A Proportional Random Effect Block Bootstrap for Highly Unbalanced Clustered Data

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Overview

Motivation

Motivation

Figure: Different ioniser designs used in the Oman rainfall enhancement trial.

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Oman rainfall enhancement trial dataset (2013-2018):

- Unit of observation: Rain gauges nested within day (i.e., days as clusters)
- Response: Log-transformed rainfall
- Covariates: Orographic covariates (e.g., elevation), meteorological covariates (e.g., temperature), and binary indicators of exposure to each of ten ionizer (H1-H10)

Research Question: Does exposure to an operating ionizer increases rainfall at a gauge?

Motivation (Cont'd)

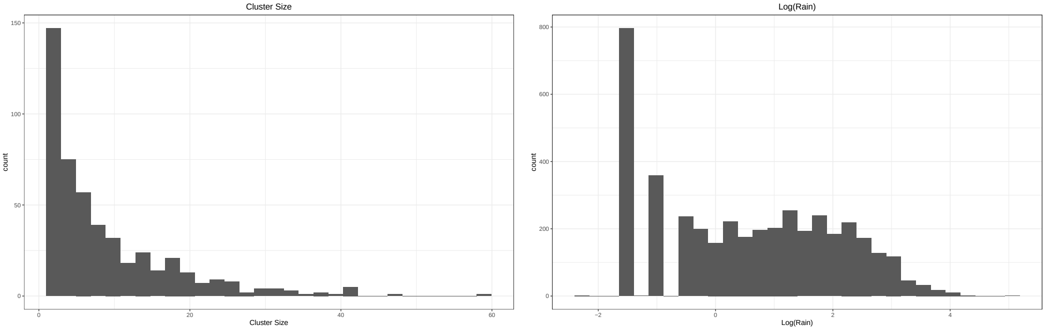


Figure: Histograms of cluster sizes (left) and log-transformed rainfall (right) in the Oman rainfall enhancement trial data.

Motivation (Cont'd)

Linear mixed model (LMM, Pinheiro and Bates, 2000; Bates et al., 2015) used to model log-rainfall.

- Need to estimate attribution and sample average treatment effect (SATE) - complicated functions of model parameters
- Perform bootstrap inference on the attribution and SATE

Existing bootstrap methods for LMM:

- Parametric Bootstrap (Butar and Lahiri, 2003)
  - Easy to implement, but sensitive to stochastic assumptions of the model
- Random Effect Block (REB) Bootstrap (Chambers and Chandra, 2013)
  - Semiparametric bootstrap that is less sensitive to stochastic assumption
  - Implicitly assumes balanced clusters

Motivation (Cont'd)

Another line of bootstrap methods for clustered data, which does not depend on LMM:

- Cluster Bootstrap (Davison and Hinkley, 1997; McCullagh, 2000)
  - Bootstrap sampling of cluster-level response vectors and model matrices, rather than unit-level
- Generalized Cluster Bootstrap (Field et al., 2010; Pang and Welsh, 2014)
  - Bootstrap sampling of weights for estimators defined as solutions to weighted estimating functions.

Model Set-Up

Model Set-Up

Let $i = 1, \cdots, D$ denote clusters and $j = 1, \cdots, n_i$ denote units within clusters with n_i representing cluster sizes. The linear mixed model is given as:

$$y_{ij} = \boldsymbol{x}_{ij}^\top \boldsymbol{\beta} + u_i + e_{ij}, \forall i, j \tag{1}$$

- y_{ij} = response, $\boldsymbol{x}_{ij}$ = covariates, $\boldsymbol{\beta}$ = fixed effect
- $u_i \overset{i.i.d.}{\sim} (0, \sigma_u^2)$ are cluster-level random intercepts
- $e_{ij} \overset{i.i.d.}{\sim} (0, \sigma_e^2)$ are unit-level error terms

Total sample size $N = \sum_{i=1}^{D} n_i$, we are interested in comparing the bootstraps under two cases:

- Balanced: $n_i = N/D$ for all $i = 1, \cdots, D$
- Highly Unbalanced: $n_i = 1$ for some clusters while other clusters have $n_i > 50$

Model Set-Up

Often convenient to rewrite (1) into an equivalent vector form:

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{Z}\boldsymbol{u} + \boldsymbol{e} \tag{2}$$

- $\boldsymbol{y} = (\boldsymbol{y}_1, \cdots, \boldsymbol{y}_D)^\top$ and $\boldsymbol{X} = (\boldsymbol{X}_1^\top, \cdots, \boldsymbol{X}_D^\top)^\top$ are obtained by stacking $\boldsymbol{y}_i$ response vectors and $\boldsymbol{X}_i$ model matrices
- $\boldsymbol{Z} = \mathrm{diag}(\boldsymbol{1}_{n_1}, \cdots, \boldsymbol{1}_{n_D})$ is matrix of cluster indicators
- $\boldsymbol{u} = (u_1, \cdots, u_D)^\top \sim (\boldsymbol{0}_D, \sigma_u^2 \boldsymbol{I}_D)$ and $\boldsymbol{e} = (\boldsymbol{e}_1, \cdots, \boldsymbol{e}_D)^\top \sim (\boldsymbol{0}_N, \sigma_e^2 \boldsymbol{I}_N)$ are obtained by stacking u_i random intercepts and $\boldsymbol{e}_i$ error vectors.

