Multilevel Models for Big Data

Approaches for handling very large datasets

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Introduction — Multilevel Models

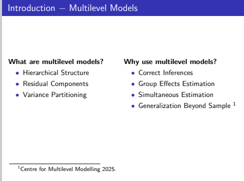
What are multilevel models?

- Hierarchical Structure
- Residual Components
- Variance Partitioning

Why use multilevel models?

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

[1] Centre 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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Statistical Model

$$y_n \sim \mathcal{N}(\mu_n, \sigma)$$
$$\mu_n = b_0 + b_1 x_{1n} + \ldots + b_p x_{pn} + \tilde{b}_{0j[n]} + \tilde{b}_{1j[n]} x_{1n} + \ldots + \tilde{b}_{pj[n]} x_{pn}$$

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
- $\tilde{b}_{pj[n]}$: 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 sizes[2]
- Design matrix construction[3]

[2] Clark 2019; Speelman, Heylen, and Geeraerts 2018.
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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 $\ell(\boldsymbol{\theta}) = \sum_i \ell(\boldsymbol{y_i}|\boldsymbol{\theta})$ where $\boldsymbol{y_i}$ is the vector of all observations in group i
- Replaces the log-likelihood contribution $\ell(\boldsymbol{y_i}|\boldsymbol{\theta})$ by a weighted sum of log-likelihood contributions for sub-vectors $\boldsymbol{Y_i}^{(s)}$
- More specifically, the pseudo-log-likelihood function:

$$p\ell(\psi) = \sum_i \sum_s \delta_s \, \ell(\boldsymbol{y_i}^{(s)}|\psi)$$

  is maximized instead with respect to ψ, which is not necessarily identical to $\boldsymbol{\theta}$
- Although $\hat{\psi}$ is not the MLE estimate, it still has similar properties such as consistency and asymptotic normality[4]

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- Now, how do we split $\boldsymbol{y_i}$ into sub-vectors $\boldsymbol{Y_i}^{(s)}$? 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

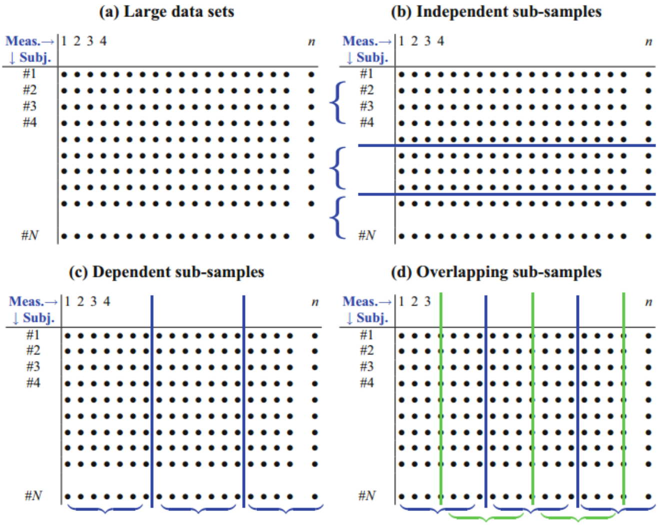

Figure 1: Graphical representation of different ways to split large samples

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 $m = 1, \ldots, M$
- In each subsample, the model is fitted, yielding an estimate $\hat{\boldsymbol{\theta}}_m$ of $\boldsymbol{\theta}$, equivalent to maximizing

$$p\ell(\boldsymbol{\psi}) = \sum_{m} \sum_{i \in S_m} \ell(\mathbf{Y}_{\boldsymbol{i}} | \boldsymbol{\theta}_m)$$

  with respect to $\boldsymbol{\psi} = \{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_M\}$
- All $\boldsymbol{\theta}_m$ are equal to $\boldsymbol{\theta}$, therefore the estimates $\hat{\boldsymbol{\theta}}_m$ can be averaged to obtain an overall estimate $\hat{\boldsymbol{\theta}}$

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- $\boldsymbol{\theta}_m$ are all equal to $\boldsymbol{\theta}$ 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 $m = 1, \ldots, M$
- Fitting the model on each subsample, equivalent to maximizing

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

  with respect to $\psi = \{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_M\}$, where $\boldsymbol{Y_i}^{(m)}$ is the observations in $\boldsymbol{Y_i}$ belonging to subsample S_m.
- All $\boldsymbol{\theta}_m$ are not necessarily equal to $\boldsymbol{\theta}$, therefore the combination of all $\hat{\boldsymbol{\theta}}_m$ into a single estimator $\hat{\boldsymbol{\theta}}$ depends on the precise model and data structure.

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- $\boldsymbol{\theta}_m$ are not necessarily equal to $\boldsymbol{\theta}$ 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 $\hat{\boldsymbol{\theta}}_m$ into a single estimator $\hat{\boldsymbol{\theta}}$ can be done using various methods, such as meta-analysis techniques, or by fitting a model to the estimates $\hat{\boldsymbol{\theta}}_m$ 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 $\{\boldsymbol{Y_i}^{(p)}, \boldsymbol{Y_i}^{(q)}\}$ by $\boldsymbol{\theta}_{p,q}$, fitting the models on all pairs is equivalent to maximizing

$$p\ell(\psi) = \sum_{p<q} \sum_{i} \ell(\boldsymbol{Y_i}^{(p)}, \boldsymbol{Y_i}^{(q)} | \boldsymbol{\theta}_{p,q})$$

  with respect to $\psi = \{\boldsymbol{\theta}_{1,2}, \boldsymbol{\theta}_{1,3}, \ldots, \boldsymbol{\theta}_{Q-1,Q}\}$, where $\boldsymbol{Y_i}^{(p)}$ and $\boldsymbol{Y_i}^{(q)}$ are the observations in $\boldsymbol{Y_i}$ belonging to subsamples S_p and S_q, respectively.
- Similarly, the combination of all $\hat{\boldsymbol{\theta}}_{p,q}$ into a single estimator $\hat{\boldsymbol{\theta}}$ depends on the precise model and data structure.

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- Similarly, the combination of all $\hat{\boldsymbol{\theta}}_{p,q}$ into a single estimator $\hat{\boldsymbol{\theta}}$ 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, $\boldsymbol{\psi} = \{\boldsymbol{\theta}_{1,2}, \boldsymbol{\theta}_{1,3}, \ldots, \boldsymbol{\theta}_{Q-1,Q}\} = \{\boldsymbol{\theta}_{p,q} : p < q\}$
- 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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R Packages — `lme4` and `mgcv`

`lme4`

- an R package for fitting linear and generalize linear mixed-effects (multilevel) models[5]
- 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 models[6]
- Modeling functions: `gam()` and `bam()`

[5] Bates et al. 2015.

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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. `bam()`: 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 decomposition[7]
  - (i) Efficient fitting algorithm, (ii) Parallel computation, and (iii) Covariate discretization[8]
  - Efficient crossproduct matrix $X^\top WX$ computation[9]
- Discretization on large datasets leads to tradeoff between accuracy and speed

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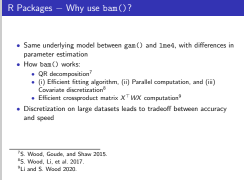

- The underlying model between `gam()` function and `lme4` is the same, with differences only in the way parameters are estimated.
- `bam()` employs parallelized computation on model matrix subsets and optional data discretization to extract minimal necessary information, enabling efficient estimation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

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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 decompostion
- (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 $X^\top WX$ 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

R Packages — When to use bam()?

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- bam() is particularly useful for:
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  - 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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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

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- 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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