illustrate that the total population-specific variance often contributes the largest part to the explained variation associated with random effects and their respective covariates. The data-specific explained variation seems to contribute strongly if the covariates associated with random effects are highly correlated and is the main driver in our novel parameter-wise dispersion relevance profile, making individual covariates more distinguishable. These individual contributions are, however, not restricted to be positive, and often do not contribute largely in sum to the overall explained variation if the covariates are uncorrelated.

The empirical covariance $\beta^T \Sigma_{XZ} u$ between the vector $X \beta$ and $Z u$ always has unconditional expectation (population-specific explained variation) 0 and conditional expectation (data-specific explained variation) $\hat{S}_{XZ}^2$. For this reason, the cross-terms do not contribute in Equation (5) but do so in decomposition (4).

### 3.3 Coefficients of Determination

The explained variations defined in Lemma 3.1 depend on the amount of observed variation. Coefficients of determination are often defined as explained variance scaled with respect to the total observed variation or the residual variance of a reference model, respectively, in order to enable comparability of variation explained in different settings. In Section 2.2, the reference model is the intercept-only model where the residual variance coincides with $\hat{\sigma}_u^2$, leading to a consistent scaling. In general, however, there need not be a unique reference model, leading to a variety of potential $R^2$'s.

In accordance to $\hat{R}^2$ in Section 2.2, we propose to utilize decomposition (4) to define

$$\hat{R}^2 = \frac{1}{\hat{\sigma}_y^2} \left( \hat{S}_X^2 + \hat{S}_Z^2 + \hat{S}_{XZ}^2 \right) = \frac{\hat{S}_X^2 + \hat{S}_Z^2 + \hat{S}_{XZ}^2}{\hat{S}_X^2 + \hat{S}_Z^2 + \hat{S}_{XZ}^2 + \hat{\sigma}_u^2} = 1 - \frac{\hat{\sigma}_u^2}{\hat{\sigma}_y^2}$$

as the adjusted coefficient of determination for the LMM (1). The terminology refers to the fact that (6) reduces to $\hat{R}^2$, see Section 2.2 and uses bias-corrected estimates by adjusting for estimation uncertainty of the effects sizes. The total observed variance or the residual variance in the model with only a fixed intercept (reference model), implying all observations to be uncorrelated, is used for scaling. The $\hat{R}^2$ has, by definition, the interpretation as proportion of explained variance, and as the additive inverse to the coefficient of alienation (proportion of unexplained variance). Therefore, (6) is in line with the $r_d^2$ introduced in Xu (9), which also reduces to the adjusted coefficient of determination in the LM in the case that REML estimation is used (9). Our main focus, however, is on explicitly investigating and interpreting the explained variation in detail.

The $\hat{R}^2$ is an analytic function of the estimates returned after a model fit with REML, making its computation straightforward. Due to the explicit and additive nature of decomposition (4), we can easily define proportions of variance explained by the coefficients associated with fixed or with random effects. Due to Lemma 3.1 the quantity $\hat{R}^2$ is dimensionless, i.e. it is invariant to scaling and centring the data $y$, $X$, and $Z$.

Alternatively, based on the further decomposition given in Section 3.2, we can define a population coefficient of determination

$$\hat{R}_p^2 = \frac{\hat{S}_X^2 + \sum_{i=1}^m \hat{\sigma}_i^2 \text{ tr } \left( \hat{\Sigma}_Z \right)}{\hat{S}_X^2 + \sum_{i=1}^m \hat{\sigma}_i^2 \text{ tr } \left( \hat{\Sigma}_Z \right) + \hat{\sigma}_u^2}$$

which constitutes the relative population average explained variation. The scaling has been chosen to resemble the unconditional expectation, see Section 3.2. However, the implied null model is not obvious. As mentioned above, the estimator for the average semisquared bias in Piepho (10) for the mean structure equals $\hat{S}_X^2$ in the variance components.
form of the LMM. Naturally, the coefficient of determination introduced in Piepho\cite{Piepho2003} is identical to $\hat{R}_p^2$ in (7) already introduced in an earlier preprint.