Typically estimated using maximum likelihood (ML) or restricted maximum likelihood (REML, Patterson and Thompson, 1971; Harville, 1977; Bates et al., 2015), with resulting estimates denoted as $\hat{\boldsymbol{\theta}} = (\hat{\boldsymbol{\beta}}, \hat{\sigma}_u^2, \hat{\sigma}_e^2)^\top$.

Proportional Random Effect Block (PREB) and Modified REB (MREB) Bootstrap

PREB Bootstrap

Existing bootstrap methods consider different ways of generating bootstrap samples u_i^* and e_{ij}^* based on the estimated $\hat{\boldsymbol{\theta}}$, to construct $y_{ij}^* = \boldsymbol{x}_{ij}^\top \hat{\boldsymbol{\beta}} + u_i^* + e_{ij}^*$

- Parametric bootstrap: generate u_i^* and e_{ij}^* from normal distributions with zero mean and estimated variances $\hat{\sigma}_u^2$ and $\hat{\sigma}_e^2$, respectively.
- REB bootstrap: compute marginal residuals $r_{ij} = y_{ij} - \boldsymbol{x}_{ij}^\top \hat{\boldsymbol{\beta}}$ first, then sample u_i^* and e_{ij}^* from functions of these marginal residuals.

Our proposed PREB bootstrap is similar to REB bootstrap, with three variants:

- Simple PREB bootstrap (PREB-0)
- Prescaled PREB bootstrap (PREB-1)
- Postscaled PREB bootstrap (PREB-2)

Prescaled PREB-1 Bootstrap

1. Compute residuals
   - Marginal residuals $r_{ij} = y_{ij} - \boldsymbol{x}_{ij}^\top \hat{\boldsymbol{\beta}}$
   - Cluster-level average residuals $\hat{u}_i = n_i^{-1} \sum_{j=1}^{n_i} r_{ij}$
   - Unit-level residuals as $\hat{e}_{ij} = r_{ij} - \hat{u}_i$
2. Reflating:
   - $\hat{u}_i^{sc} = \hat{u}_i^c \frac{\hat{\sigma}_u}{\sqrt{D^{-1} \sum_{i'=1}^{D} (\hat{u}_{i'}^c)^2}}$, where $\hat{u}_i^c = \hat{u}_i - D^{-1} \sum_{i'=1}^{D} \hat{u}_{i'}$
   - $\hat{e}_{ij}^s = \hat{e}_{ij} \frac{\hat{\sigma}_e}{\sqrt{N^{-1} \sum_{i'=1}^{D} \sum_{j'=1}^{n_{i'}} \hat{e}_{i'j'}^2}}$
3. Bootstrap cluster effects u_i
   - $u_i^* = \mathrm{SRSWR}((\hat{u}_1^{sc}, \cdots, \hat{u}_D^{sc}), 1)$
4. Bootstrap unit-level residuals $\boldsymbol{e}_i^* = (e_{i1}^*, \cdots, e_{in_i}^*)^\top$
   - First, sample the donor cluster $d_i = \mathrm{PPSWR}((1, \cdots, D), (n_1/N, \cdots, n_D/N), 1)$
   - Sample within the donor cluster: $\boldsymbol{e}_i^* = \mathrm{SRSWR}((\hat{e}_{d_i 1}^s, \cdots, \hat{e}_{d_i n_{d_i}}^s), n_i)$
5. Construct bootstrapped response
   - $y_{ij}^* = \boldsymbol{x}_{ij}^\top \hat{\boldsymbol{\beta}} + u_i^* + e_{ij}^*$

Prescaled PREB-1 Bootstrap

- Repeat Steps 2a–2d to obtain bootstrap replicates of $\hat{\boldsymbol{\theta}}^*$
  - Enables performing inference, e.g., constructing bootstrap percentile confidence intervals
- Reflating $\hat{u}_i$ to $\hat{u}_i^{sc}$ and $\hat{e}_{ij}$ to $\hat{e}_{ij}^{s}$ (together with PPS sampling of d_i) ensures that, for general cluster sizes n_i,
  - $\mathrm{E}^*(u_i^*) = 0$, $\mathrm{E}^*(e_{ij}^*) = 0$, where $\mathrm{E}^*(\cdot)$ is the bootstrap expectation operator.
  - $\mathrm{var}^*(u_i^*) = \hat{\sigma}_u^2$, $\mathrm{var}^*(e_{ij}^*) = \hat{\sigma}_e^2$, where $\mathrm{var}^*(\cdot)$ is the bootstrap variance operator
- Only requires correct specification of the fixed effect structure to calculate the marginal residuals $r_{ij} = y_{ij} - \boldsymbol{x}_{ij}^\top \hat{\boldsymbol{\beta}}$

