

Multilevel Models for Big Data

Approaches for handling very large datasets

Ömercan Mısırlıoğlu, Yordan Saputra

Department of Statistics
TU Dortmund University

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What are multilevel models?

- Hierarchical Structure
- Residual Components
- Variance Partitioning

Why use multilevel models?

- Correct Inferences
- Group Effects Estimation
- Simultaneous Estimation
- Generalization Beyond Sample ¹

Statistical Model

$$y_n \sim \mathcal{N}(\mu_n, \sigma)$$

$$\mu_n = b_0 + \sum_{p=1}^P b_p x_{pn} + \tilde{b}_{0j[n]} + \sum_{p=1}^P \tilde{b}_{pj[n]} x_{pn}$$

¹Centre for Multilevel Modelling 2025.

Multilevel Models for Big Data

Introduction

Multilevel Models

Introduction – Multilevel Models

What are multilevel models?

- Hierarchical Structure
- Residual Components
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Why use multilevel models?

- Correct Inferences
- Group Effects Estimation
- Simultaneous Estimation
- Generalization Beyond Sample¹

Statistical Model

$$y_{it} \sim \mathcal{N}(\mu_{it}, \sigma^2)$$

$$\mu_{it} = \beta_0 + \sum_{p=1}^P \beta_p x_{pit} + \tilde{\beta}_{0[iq]} + \sum_{p=1}^P \tilde{\beta}_{p[iq]} x_{pit}$$

¹Centre for Multilevel Modelling 2025.

What are multilevel models?

- **Hierarchical Structure:** Observational data often feature individuals nested within higher-level groups, such as schools, workplaces, or geographical areas.
- **Residual Components:** Multilevel models account for these hierarchies by incorporating residual components at every level of the data structure.
- **Variance Partitioning:** These models divide residual variance into between-group and within-group components to capture unobserved factors influencing outcomes.

Why use multilevel models?

- **Correct Inferences:** Traditional methods assume independent observations, which are often false. Additionally, ignoring hierarchical structures can lead to underestimated standard errors and overstated statistical significance.
- **Group Effects Estimation:** Directly quantify between-group variation and identify outlying groups.
- **Simultaneous Estimation:** Unlike fixed effects models, the separation of observed and unobserved group characteristics is possible, allowing for simultaneous estimation of group-level and individual-level effects.
- **Generalization Beyond Sample:** Unlike fixed effects models which only describe sampled groups, multilevel models treat groups as random samples from a population, enabling generalizations to unobserved groups.

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Introduction – Multilevel Models

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Why use multilevel models?

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Statistical Model

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¹Centre for Multilevel Modelling, 2025.

Statistical Model

$$y_n \sim \mathcal{N}(\mu_n, \sigma)$$

$$\mu_n = b_0 + b_1 x_{1n} + \dots + b_p x_{pn} + \tilde{b}_{0[j]} + \tilde{b}_{1[j]} x_{1n} + \dots + \tilde{b}_{pj[j]} x_{pn}$$

where:

- y_n : dependent variable for observation n
- x_{pn} : predictor variable p for observation n
- b_p : overall slope (or intercept for $p = 0$) for predictor p across all groups
- $\tilde{b}_{pj[j]}$: random effect of predictor p for group j that observation n belongs to
- σ : residual standard deviation (assumed constant across observations)

Introduction — Issues with Large Datasets

As hierarchical data scales (N groups \times n individuals), massive datasets create the following issues:

- High number of groups
- Large group sizes²
- Design matrix construction³

²Clark 2019; Speelman, Heylen, and Geeraerts 2018.

³S. Wood, Goude, and Shaw 2015.

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└ Introduction

└ Issues with Large Datasets

└ Introduction – Issues with Large Datasets

As hierarchical data scales (N groups \times n individuals), massive datasets create the following issues:

- High number of groups
- Large group sizes²
- Design matrix construction³

²Clark 2019; Spielman, Høyen, and Geeraerts 2018.

³S. Wood, Gouldie, and Shao 2015.