The widely employed marginal ($R_{m}^2$) and conditional ($R_{c}^2$) coefficients of determination by Nakagawa and Schielzeth\cite{Nakagawa&Schielzeth2013} and Johnson\cite{Johnson2010} are given by

$$R_{m}^2 = \frac{\hat{\sigma}_{\hat{f}}^2}{\hat{\sigma}_{\hat{f}}^2 + \hat{\sigma}_\varepsilon^2 + \hat{\sigma}_\zeta^2}, \quad R_{c}^2 = \frac{\hat{\sigma}_{\hat{f}}^2 + \hat{\sigma}_i^2}{\hat{\sigma}_{\hat{f}}^2 + \hat{\sigma}_i^2 + \hat{\sigma}_\zeta^2}$$

(8)

where $\sigma_i^2 = \text{tr}(\mathbf{Z} \mathbf{D} \mathbf{Z}^T)/n$ is termed the mean random effect variance, resembling the unconditional estimate in Section 3.2. The term $\hat{\sigma}_{\hat{f}}^2$ is defined in the context of model (1), thus allowing for fixed effects and an arbitrary number of independent random effects. Consequently, $\hat{\sigma}_{\hat{f}}^2$ resembles the unconditional expectation, see Section 3.2, and that $\hat{\sigma}_{\hat{f}}^2$ is biased. The main differences of (8) and (6) are that we use a bias-corrected, variance adjusted estimator, $\hat{S}_X$, for the explained variance of the mean structure and that we include not only population averages for the covariance structure, but also data set specific deviations. These deviations might be present for the coefficients of random effects but also in terms of correlations between the coefficients associated with fixed and random effects (given by $\hat{S}_{X \times X}$). The data set specific contributions are in particular vital for parameter-wise relevance profiles, as illustrated, for instance, in Figure 2 and described in detail in the next section.

In GWAS, the simultaneous effect of markers is typically modeled using the variance components form of a random effect model, $y = \mu \mathbf{1}_n + \mathbf{Z} \mathbf{u} + \epsilon = \mu \mathbf{1}_n + \mathbf{g} + \epsilon, \quad \mathbf{g} \sim \mathcal{N}(0, \sigma_g^2 \mathbf{I})$, where $\mathbf{Z}$ denotes the design matrix of the genomic markers e.g.\cite{Yang2013}. The most popular approach for the estimation of the relative genomic variance has been introduced by Yang et al.\cite{Yang2013} who use the estimator $\hat{\sigma}_g^2$ as an improved estimator of the genomic variance while $\hat{\sigma}_f^2$, for the explained variance used in Nakagawa and Schielzeth\cite{Nakagawa&Schielzeth2013} and the references therein. The estimator $\hat{S}_X$, however, is in accordance to quantitative genetics theory and in particular includes the contribution of linkage disequilibrium\cite{Johnson2010}. Consequently, $\hat{S}_X$ can be viewed as an improved estimator of the genomic variance while being defined in the context of model (1), thus allowing for fixed effects and an arbitrary number of independent random effects. Heritability estimates, i.e. proportion of genomic variance, can be obtained by coefficients of determination based on (8).

### 3.4 Components of Explained Variation

We believe that partitioning the explained variation is the best and possibly only option for a simultaneous assessment of parameter-wise relevance for covariates associated with fixed and random effects in the LMM. To this end, we utilize a similar reasoning as Hoffmann\cite{Hoffmann2017} and Pratt\cite{Pratt2017}, see Section 2.3, to further partition the explained variations in decomposition (4) to parameter-wise components. We assign equal shares of the joint contribution to the direct contribution of parameters to obtain their total contribution.

We partition the bias-corrected $\hat{S}_X$, see Lemma 3.1, into the $k$ contributions of the covariates associated with fixed effects $\hat{S}_{X \times X} = \sum_{j=1}^{k} \left\langle \begin{array}{l} \hat{\Sigma}_{X} \end{array} \right\rangle_{jj} \left[ \hat{\beta}_j - (\hat{\Sigma}_{\hat{\beta}})_{jj} \right] + \sum_{j \neq i} \left\langle \begin{array}{l} \hat{\Sigma}_{X} \end{array} \right\rangle_{ij} \left[ \hat{\beta}_i \hat{\beta}_j - (\hat{\Sigma}_{\hat{\beta}})_{ij} \right]$. We attribute the data set specific term $\hat{S}_{X \times Z}^2$ to each of the $k$ fixed effects and to each of the $m$ random effect vectors by summing over the contributions of the covariances with the random and fixed effects, respectively $\hat{S}_{X \times Z}^2 = \sum_{j=1}^{k} \hat{\beta}_j \sum_{i=1}^{m} \left\langle \begin{array}{l} \hat{\Sigma}_{XZ} \end{array} \right\rangle_{ij} \left[ \hat{\beta}_i \hat{\beta}_j - (\hat{\Sigma}_{\hat{\beta}})_{ij} \right] + \sum_{i=1}^{m} \hat{\beta}_j \sum_{i=1}^{m} \left\langle \begin{array}{l} \hat{\Sigma}_{XZ} \end{array} \right\rangle_{ij} \left[ \hat{\beta}_i \hat{\beta}_j - (\hat{\Sigma}_{\hat{\beta}})_{ij} \right]$. In this way, a certain contribution of data set specific explained variance can be attributed to each covariate, whether associated with a fixed or random effect. To sum up, we assign the $j$-th covariate associated with a fixed effect the share