Modified REB-1 (MREB-1) Bootstrap

1. Compute residuals
   - Marginal residuals $r_{ij} = y_{ij} - \boldsymbol{x}_{ij}^\top \hat{\boldsymbol{\beta}}$
   - Cluster-level average residuals $\hat{u}_i = n_i^{-1} \sum_{j=1}^{n_i} r_{ij}$
   - Unit-level residuals as $\hat{e}_{ij} = r_{ij} - \hat{u}_i$
2. Reflating:
   - $\hat{u}_i^{sc} = \hat{u}_i^c \frac{\hat{\sigma}_u}{\sqrt{D^{-1} \sum_{i'=1}^{D} (\hat{u}_{i'}^c)^2}}$, where $\hat{u}_i^c = \hat{u}_i - D^{-1} \sum_{i'=1}^{D} \hat{u}_{i'}$
   - $\tilde{e}_{ij}^s = \hat{e}_{ij} \frac{\hat{\sigma}_e}{\sqrt{\sum_{i'=1}^{D} \sum_{j'=1}^{n_{i'}} D^{-1} n_{i'}^{-1} \hat{e}_{i'j'}^2}}$
3. Bootstrap cluster effects u_i
   - $u_i^* = \mathrm{SRSWR}((\hat{u}_1^{sc}, \cdots, \hat{u}_D^{sc}), 1)$
4. Bootstrap unit-level residuals $\boldsymbol{e}_i^* = (e_{i1}^*, \cdots, e_{in_i}^*)^\top$
   - First, sample the donor cluster $d_i = \mathrm{SRSWR}((1, \cdots, D), 1)$
   - Sample within the donor cluster: $\boldsymbol{e}_i^* = \mathrm{SRSWR}((\tilde{e}_{d_i 1}^s, \cdots, \tilde{e}_{d_i n_{d_i}}^s), n_i)$
5. Construct bootstrapped response
   - $y_{ij}^* = \boldsymbol{x}_{ij}^\top \hat{\boldsymbol{\beta}} + u_i^* + e_{ij}^*$

Comparison among PREB-1, MREB-1 and REB-1

	PREB-1	MREB-1	REB-1
Cluster-level Random Effect	$\hat{u}_i^{sc}$	$\hat{u}_i^{sc}$	$\hat{u}_i^{cs}$
Donor Cluster Sampling Scheme	PPSWR	SRSWR	SRSWR
Unit-level Residuals	$\hat{e}_{ij}^s$	$\tilde{e}_{ij}^s$	$\hat{e}_{ij}^s$
Balanced n_i	✓	✓	✓
Unbalanced n_i	✓	✓	×

- PREB-1 and MREB-1 are generalized cases of REB-1 to accommodate unbalanced n_i
- Centering before scaling $\hat{u}_i$
    - Should sample from $\hat{u}_i^{sc}$ instead of $\hat{u}_i^{cs}$
- Proper combinations of donor cluster sampling scheme and scaling of unit-level residuals
    - PPSWR + $\hat{e}_{ij}^s$ (with N^{-1}) in PREB-1
    - SRSWR + $\tilde{e}_{ij}^s$ (with $D^{-1}n_i^{-1}$) in MREB-1

Comparison among PREB-1, MREB-1 and REB-1

In fact, PREB-1, MREB-1 and REB-1 are all equivalent when n_i's are balanced i.e., $n_i = N/D$, because

- $\hat{u}_i^{sc} = \hat{u}_i^{cs}$, since they are mean-zero.

$$D^{-1}\sum_{i=1}^{D}\hat{u}_i = D^{-1}\sum_{i=1}^{D} n_i^{-1}\sum_{j=1}^{n_i} r_{ij} = N^{-1}\sum_{i=1}^{D}\sum_{j=1}^{N/D} r_{ij} = 0$$

- SRSWR = PPSWR, since the probabilities in PPSWR are $n_i/N = (N/D)/N = 1/D$.
- $\hat{e}_{ij}^s = \tilde{e}_{ij}^s$, as their denominators of scaling factor are equal.

$$\sqrt{N^{-1}\sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}}\hat{e}_{i'j'}^2} = \sqrt{\sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} D^{-1} n_{i'}^{-1}\hat{e}_{i'j'}^2}$$

Simple PREB-0 and Postscaled PREB-2 Bootstrap

PREB-0: Does not consider reflating, i.e., by directly sampling from $\hat{u}_i$ and $\hat{e}_{ij}$

PREB-2: Post-processes bootstrap replicates $\hat{\boldsymbol{\theta}}^*$ from PREB-0

