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]

Statistical Model

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

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

[1] Centre for Multilevel Modelling 2025.

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.

[3] S. Wood, Goude, and Shaw 2015.

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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]

[4] Clark 2019.

The split-sample approach — Graphical representation

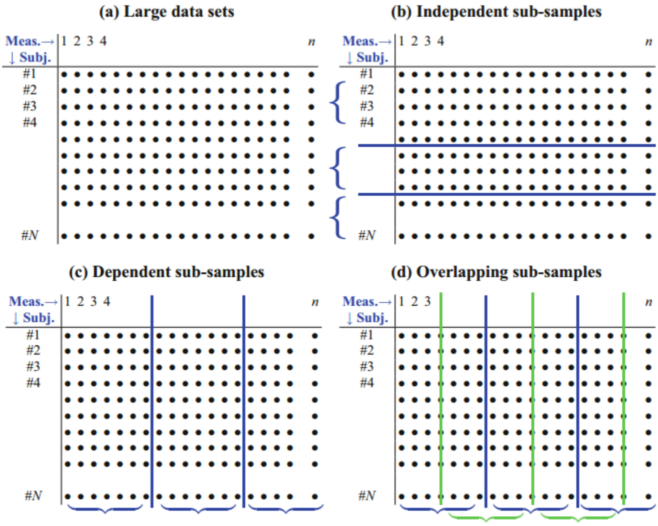

Figure 1: Graphical representation of different ways to split large samples

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 $\hat{\boldsymbol{\theta}}$

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.

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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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.

[6] S. N. Wood 2011.

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

[7] S. Wood, Goude, and Shaw 2015.
[8] S. Wood, Li, et al. 2017.
[9] Li and S. Wood 2020.

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

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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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