$$\hat{S}_{Xj} = \left\langle \begin{array}{l} \hat{\Sigma}_{X} \end{array} \right\rangle_{jj} \left[ \hat{\beta}_j^2 - (\hat{\Sigma}_{\hat{\beta}})_{jj} \right] + \sum_{i \neq j} \left\langle \begin{array}{l} \hat{\Sigma}_{X} \end{array} \right\rangle_{ij} \left[ \hat{\beta}_i \hat{\beta}_j - (\hat{\Sigma}_{\hat{\beta}})_{ij} \right] + \hat{\beta}_j \sum_{i=1}^{m} \left\langle \begin{array}{l} \hat{\Sigma}_{XZ} \end{array} \right\rangle_{ij} \left[ \hat{\beta}_i \hat{\beta}_j - (\hat{\Sigma}_{\hat{\beta}})_{ij} \right]$$

(9)

including data set specific contributions.
It is straightforward to partition the population explained variance \( \sum_{i=1}^{m} \hat{\sigma}_i^2 \) to specific random effects. The data set specific part can be partitioned using \( \sum_{i=1}^{m} \left\{ \text{tr}(\Sigma Z_i [\hat{u}_i \hat{u}_i^\top - \Sigma \alpha_{i}]) + \sum_{j \neq i} \text{tr}(\Sigma Z_i [\hat{u}_j \hat{u}_j^\top - \Sigma \alpha_{j}]) \right\} \). Similar to \( \hat{\sigma}_i^2 \), we define the contribution of the \( i \)-th covariate associated with random effects to the explained variance including data set specific deviations as
\[
\hat{S}_{Z_i}^2 = \sigma_{u_i}^2 \text{tr}(\Sigma Z_i) + \text{tr}(\Sigma Z_i [\hat{u}_i \hat{u}_i^\top - \Sigma \alpha_{i}]) + \sum_{j \neq i} \text{tr}(\Sigma Z_i [\hat{u}_j \hat{u}_j^\top - \Sigma \alpha_{j}]) + \beta^\top \hat{\Sigma}_Z Z_i \hat{u}_i.
\] (10)

For instance in Table 2 we illustrate how the parameter-wise contributions \( \hat{\sigma}_i^2 \) and \( \hat{S}_{Z_i}^2 \) lead to a simultaneous dispersion relevance assessment of all model covariates associated with fixed effects and random effects on the same scale. Relative parameter-wise shares of explained variations are obtained by division as in equation (6).

By similar arguments, the contribution of the covariates \( Z_i \), see Equation (10), can be even further partitioned to each column of \( Z_i \). This can be applied, for example, to obtain relevance profiles for individuals genomic markers which share the same random effect vector, as exemplified in Section 4.3 and visualized in Figure 2.

4 Real Data Applications

4.1 Hierarchical Data - Sleep Deprivation Study

Bates et al.\(^{23}\) investigate reaction time per day for subjects in a longitudinal sleep deprivation study. For each of the 18 subjects, the response variable Reaction defined as the average reaction times in milliseconds is collected on the same 10 days, implying a balanced design. The amount of sleep is unrestricted on day 0 and restricted to 3 hours afterwards. By means of a likelihood ratio test and difference in deviance, Bates et al.\(^{23}\) study whether a random slope for time should be added to the basic model including time as a covariate with fixed effect and a random subject-specific intercept (ID). They conclude that "adding a linear [random] effect of time uncorrelated with the [random] intercept leads to an enormous and significant drop in deviance". While this may be convincing from a modeling perspective, the magnitude of a deviance drop is inherently difficult to interpret.