- Modifying the bootstrap distributions of logarithm of $\hat{\sigma}_u^{2*}$ and $\hat{\sigma}_e^{2*}$ to be empirically uncorrelated.
- Then, apply mean and ratio corrections to center:
  - $\hat{\boldsymbol{\beta}}^*$ at $\hat{\boldsymbol{\beta}}$
  - $(\hat{\sigma}_u^{2*}, \hat{\sigma}_e^{2*})$ at $(\hat{\sigma}_u^2, \hat{\sigma}_e^2)$

Consistency Properties of PREB and MREB Bootstrap

Consistency Requirements

Requirement for consistency of bootstrap estimator $\hat{\boldsymbol{\theta}}^*$ based on ML estimating function is then

$$\mathrm{E}^* \left\{ \frac{\partial l(\hat{\boldsymbol{\theta}}; \boldsymbol{y}^*)}{\partial \boldsymbol{\theta}} \right\} = \mathbf{0}_{p+2}$$

which is equivalent to

- $\mathrm{E}^*(u_i^*) = 0$, $\mathrm{E}^*(e_{ij}^*) = 0$
- $\mathrm{E}^*(u_i^{*2}) = \hat{\sigma}_u^2$, $\mathrm{E}^*(e_{ij}^{*2}) = \hat{\sigma}_e^2$

	PREB-1	MREB-1	REB-1	PREB-0
Balanced n_i	✓	✓	✓	×
Unbalanced n_i	✓	✓	×	×

Table: PREB-2 not applicable

Simulation Studies

Simulation Settings

Data generating process follows a LMM:

$$y_{ij} = \beta_0 + \beta_1 x_{ij} + u_i + e_{ij}$$

- Covariate: $x_{ij} \sim \text{Uniform}(0, 1)$
- Number of clusters: $D = 100$
- Total 500 simulated datasets for each setting

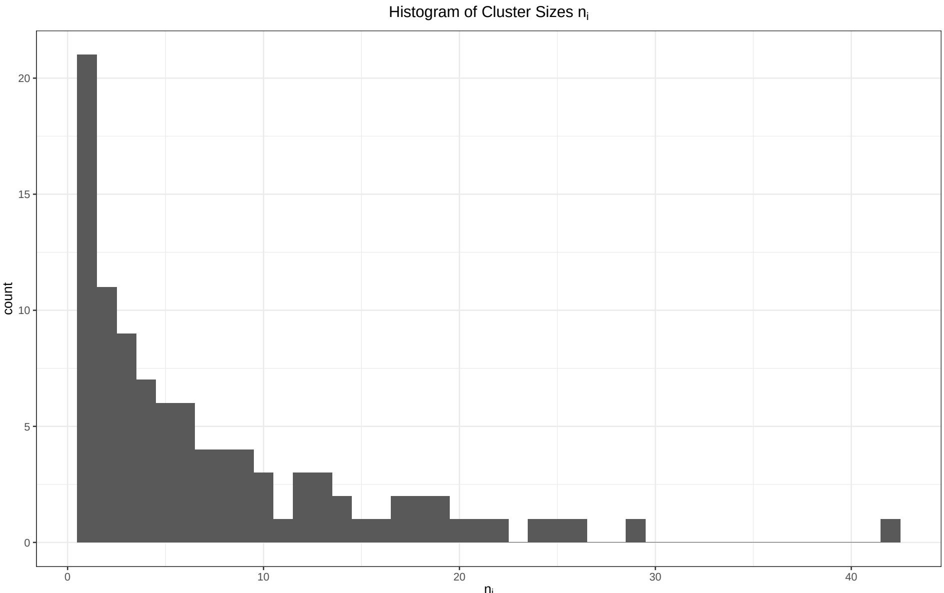
Distribution of u_i and e_{ij}

- Normal: $u_i \overset{i.i.d.}{\sim} N(0, \sigma_u^2)$, $e_{ij} \overset{i.i.d.}{\sim} N(0, \sigma_e^2)$, where $\sigma_u = 0.2$ and $\sigma_e = 0.4$
- Chi-squared: $u_i \overset{i.i.d.}{\sim} \sigma_u\{(\chi_1^2 - 1)/\sqrt{2}\}$, $e_{ij} \overset{i.i.d.}{\sim} \sigma_e\{(\chi_1^2 - 1)/\sqrt{2}\}$

Cluster size setting

- Balanced: $n_i = 20$ for all $i = 1, \cdots, D$
- Unbalanced: n_i summarized in Figure 3

Simulation Settings (Cont'd)



Simulation Settings (Cont'd)

Comparison of the following bootstrap methods, each with 500 bootstrap replicates:

- PREB bootstraps: PREB-0, PREB-1, PREB-2
- MREB-1
- REB bootstraps: REB-0, REB-1, REB-2
- Parametric bootstrap

Evaluation metric:

- Empirical coverage rate of 95% bootstrap percentile confidence intervals
- Parameters assessed: $(\beta_0, \beta_1, \sigma_u^2, \sigma_e^2)$

Results for Normal Distribution

Balanced: Comparable performances among all methods

	PREB-0	PREB-1	PREB-2	MREB-1	REB-0	REB-1	REB-2	Parametric
β_0	0.938	0.916	0.936	0.926	0.942	0.914	0.936	0.912
β_1	0.926	0.932	0.924	0.932	0.924	0.932	0.924	0.938
σ_u^2	0.870	0.924	0.918	0.920	0.870	0.930	0.922	0.942
σ_e^2	0.854	0.994	0.992	0.998	0.860	0.994	0.992	0.958

Unbalanced: Undercoverage for β_1 and σ_e^2 using REB bootstraps

	PREB-0	PREB-1	PREB-2	MREB-1	REB-0	REB-1	REB-2	Parametric
β_0	0.972	0.950	0.988	0.946	0.956	0.916	0.972	0.956
β_1	0.938	0.950	0.938	0.956	0.896	0.910	0.896	0.954
σ_u^2	0.014	0.954	0.884	0.968	0.014	0.944	0.860	0.910
σ_e^2	0.680	1.000	1.000	1.000	0.012	0.252	1.000	0.936

Results for Chi-Squared Distribution

Balanced: Undercoverage for σ_u^2 and σ_e^2 using parametric bootstrap

	PREB-0	PREB-1	PREB-2	MREB-1	REB-0	REB-1	REB-2	Parametric
β_0	0.960	0.944	0.956	0.938	0.954	0.948	0.954	0.946
β_1	0.944	0.950	0.944	0.954	0.938	0.950	0.944	0.950
σ_u^2	0.938	0.830	0.840	0.836	0.930	0.842	0.852	0.618
σ_e^2	0.934	0.978	0.978	0.974	0.938	0.974	0.976	0.540

Unbalanced: Undercoverage for β_1 and σ_e^2 using REB bootstraps, undercoverage for σ_u^2 and σ_e^2 using parametric bootstrap.

	PREB-0	PREB-1	PREB-2	MREB-1	REB-0	REB-1	REB-2	Parametric
β_0	0.948	0.926	0.966	0.926	0.924	0.886	0.948	0.942
β_1	0.928	0.934	0.926	0.932	0.876	0.892	0.874	0.936
σ_u^2	0.392	0.886	0.798	0.922	0.340	0.890	0.784	0.708
σ_e^2	0.908	0.990	0.984	0.998	0.468	0.768	1.000	0.584

Application

Application: Oman Rainfall Enhancement Trial Dataset

Analysis of rainfall enhancement trial data (2013–2018):

$$y_{ij} = \boldsymbol{x}_{ij,non-ionizer}^{\top} \boldsymbol{\beta}_{non-ionizer} + \boldsymbol{x}_{ij,ionizer}^{\top} \boldsymbol{\beta}_{ionizer} + u_i + e_{ij},$$

- i = day (cluster), j = rain gauge with positive rainfall
- y_{ij} = log-transformed rainfall
- $\boldsymbol{x}_{ij,non-ionizer}$ = orographic covariates (e.g., elevation)
- $\boldsymbol{x}_{ij,ionizer}$ = indicators for exposure to active ionizer
- $D = 488$ clusters, with highly unbalanced cluster sizes ranging from $n_i = 1$ to $n_i = 58$
- $N = 4168$ total gauge-day observations

Application: Oman Rainfall Enhancement Trial Dataset

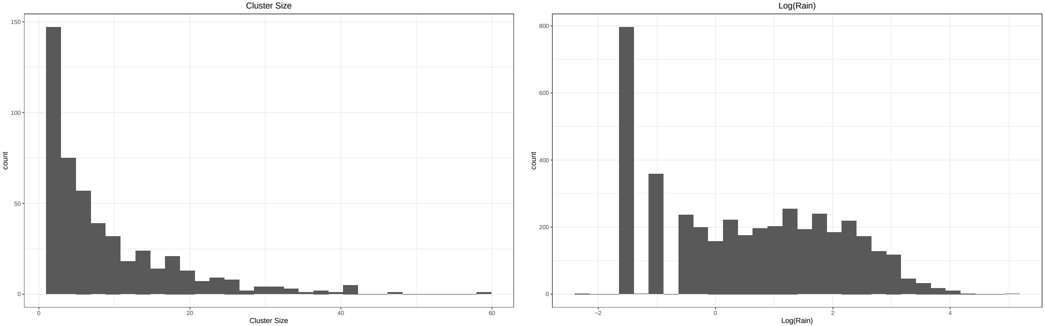
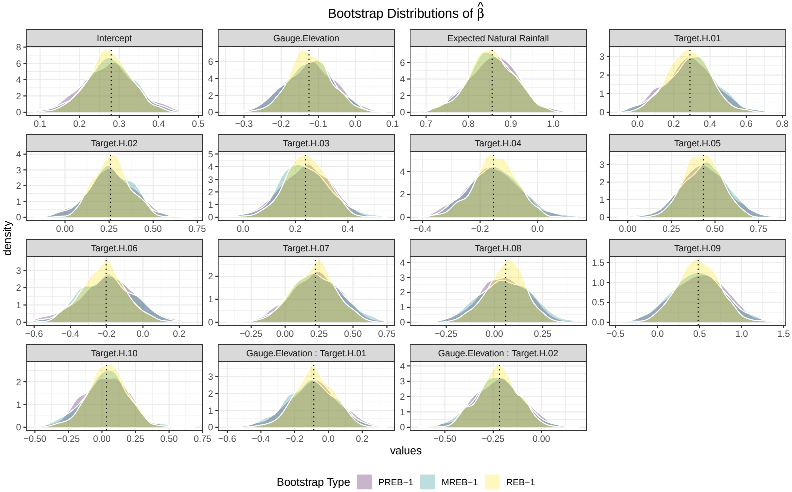