Issues with Large Datasets

- Large number of groups: Computational bottleneck from numerical integration over random effects for each group at every optimization step, leading to high computational costs
- Large group sizes: High-dimensional multivariate distributions create numerical issues with large covariance matrix inversion, even in linear models
- construction of the full design matrix X leads to high computational costs. In GAM, the estimator $\hat{\beta} = (X^T X + \sum \lambda_j S_j)^{-1} X^T y$ is hard to compute when X is large.
- it's even worse when we add another level to the hierarchy, e.g. students nested within classes nested within schools, which is common in educational research.

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The split-sample approach – Pseudo Likelihood

- Consider the log-likelihood function $\ell(\boldsymbol{\theta}) = \sum_i \ell(\mathbf{y}_i | \boldsymbol{\theta})$ where \mathbf{y}_i is the vector of all observations in group i
- Replaces the log-likelihood contribution $\ell(\mathbf{y}_i | \boldsymbol{\theta})$ by a weighted sum of log-likelihood contributions for sub-vectors $\mathbf{Y}_i^{(s)}$
- More specifically, the pseudo-log-likelihood function:

$$p\ell(\boldsymbol{\psi}) = \sum_i \sum_s \delta_s \ell(\mathbf{y}_i^{(s)} | \boldsymbol{\psi})$$

is maximized instead with respect to $\boldsymbol{\psi}$, which is not necessarily identical to $\boldsymbol{\theta}$

- Although $\hat{\boldsymbol{\psi}}$ is not the MLE estimate, it still has similar properties such as consistency and asymptotic normality⁴

⁴Clark 2019.

Multilevel Models for Big Data

└ The split-sample approach

└ Pseudo Likelihood

└ The split-sample approach – Pseudo Likelihood

- Consider the log-likelihood function $l(\theta) = \sum_i l(y_i|\theta)$ where y_i is the vector of all observations in group i
- Replaces the log-likelihood contribution $l(y_i|\theta)$ by a weighted sum of log-likelihood contributions for sub-vectors $\mathbf{y}_i^{(s)}$
- More specifically, the pseudo-log-likelihood function:

$$p(\psi) = \sum_i \sum_s \delta_i l(y_i^{(s)}|\psi)$$

is maximized instead with respect to ψ , which is not necessarily identical to θ

- Although ψ is not the MLE estimate, it still has similar properties such as consistency and asymptotic normality⁴

⁴Clark 2018.

- Now, how do we split \mathbf{y}_i into sub-vectors $\mathbf{Y}_i^{(s)}$? There are different ways to do this, and we will discuss some of them in the next slides.
- Going back to the slide on “issues with large datasets”, it’s obvious that we can split the data in two (technically three) different ways: either we can split the data by groups, or we can split the data by observations within groups. The first one is more suitable when we have a large number of groups, while the second one is more suitable when we have a large number of observations within groups.

The split-sample approach – Graphical representation

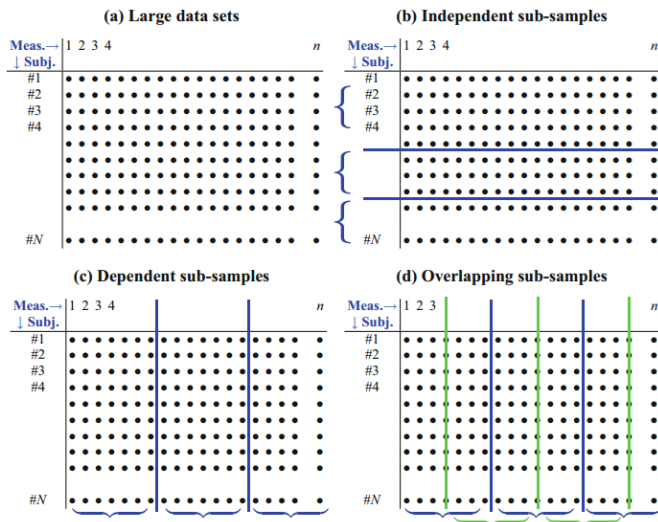


Figure 1: Graphical representation of different ways to split large samples

The split-sample approach — Independent subsamples

- Shown in panel (b) of Figure 1, dataset with large N is partitioned into M independent sets S_m of groups, where $m = 1, \dots, M$
- In each subsample, the model is fitted, yielding an estimate $\hat{\theta}_m$ of θ , equivalent to maximizing