We fit model (1) and use Equation (4) to additively decompose the observed variance of Reaction (\( \hat{\sigma}_y^2 = 3172.93 \)) into the estimate \( \hat{S}_{Z}^2 = 888.78 (\approx 28\%) \) for the adjusted explained variation of time associated with a fixed effect, an estimate of the unbiased predictor \( \hat{S}_{Z}^2 = 1630.57 (\approx 51\%) \) for the explained variation of time and ID associated with random effects and the REML estimate \( \hat{\sigma}_z^2 = 653.58 (\approx 21\%) \) for the residual variance. The estimate of \( \hat{S}_{Z}^2 = 653.58 \) is negligible here (\( < 0.01 \)), similar to \( \hat{S}_{Z}^2 \). This yields \( \hat{R}^2 \approx 0.79 \) which is very close to the population coefficient \( \hat{R}_p^2 \).

| Effect Type | Covariable | Estimate | Std. Error | Pr(>|t|) | \( \hat{R}^2 \) (in %) | 2.5% | 97.5% |
|-------------|------------|----------|------------|---------|----------------------|------|------|
| Fixed       | (Intercept)| 251.41   | 6.89       | < 0.001 | -                    | -    | -    |
|             | time       | 10.47    | 1.56       | < 0.001 | 28.01                | 15.43| 44.48|
| Random      | ID         | 0.20     | -          | -       | 19.53                | 4.56 | 33.77|
|             | time       | 0.01     | -          | -       | 31.86                | 14.04| 48.87|
|             |            | 0.21     | -          | -       | 20.60                | 14.10| 32.04|

In Table 1 we present the relative contributions of the individual covariates to the explained variance. This enables us to compare the relevance of all covariates on the same scale, which is not possible by using only the standard output including effect estimates, standard errors, p-values and variance component estimates (relative to \( \hat{\sigma}_y^2 \)). Time as a covariate associated with a random slope explains about 32% of the observed variation in Reaction, substantiating the result from the likelihood ratio test. ID contributes similarly as the residual variance (about 20% each) to the observed variance. Notably, when comparing only the variance components of the covariates associated with random effects,
the variance of ID is about 20 times the variance of time. Clearly, this naive approach ignoring the variance $\hat{\Sigma}_Z$ of the data-generating process of time is not advisable. Time as a covariate associated with a fixed effect contributes similarly (about 28%) to the covariate time associated with a random slope. Thus, variability in Reaction explained by time associated with both a fixed and random effect amounts to a total of about 60%, which is considerably more than the subject-specific explained variation.

In sum, explained variances are more intuitively interpretable than differences in deviance, capturing relevance of the covariates rather than statistical significance in sequential testing. The novel importance ranking provides complementary information to the standard LMM model output by assessing the relevance of all covariates on a common scale.

4.2 Multilevel Data - Income Inequality in Burkina Faso

Gräb and Grimm\cite{24} investigate income inequality in Burkina Faso in the year 1994. At that time, the country was organized in 13 regions, 45 provinces and 434 communities. Household data were drawn from nationwide household surveys covering $n = 8374$ households. The overall aim of Gräb and Grimm\cite{24}'s study was to “[…] provide a decomposition of the variance of observed living standards into components due to factors that vary within and factors that vary between spatial units” to potentially “[…] help to target poverty reduction policies more effectively”. Thus, the authors were not primarily interested in estimating regression coefficients, but in decomposing the variance of the logarithm of household expenditure as a proxy for income inequality. Consequently, the components of explained variation rather than the coefficients were actually the estimand of interest. Gräb and Grimm\cite{24} use nested random intercepts to model the spatial (co)-variation due to communities, provinces and regions while including household and community characteristics as covariates associated with fixed effects. Their model M2 utilizes selected covariates on the household level, including the household size (hh.size), the kid-per-adult ratio (hh.kid.adult), the youth-per-adult ratio (hh.youth.adult), the age of the household head (hh.age.head), whether the household head was literate (hh.lit.head), the literacy percentage of adult household members (hh.lit.adult) and whether the household head was christian (hh.christian). Selected community level covariates include the ethnic fragmentation in the community (com.ethnic), the adult literacy fraction in the community (com.lit.adult), the community youth-adult ratio (com.youth.adult), whether at least one household in the community has electricity (com.electricity) and whether the community was urban (com.urban). The authors utilize the ICC to judge the contribution of each spatial level to the variance in the outcome. However, the ICC ignores the variation induced by the covariates associated with fixed effects, additionally to ignoring the variance of the data-generating process of the covariates associated with random effects. The variation attributable to the mean structure is determined by the proportional change of the ICC in a pure random intercept model compared to the ICC in a LMM with the fixed effects. Clearly, this is a rather heuristic approach, and a simultaneous modeling of the variance due to covariates associated with fixed and random effects is not possible this way.