Figure: Histograms of cluster sizes (left) and log-transformed rain (right) in the Oman rainfall enhancement trial data.

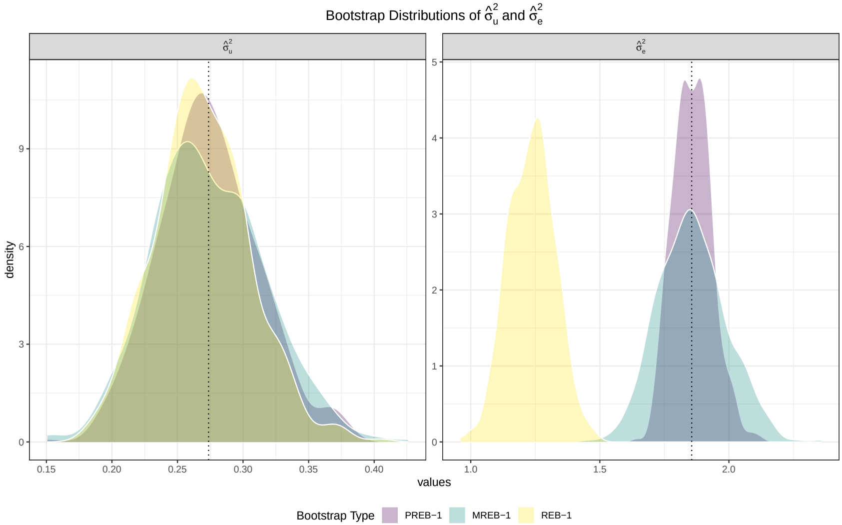
Bootstrap Distributions for $\hat{\beta}$

PREB-1 and MREB-1 bootstrap distributions are consistently more dispersed than REB-1



Bootstrap Distributions for $(\hat{\sigma}_u^2, \hat{\sigma}_e^2)$

REB-1 bootstrap distribution for $\hat{\sigma}_e^2$ exhibits clear negative bias.



SATE and Attribution

- Sample average treatment effect (SATE) estimate:

$$\frac{\sum_{(i,j)} 1_{\{\boldsymbol{x}_{ij,ioniser} \neq \mathbf{0}\}} \boldsymbol{x}_{ij,ioniser}^{\top} \hat{\boldsymbol{\beta}}_{ioniser}}{\sum_{(i,j)} 1_{\{\boldsymbol{x}_{ij,ioniser} \neq \mathbf{0}\}}}$$

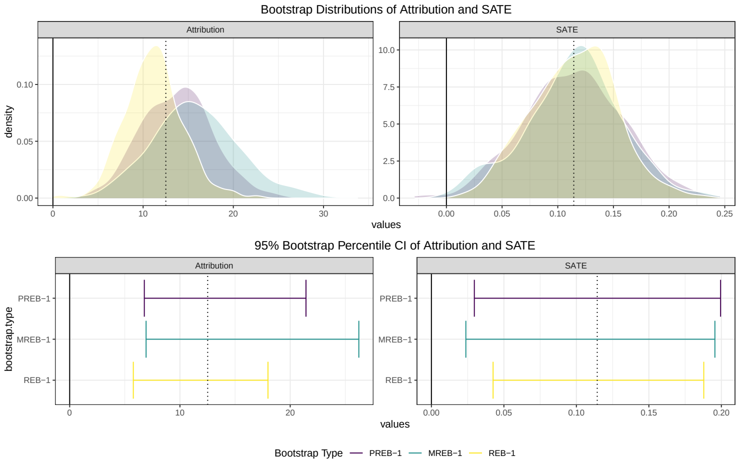
- Attribution = Percentage increase/decrease in rainfall attributed to the ionisers:

$$100\% \times \frac{\sum_{(i,j)} \exp(y_{ij})\{1 - \kappa^{-1}(\boldsymbol{y}, \hat{\boldsymbol{\theta}}) \exp(-\boldsymbol{x}_{ij,ioniser}^{\top} \hat{\boldsymbol{\beta}}_{ioniser})\}}{\sum_{(i,j)} \exp(y_{ij}) \kappa^{-1}(\boldsymbol{y}, \hat{\boldsymbol{\theta}}) \exp(-\boldsymbol{x}_{ij,ioniser}^{\top} \hat{\boldsymbol{\beta}}_{ioniser})}$$