$$p\ell(\psi) = \sum_m \sum_{i \in S_m} \ell(\mathbf{y}_i | \theta_m)$$

with respect to $\psi = \{\theta_1, \dots, \theta_M\}$

- All θ_m are equal to θ , therefore the estimates $\hat{\theta}_m$ can be averaged to obtain an overall estimate $\hat{\theta}$

Multilevel Models for Big Data

- └ The split-sample approach
 - └ Independent subsamples
 - └ The split-sample approach — Independent subsamples

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with respect to $\psi = (\theta_1, \dots, \theta_M)$

- All θ_m are equal to θ , therefore the estimates $\hat{\theta}_m$ can be averaged to obtain an overall estimate $\hat{\theta}$

- θ_m are all equal to θ because the subsamples are independent
- Mention parallelization here, since we can fit the model on each subsample in parallel, which can significantly reduce the computational time.

The split-sample approach – Dependent subsamples

- Shown in panel (c) of Figure 1, dataset with large n is partitioned into M (not independent) sets S_m of groups, where $m = 1, \dots, M$
- Fitting the model on each subsample, equivalent to maximizing

$$p\ell(\psi) = \sum_m \sum_i \ell(\mathbf{Y}_i^{(m)} | \theta_m)$$

with respect to $\psi = \{\theta_1, \dots, \theta_M\}$, where $\mathbf{Y}_i^{(m)}$ is the observations in \mathbf{Y}_i belonging to subsample S_m .

- All θ_m are not necessarily equal to θ , therefore the combination of all $\hat{\theta}_m$ into a single estimator $\hat{\theta}$ depends on the precise model and data structure.

Multilevel Models for Big Data

- └ The split-sample approach
 - └ Dependent subsamples
 - └ The split-sample approach – Dependent subsamples

- Shown in panel (c) of Figure 1, dataset with large n is partitioned into M (not independent) sets S_m of groups, where $m = 1, \dots, M$
- Fitting the model on each subsample, equivalent to maximizing

$$p(\psi) = \sum_m \sum_i \ell(Y_i^{(m)} | \theta_m)$$

with respect to $\psi = \{\theta_1, \dots, \theta_M\}$, where $Y_i^{(m)}$ is the observations in Y_i belonging to subsample S_m .

- All θ_m are not necessarily equal to θ , therefore the combination of all $\hat{\theta}_m$ into a single estimator $\hat{\theta}$ depends on the precise model and data structure.

- θ_m are not necessarily equal to θ because the subsamples are not independent, and there may be some correlation between the observations in different subsamples.
- (GPT warning, dont trust 100%) The combination of all $\hat{\theta}_m$ into a single estimator $\hat{\theta}$ can be done using various methods, such as meta-analysis techniques, or by fitting a model to the estimates $\hat{\theta}_m$ themselves.

The split-sample approach — Overlapping subsamples

- Shown in panel (d) of Figure 1, dataset with large n is partitioned similarly to dependent subsamples, but association between observations is accounted for by letting the subsamples overlap
- Denoting the parameters in pair $\{\mathbf{Y}_i^{(p)}, \mathbf{Y}_i^{(q)}\}$ by $\theta_{p,q}$, fitting the models on all pairs is equivalent to maximizing

$$p\ell(\psi) = \sum_{p < q} \sum_i \ell(\mathbf{Y}_i^{(p)}, \mathbf{Y}_i^{(q)} | \theta_{p,q})$$

with respect to $\psi = \{\theta_{1,2}, \theta_{1,3}, \dots, \theta_{Q-1,Q}\}$, where $\mathbf{Y}_i^{(p)}$ and $\mathbf{Y}_i^{(q)}$ are the observations in \mathbf{Y}_i belonging to subsamples S_p and S_q , respectively.