We fit model (1) to represent M2 and illustrate how our novel variance decomposition provides a formal approach to simultaneously judge the contribution of each spatial level and each household and community level covariate to the variability of the logarithm of household expenditures.

We additively decompose $\hat{\sigma}^2_y = 0.883$ of the logarithm of household expenditures. The estimate $\hat{\Sigma}_X^2$ equals 0.375 ($\approx 42\%$). The estimate of the unbiased predictor for the explained variation of community, province, and region associated with random effects is $\hat{\Sigma}_Z^2 = 0.050$ ($\approx 6\%$). The data set specific explained variance $\hat{\Sigma}_{Z_d}^2$ is 0.005 ($\approx 0.4\%$) and the population explained variance is $\hat{\Sigma}_{Z_p}^2$ is 0.05 ($\approx 5.6\%$). The estimate of the data set specific covariance term $\hat{\Sigma}_{X \times Z}$ represents a substantial contribution of 0.058 ($\approx 6.6\%$ which should not be ignored. The REML estimate $\hat{\sigma}^2_\varepsilon = 0.395$ ($\approx 45\%$) for the residual variance. This yields an adjusted coefficient of determination $R^2 \approx 55\%$, see definition (6). The population coefficient $R^2_p$ in equation (7) amounts to $\approx 52\%$ which approximately equals $R^2$. In Table 2 we present relative contributions of the individual covariates, including data set specific contributions, to the explained variance. The combined explained variation by the spatial levels is about 9.5% including its share of
\[ \hat{S}_{X \times z}^2, \text{see Equation (10).} \] The covariates associated with fixed effects that are most relevant with respect to dispersion are household size (8.2%) and variables associated with literacy (22.6% combined with bootstrap confidence interval (19.6%; 25.8%). Characteristics on the household level explain a combined amount of \( \approx 25\% \) and the characteristics on the community level explain about 24% including community and its random effect.

**Table 2: Inequality in Burkina Faso.** \( \hat{R}_{(i)}^2 \) denotes parameter-wise contributions to dispersion relevance, as defined in equation and \( \hat{\sigma}^2_y \). We include 95% parametric bootstrap confidence intervals.

| Effect Type | Covariable           | Estimate | Std. Error | Pr(>|t|) | \( \hat{R}_{(i)}^2 \) (in %) | 2.5%   | 97.5%   |
|-------------|-----------------------|----------|------------|---------|-----------------------------|--------|---------|
| Fixed       | (Intercept)           | 11.13    | 0.05       | < 0.001 | 8.24 7.18 9.35              | 45.74  | 43.40  48.18 |
|             | hh.size               | -0.04    | 0.001      | < 0.001 | 0.66 0.42 0.99              | 4.96   | 3.86   6.13  |
|             | hh.kid.adult          | -0.05    | 0.006      | < 0.001 | 1.49 1.21 1.62              | 0.66   | 0.42   0.99  |
|             | hh.youth.adult        | -0.004   | < 0.001    | < 0.001 | 2.06 1.49 2.69              | 0.35   | 0.23   0.47  |
|             | hh.age.head           | 0.35     | 0.023      | < 0.001 | 9.30 6.88 11.90             | 4.96   | 3.86   6.13  |
|             | hh.lit.head           | 0.20     | 0.023      | < 0.001 | 6.13 4.88 7.48              | 0.35   | 0.23   0.47  |
|             | hh.lit.adult          | 0.03     | 0.019      | 0.071   | 0.85 0.58 1.12              | 0.35   | 0.23   0.47  |
|             | hh.christian          | 0.35     | 0.059      | < 0.001 | 5.09 3.86 6.37              | 0.35   | 0.23   0.47  |
|             | com.ethnic            | 0.50     | 0.070      | < 0.001 | 12.67 9.96 15.39            | 0.35   | 0.23   0.47  |
|             | com.lit.adult         | -0.09    | 0.041      | 0.035   | 0.92 0.66 1.18              | 0.35   | 0.23   0.47  |
|             | com.electricity       | 0.14     | 0.041      | < 0.001 | 4.95 4.00 5.90              | 0.35   | 0.23   0.47  |
|             | com.urban             | -0.15    | 0.046      | 0.001   | 6.21 4.54 7.87              | 0.35   | 0.23   0.47  |
| Fixed total |                       |          |            |         | 45.74 43.40 48.18            | 45.74  | 43.40  48.18 |
| Random      | community             | \( \hat{\sigma}^2_{y_1}/\hat{\sigma}^2_y = 0.035 \) | - | - | 3.72 2.62 4.81          | 0.35   | 0.23   0.47  |
|             | province              | \( \hat{\sigma}^2_{y_2}/\hat{\sigma}^2_y = 0.006 \) | - | - | 2.51 1.87 3.15          | 0.35   | 0.23   0.47  |
|             | region                | \( \hat{\sigma}^2_{y_3}/\hat{\sigma}^2_y = 0.017 \) | - | - | 6.12 4.37 8.14          | 0.35   | 0.23   0.47  |
| Random total|                       |          |            |         | 9.52 5.92 11.00            | 0.35   | 0.23   0.47  |
| Residual    | \( \hat{\sigma}^2_{\epsilon}/\hat{\sigma}^2_y = 0.447 \) | - | - | 52.66 43.44 61.90 | 0.447   | 0.31   0.64  |