  - $\kappa^{-1}(\boldsymbol{y}, \hat{\boldsymbol{\theta}})$ is a smearing-type adjustment to account for bias introduced by exponentiating log-rainfall to obtain raw-scale rainfall (Chambers et al., 2022)
  - Provides *an estimate of the precipitation increase along with the confidence intervals in which the true impact lies* (WMO, 2010).

Bootstrap Inference for SATE and Attribution

PREB-1 and MREB-1 bootstrap distributions are more dispersed than REB-1, but all methods yield significant positive ioniser effects.



Conclusion and Future Work

Conclusion and Future Work

- PREB-1 and MREB-1 are useful for highly unbalanced clustered data with potentially non-normal random effects and error terms.
- Core ideas:
  - Performing proper 'reflating' on $\hat{u}_i$ and $\hat{e}_{ij}$ before bootstrapping
  - Block bootstrapping of unit-level residuals, by treating clusters as blocks
  - Using appropriate combination of sampling scheme for donor cluster and scaling for unit-level residuals
- Extensions:
  - Bootstrap inference on linear combinations of fixed effects and random effects $\boldsymbol{l}_i^\top \boldsymbol{\beta} + u_i$ (known as cluster-level mixed effects parameters, see Reluga et al., 2023, 2024)
  - Extend from LMM to M-quantile based model (e.g., Dawber and Chambers, 2019)

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THE END

THANKS!

Appendix

PREB-1 - u_i^*

- $u_i^* = \text{SRSWR}((\hat{u}_1^{sc}, \cdots, \hat{u}_D^{sc}), 1)$ where $\hat{u}_i^{sc} = \frac{\hat{\sigma}_u}{\sqrt{D^{-1}\sum_{i'=1}^{D}(\hat{u}_i^c)^2}}\hat{u}_i^c$ and $\hat{u}_i^c = \hat{u}_i - D^{-1}\sum_{i'=1}^{D}\hat{u}_{i'}$

$$\begin{aligned}
\mathrm{E}^*(u_i^*) &= \sum_{i'=1}^{D}\frac{1}{D}\hat{u}_{i'}^{sc} = \sum_{i'=1}^{D}\frac{1}{D}\frac{\hat{\sigma}_u}{\sqrt{\frac{1}{D}\sum_{l=1}^{D}\left(\hat{u}_l^c\right)^2}}\hat{u}_{i'}^c \\
&= \frac{\hat{\sigma}_u}{\sqrt{\frac{1}{D}\sum_{l=1}^{D}\left(\hat{u}_l^c\right)^2}}\frac{1}{D}\sum_{i'=1}^{D}\left(\hat{u}_{i'} - \frac{1}{D}\sum_{l=1}^{D}\hat{u}_l\right) = 0,
\end{aligned}$$

$$\mathrm{E}^*(u_i^{*2}) = \sum_{i'=1}^{D}\frac{1}{D}\left(\hat{u}_{i'}^{sc}\right)^2 = \frac{\hat{\sigma}_u^2}{\frac{1}{D}\sum_{l=1}^{D}\left(\hat{u}_l^c\right)^2}\frac{1}{D}\sum_{i'=1}^{D}\left(\hat{u}_{i'}^c\right)^2 = \hat{\sigma}_u^2,$$

PREB-1 - e^*_{ij}

- $d_i = \text{PPSWR}((1, \cdots, D), (n_1/N, \cdots, n_D/N), 1)$, then $\boldsymbol{e}_i^* = \text{SRSWR}((\hat{e}^s_{d_i 1}, \cdots, \hat{e}^s_{d_i n_{d_i}}), n_i)$, where $\hat{e}^s_{ij} = \frac{\hat{\sigma}_e}{\sqrt{N^{-1}\sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \hat{e}^2_{i'j'}}}\hat{e}_{ij}$ and $\hat{e}_{ij} = r_{ij} - n_i^{-1}\sum_{j'=1}^{n_i} r_{ij'}$

$$
\begin{aligned}
\text{E}^*(e^*_{ij}) &= \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{n_{i'}}{N}\frac{1}{n_{i'}}\hat{e}^s_{i'j'} \\
&= \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{n_{i'}}{N}\frac{1}{n_{i'}}\frac{\hat{\sigma}_e}{\sqrt{\frac{1}{N}\sum_{l=1}^{D}\sum_{m=1}^{n_l}\hat{e}^2_{lm}}}\hat{e}_{i'j'} \\
&= \frac{\hat{\sigma}_e}{\sqrt{\frac{1}{N}\sum_{l=1}^{D}\sum_{m=1}^{n_l}\hat{e}^2_{lm}}}\sum_{i'=1}^{D}\frac{n_{i'}}{N}\frac{1}{n_{i'}}\sum_{j'=1}^{n_{i'}}\left(r_{i'j'} - \frac{1}{n'_i}\sum_{m=1}^{n_{i'}} r_{i'm}\right) \\
&= 0
\end{aligned}
$$