- Similarly, the combination of all $\hat{\theta}_{p,q}$ into a single estimator $\hat{\theta}$ depends on the precise model and data structure.

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- └ The split-sample approach
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with respect to $\psi = (\theta_{1,2}, \theta_{1,3}, \dots, \theta_{Q-1,Q})$, where $\mathbf{Y}_i^{(p)}$ and $\mathbf{Y}_i^{(q)}$ are the observations in \mathbf{Y}_i belonging to subsamples S_p and S_q , respectively.

- Similarly, the combination of all $\hat{\theta}_{p,q}$ into a single estimator $\hat{\theta}$ depends on the precise model and data structure.

- without the pairwise fitting, we have to fit the model on the entire dataset, which is computationally infeasible when n is very large. By fitting the model on pairs of subsamples, we can reduce the computational burden while still accounting for the association between longitudinal observations.
- not gonna go into details here since this is more suitable for longitudinal data, which is not the focus of our presentation, but the idea is similar to dependent subsamples
- similarly, $\psi = \{\theta_{1,2}, \theta_{1,3}, \dots, \theta_{Q-1,Q}\} = \{\theta_{p,q} : p < q\}$
- what if both n and N are large? there is no mention of this in the literature, should we mention this?

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- lme4 and mgcv
- Why use bam()?
- When to use bam()?

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lme4

- an R package for fitting linear and generalized linear mixed-effects (multilevel) models⁵
- efficient, able to handle large sample sizes for simple model, and process hundreds of thousands observations on a typical laptop
- Modeling functions: `lmer()` and `glmer()`

mgcv

- an R package for fitting generalized additive model and generalized additive mixed models⁶
- Modeling functions: `gam()` and `bam()`

⁵Bates et al. 2015.

⁶S. N. Wood 2011.

Multilevel Models for Big Data

└ R Packages

└ lme4 and mgcv

└ R Packages – lme4 and mgcv

lme4

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- efficient, able to handle large sample sizes for simple model, and process hundreds of thousands of observations on a typical laptop
- Modeling functions: `lmer()` and `glmer()`

mgcv

- an R package for fitting generalized additive model and generalized additive mixed models⁴
- Modeling functions: `gam()` and `bsm()`

³Bates et al. 2015.

⁴S. N. Wood 2011.

can start by saying "in practice, optimization on large datasets are much more complex than what we have shown here, and a short presentation is not enough to cover all the details. we have two packages (used for large datasets) that we want to cover here, that is lme4 and mgcv"

lme4:

- is an R package for fitting linear and generalized linear mixed-effects (multilevel) models using 'Eigen' C++ library and S4 classes. (or just say using C++ library). Eigen is a high-level C++ template library for linear algebra that provides efficient, header-only classes for managing matrices, vectors, and numerical solvers. S4 is a formal system in R for object-oriented programming that uses strictly defined classes and methods to ensure data integrity and facilitate complex statistical modeling.
- It's computationally efficient, enabling it to handle very large sample sizes for simpler mixed models and to process hundreds of thousands of observations with random effects on a typical laptop.
- `lmer()`: fits linear multilevel model using restricted maximum likelihood (REML) or maximum likelihood estimation. `glmer()`: fits generalized linear multilevel model, accommodating non-normal response distributions. basically, `lmer()` for linear models and `glmer()` for GLM

mgcv:

- is an R package for fitting generalized additive models (GAMs) and generalized additive mixed models (GAMMs) using penalized regression splines.
- `gam()`: fits generalized additive multilevel models using penalized regression splines with smooth terms that can incorporate multilevel structure through random effect splines. `bsm()`: a computationally efficient version of `gam()` optimized for very large datasets.

R Packages – Why use bam()?

- Same underlying model between `gam()` and `lme4`, with differences in parameter estimation
- How `bam()` works:
 - QR decomposition⁷
 - (i) Efficient fitting algorithm, (ii) Parallel computation, and (iii) Covariate discretization⁸
 - Efficient crossproduct matrix $X^T W X$ computation⁹
- Discretization on large datasets leads to tradeoff between accuracy and speed

⁷S. Wood, Goude, and Shaw 2015.