In Figure 1, we illustrate the parameter-wise relevance profiles of the spatial levels region, province and community. The region as well as the province with ID 11 contribute prominently to the explained variance compared to the other regions and provinces. Interestingly, we identified ID 11 as Centre, which is the region in Burkina Faso with the highest population density and with the only large town in the country (Ouagadougou, the capital city). Unfortunately, we were not able to assign the community ID's.
Our novel variance decomposition provides a formal tool to simultaneously judge the relevance of hierarchical levels and covariates associated with fixed effects on the same scale. Thus, we were able to contrast the sum of contributions of multiple fixed effects covariates to the contribution of random effects capturing spatial structure. Income inequality, which is measured by the variability in household expenditures, could be associated with literacy as a main contributor while the spatial levels contributed less. Further, relevance profiles for province and region revealed that the region “Centre/Ouagadougou” contributed the most to the spatial inequality while accounting for covariates associated with fixed effects.

4.3 High-Dimensional GWAS - Arabidopsis Thaliana

GWAS focus on finding associations between complex phenotypes and marker loci often spread on the whole genome. In this context, model [1] is widely applied to fit all markers on the genome simultaneously e. g. This enables a more realistic analysis than marker-wise comparisons because a combined model allows for controlling confounding effects of the often highly correlated markers. It is of central interest to identify genetic variants that explain variation in a phenotype, as well as to attribute the observed variation to specific covariates, in particular to certain regions of the genome such as chromosomes or even single markers e. g. This reinforces the need for a dispersion relevance profile in the LMM, in particular for genomic markers, which are represented by covariates associated with random effects.

The publicly available data set for the model organism “Arabidopsis thaliana” comprises \( n = 1057 \) lines which were genotyped for \( p = 193,697 \) single nucleotide polymorphism (SNP) markers split on \( m = 5 \) chromosomes \( (p_1 = 47,518, p_2 = 25,550, p_3 = 38,813, p_4 = 33,240, p_5 = 48,576) \). We relate the phenotype flowering time at 10°C, \( ft10 \), to the marker genotypes on the \( m = 5 \) chromosomes of the organism to investigate the proportion of variation of \( ft10 \) each chromosome, and subsequently each individual SNP, explains. To this end, we fitted a LMM (using R package sommer\( ^{23} \)) in which we model each chromosome as a covariate associated with a random effect vector (of size \( p_i, i = 1, \ldots, 5 \)). We include a fixed intercept, but no other covariates associated with fixed effects.

The REML estimate of the unexplained variation and the estimate of \( \hat{S}_Z^2 \) contributed 7.75% and 92.25% to the sample variance of \( ft10 \), respectively. The population explained variation amounted to 47.80% together with large data set specific contributions (44.46% in sum). The latter has already been shown to be the contribution of linkage disequilibrium, i. e. when covariates (markers) are correlated\( ^{29} \).

In Table 3 we give a detailed overview of the explained variation between and among the five chromosomes, as derived in Equation (10). Chromosome five explains by far the largest amount of variance of \( ft10 \) compared to the other chromosomes. In particular, the first three chromosomes explain very little variance by themselves. About one third of the explained variation can be attributed to effects between pairs of chromosomes where pairs that contain chromosome five contribute the largest. Based on this high-level overview, we investigate single chromosomes in greater detail, in particular chromosome five.

| Chromosomes | 1   | 2   | 3   | 4   | 5   | \( \hat{R}_Z^2 \) |
|-------------|-----|-----|-----|-----|-----|-----------------|
| 1           | 4.32 (3.94) | 0.63 | 0.19 | 1.06 | 2.06 | 8.25 (3.94) |
| 2           | 0.63 | 6.43 (5.20) | 0.25 | 1.57 | 2.58 | 11.46 (5.20) |
| 3           | 0.19 | 0.25 | 2.67 (2.62) | 0.50 | 1.06 | 4.67 (2.62) |
| 4           | 1.05 | 1.57 | 0.50 | 14.11 (11.76) | 5.12 | 22.35 (11.76) |
| 5           | 2.06 | 2.58 | 1.06 | 5.12 | 34.70 (22.28) | 45.52 (22.28) |
| \( \hat{R}_Z^2 \) | 8.25 (3.94) | 11.46 (5.20) | 4.67 (2.62) | 22.35 (11.76) | 45.52 (22.28) | 92.25 (47.80) |
In Figure 2A, we illustrate the coefficient p-values based on univariable LM’s where single markers on chromosome 5 are regressed on ft10 (Manhattan plot). However, these univariable models suffer strongly from confounding, in particular because markers close on the genome tend to be highly correlated. Additionally, significance does not necessarily imply any relevance. To mitigate these issues, we introduce a novel dispersion relevance plot in Figures 2B to visualize the parameter-wise contributions of individual SNP’s to the observed variation in ft10 as described in the end of Section 3.4.

Several regions on chromosome 5 indicated by the Manhattan-type plot in Figure 2A cannot be replicated to the same extent in the relevance profile in Figure 2B, reflecting the above mentioned fact that significance does not imply relevance. The region on the genome around SNP ID 34000 is, however, prominent in both the Manhattan-type plot as well as the relevance profile. Some significant SNPs in univariate analysis have negative contributions to the explained variation. This suggests that these regions might not be particularly important with respect to dispersion relevance in the fitted LMM. Naturally, in the context of this paper, we cannot give definitive answers of important regions or even individual SNPs. However, the simultaneous relevance assessment mitigates confounding and problems concerned with
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significance-based analyses. Thus, it might be meaningful to direct the main focus on spikes present in both approaches and investigate differences.

The population variation (Figure 2C) is relatively constant and always positive over the whole chromosome, but comparably low for each marker. Differences arise solely to differences of the diagonal of $\hat{\Sigma}_Z$, but are almost completely mitigated by the small value of $\hat{\sigma}_u^2$. These characteristics arise from the derivation of the population explained variance as the unconditional expectation of $\sigma^2_r$ combined with the model assumptions about the random effects, see Section 3.2 and Equation (1). The data set specific explained variation (Figure 2D) determines the shape of the relevance profile which supports their importance in particular for parameter-wise or individual relevance assessments. The dispersion relevance profiles for the chromosomes 1 – 4 are illustrated in the Supplementary Material, as well as an additional example (mice data) including coefficients associated with fixed effects.

5 Discussion

We have rigorously proven a novel proper decomposition of the observed sum of squares in the variance components form of the LMM, where only estimates that result from the model fit using REML are involved. The components of this decomposition have been shown to represent unbiased estimators of empirical explained variances, which constitute easily interpretable estimands within the scope of our paper. We have introduced a bias-corrected estimator for the explained variance of covariates associated with fixed effects. Our estimator of the explained variation of covariates associated with random effects consists of what we call a population and a purely additive data set specific contribution. The population part often constitutes the main contribution to the explained variation, while the data set specific part is particularly important for the parameter-wise dispersion relevance profile. The explained variance attributed to correlations between the covariates associated with fixed and random effects has a non-zero data set specific contribution but zero population mean. On the one hand, we have utilized our decomposition to define an extension of the adjusted coefficient of determination from the LM to the LMM. On the other hand, we have introduced a parameter-wise dispersion relevance assessment for covariates associated with fixed and random effects on a common scale within a single LMM fit. To the best of our knowledge, a similar result has not been reported before. Its usefulness as a complement to the standard LMM output for hierarchical or multilevel data and its application as a novel relevance screening plot for high-dimensional genomic data has been illustrated in several real data examples.