⁸S. Wood, Li, et al. 2017.

⁹Li and S. Wood 2020.

Multilevel Models for Big Data

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- The underlying model between `gam()` function and `lme4` is the same, with differences only in the way parameters are estimated.
- `bam()` employs parallelized computation on model matrix subsets and optional data discretization to extract minimal necessary information, enabling efficient estimation of large multilevel models.
- Discretization has negligible impact on parameter estimates (differing only at high decimal precision), but leads to dramatic speed improvements.

Multilevel Models for Big Data

R Packages

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⁹Li and S. Wood 2020.

QR decomposition

- QR decomposition is a method for decomposing a matrix into a lower triangular matrix and an upper triangular matrix.
- Fitting GAM $\hat{\beta} = (X^T X + \sum \lambda_j S_j)^{-1} X^T y$ becomes $\hat{\beta} = (R^T R + \sum \lambda_j S_j)^{-1} R^T R$ where $X = QR$, X is the design matrix, S_j is the penalty matrix, and λ_j are smoothing parameters.

(i) Efficient fitting algorithm, (ii) Parallel computation, and (iii) Covariate discretization

- (i) Efficient fitting algorithm: which required only basic easily parallelized matrix computations and a pivoted Cholesky decomposition
- (ii) Parallel computation: the use of a scalable parallel block pivoted Cholesky algorithm mentioned above
- (iii) Covariate discretization: an efficient approach to model matrix storage and computations with the model matrix, using discretized covariates. For example, there are only a finite number of site locations, site labels and elevations, temperature is only recorded to within $0.1^\circ C$ (or any precision), etc
- These three elements work together, and dropping any one of them leads to an increase in fitting time of an order of magnitude or more. also, mention that this is a new algorithm that is better than QR decomposition. 3 orders of magnitude faster than QR decomposition

Efficient crossproduct matrix $X^T W X$ computation

- the most expensive part of previous algorithm is the formation of the matrix crossproduct. this approach present a simple, novel and substantially more efficient approach to the computation of this cross product

R Packages – When to use `bam()`?

- In general, `lme4` is preferred due to easy syntax and robust estimation
- `bam()` is particularly useful for:
 - Complex models that exceed `lme4`'s capabilities
 - Incorporating smooth (nonlinear) terms
 - Large datasets with memory issues
 - Leveraging parallel computing resources

Multilevel Models for Big Data

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- `bam()` is particularly useful for:
 - Complex models that exceed `lme4`'s capabilities
 - Incorporating smooth (nonlinear) terms
 - Large datasets with memory issues
 - Leveraging parallel computing resources

- In general, `lme4` is preferred for most multilevel datasets due to its straightforward syntax and robust estimation methods.
- `bam()` is particularly useful when:
 - You have complicated structure that begins to bog down `lme4`
 - You want to add smooth terms¹
 - You have memory issues
 - You have a computing setup that can take advantage of `bam`

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- Large multilevel datasets pose significant computational challenges
- The split-sample approach offers a practical solution
- R packages like `lme4` and `mgcv` provide robust tools for fitting multilevel models
- Approach and tools selection depends on dataset and research questions

Multilevel Models for Big Data

└ Summary

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Summary

- Large multilevel datasets pose significant computational challenges
- The split-sample approach offers a practical solution
- R packages like `lme4` and `mgcv` provide robust tools for fitting multilevel models
- Approach and tools selection depends on dataset and research questions

- However, large multilevel datasets pose significant computational challenges, including memory constraints and slow estimation times.
- The split-sample approach offers a practical solution by partitioning data into manageable subsamples, enabling efficient model fitting while retaining key statistical properties.
- R packages like `lme4` and `mgcv` provide robust tools for fitting multilevel models, with `bam()` in `mgcv` being particularly suited for very large datasets due to its computational efficiency.
- Choosing the right approach and tools depends on the specific characteristics of the dataset and the research questions at hand.

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