Throughout the paper we emphasize that the data-generating processes of the covariates (associated with fixed or random effects) take a key part in the generation of explained variation. For instance, we have illustrated that the explained variation is induced by the data-generating process $X$ of the covariates associated with fixed effects. As per definition, the fixed effects have no variance and contribute only as weighting factors. The LMM, however, comprises several sources of variation. Additionally to the (co-)variances of the data-generating processes of the covariates associated with fixed and random effects, the variation due to the random effects is important. Decomposition (4) illustrates how these different sources of variation interact and lead to a full decomposition of $\hat{\sigma}_y^2$.

Decomposition (4) and with it explained variances, adjusted coefficient of determination and the parameter-wise relevance ranking are foremost applicable for model (1) with continuous response and independent random effects. An extension to generalized linear mixed models and LMMs with correlated random effects is part of future research.

The homoscedastic LM (2) implies that the observations have identical variance, which in turn is decomposed into explained and residual variance. This gives rise to the proportion of variance of the observations explained by the covariates, which can be viewed as a population parameter. In most heteroscedastic models, including the LMM, there is no unique variance of the dependent variable to decompose, with the exception of purely random intercept models. We focus on the decomposition of the quadratic form $\hat{\sigma}_y^2$, which reflects an empirical variance approach. To this end, the realizations of the random effects are estimated via empirical BLUP (or equivalently parametric Gaussian empirical Bayes), which is the prominent strength of the LMM over marginal models like the general linear model.

Explicit prediction of random effects is advocated, for instance, by Robinson and is very common, amongst others, in
GWAS, and in cases were subject-specific merit is of interest, e.g. in cattle breeding\textsuperscript{21,22}. In the particular case that these estimates are of interest, we believe they should also be utilized in the calculation of explained variation leading to the \textit{data set specific} contributions. These are purely additive components of the explained variance, i.e. they can always be considered complementary to the \textit{population} contribution. To the best of our knowledge, none of the existing approaches take the data set specific contribution into account.

Similar to ANOVA, and derived in the orthogonal case, it is a favourable property that the proportions of variance attributable to each of the covariates sum to $R^2$, although it is not a strict requirement for a meaningful measure of parameter-wise relevance\textsuperscript{[1]}. In the LMM, alternative approaches such as semi-partial $R^2$’s are only available for the coefficients associated with fixed effects, because dropping covariates associated with random effects invalidates model comparisons. Additionally, semi-partial $R^2$’s suffer from drawbacks such as multiple model comparisons and lack of interpretation in terms of explained variation as they typically do not sum to the full model $R^2$. Consequently, our parameter-wise relevance assessment is based on decomposition \textsuperscript{[4]} and equal (co-)variance sharing\textsuperscript{[4,5]}. Different weights for the (co-)variance sharing are possible and easily implemented, however, in the absence of convincing alternatives, we prefer the straightforward equal weighting in this already complex context.

Parameter-wise contributions to the adjusted $R^2$ can be negative. Although potentially confusing, this happens for example when the variance of an estimate is large while the effect estimate itself is small. Additionally, individual contributions might become negative if the corresponding variable decreases the variance of the observations by a strong negative correlation with other variables\textsuperscript{[5]}. In such cases, second-guessing the model at hand might be reasonable. Moreover, using a single measure to find the explained variation is always a simplification of a very complex situation and should therefore not be expected to provide unambiguous answers in all scenarios\textsuperscript{[5]}.

Our approach does not assess \textit{independent} variance contributions of covariates associated with fixed and random effects, but contributions given a specific model context. Therefore, our parameter-wise covariate relevance assessment is not intended for variable selection purposes. As argued in Cantoni et al.\textsuperscript{[17]}, variable selection in the LMM should be based on information criteria, whereas $R^2$ provides information about the fitted model. Similarly, Edwards et al.\textsuperscript{[8]} state that the concept of explained variation has limited use in model building.

Our novel parameter-wise assignment of shares of explained variances constitutes, to the best of our knowledge, the only both practically viable and theory-based option to simultaneously judge the relevance of covariates associated with fixed and random effects on the same scale, the observed variation, within a single LMM fit. In our opinion, the parameter-wise explained variations may be valuable in complementing standard model outputs as a descriptive dispersion relevance measure of the covariates associated with both fixed and random effects in fitted LMMs.

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