PREB-1 - e^*_{ij}

- $d_i = \mathrm{PPSWR}((1, \cdots, D), (n_1/N, \cdots, n_D/N), 1)$, then
  $\boldsymbol{e}_i^* = \mathrm{SRSWR}((\hat{e}^s_{d_i 1}, \cdots, \hat{e}^s_{d_i n_{d_i}}), n_i)$, where $\hat{e}^s_{ij} = \frac{\hat{\sigma}_e}{\sqrt{N^{-1}\sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \hat{e}^2_{i'j'}}} \hat{e}_{ij}$

$$
\begin{aligned}
\mathrm{E}^*(e^{*2}_{ij}) &= \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{n_{i'}}{N}\frac{1}{n_{i'}}\left(\hat{e}^s_{i'j'}\right)^2 \\
&= \frac{\hat{\sigma}^2_e}{\frac{1}{N}\sum_{l=1}^{D}\sum_{m=1}^{n_l}\hat{e}^2_{lm}} \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{n_{i'}}{N}\frac{1}{n_{i'}}\hat{e}^2_{i'j'} \\
&= \frac{\hat{\sigma}^2_e}{\frac{1}{N}\sum_{l=1}^{D}\sum_{m=1}^{n_l}\hat{e}^2_{lm}} \frac{1}{N}\sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \hat{e}^2_{i'j'} \\
&= \hat{\sigma}^2_e.
\end{aligned}
$$

MREB-1 - u_i^* and e_{ij}^*

Same procedure as PREB-1 in bootstrapping $u_i^* \implies$ also satisfies $\mathrm{E}^*(u_i^*) = 0$ and $\mathrm{E}^*(u_i^{*2}) = \hat{\sigma}_u^2$

- $d_i = \mathrm{SRSWR}((1, \cdots, D), 1)$, then $\boldsymbol{e}_i^* = \mathrm{SRSWR}((\tilde{e}^s_{d_i 1}, \cdots, \tilde{e}^s_{d_i n_{d_i}}), n_i)$, where $\tilde{e}^s_{ij} = \frac{\hat{\sigma}_e}{\sqrt{\sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} D^{-1} n_{i'}^{-1} \hat{e}^2_{i'j'}}} \hat{e}_{ij}$ and $\hat{e}_{ij} = r_{ij} - n_i^{-1}\sum_{j'=1}^{n_i} r_{ij'}$

$$
\begin{aligned}
\mathrm{E}^*(e_{ij}^*) &= \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{1}{D}\frac{1}{n_{i'}} \tilde{e}^s_{i'j'} = \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{1}{D}\frac{1}{n_{i'}} \frac{\hat{\sigma}_e}{\sqrt{\sum_{l=1}^{D}\sum_{m=1}^{n_l} \frac{1}{D}\frac{1}{n_l}\hat{e}^2_{lm}}} \hat{e}_{i'j'} \\
&= \frac{\hat{\sigma}_e}{\sqrt{\sum_{l=1}^{D}\sum_{m=1}^{n_l} \frac{1}{D}\frac{1}{n_l}\hat{e}^2_{lm}}} \sum_{i'=1}^{D} \frac{1}{D}\frac{1}{n_{i'}} \sum_{j'=1}^{n_{i'}} \left(r_{i'j'} - \frac{1}{n_{i'}} \sum_{m=1}^{n_{i'}} r_{i'm} \right) \\
&= 0
\end{aligned}
$$

MREB-1 - e^*_{ij}

- $d_i = \mathrm{SRSWR}((1,\cdots,D),1)$, then $\boldsymbol{e}^*_i = \mathrm{SRSWR}((\tilde{e}^s_{d_i 1},\cdots,\tilde{e}^s_{d_i n_{d_i}}),n_i)$, where $\tilde{e}^s_{ij} = \frac{\hat{\sigma}_e}{\sqrt{\sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} D^{-1} n_{i'}^{-1} \hat{e}^2_{i'j'}}}\hat{e}_{ij}$ and $\hat{e}_{ij} = r_{ij} - n_i^{-1}\sum_{j'=1}^{n_i} r_{ij'}$

$$
\begin{aligned}
\mathrm{E}^*(e^{*2}_{ij}) &= \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{1}{D}\frac{1}{n_{i'}}\left(\tilde{e}^s_{ij}\right)^2 \\
&= \frac{\hat{\sigma}^2_e}{\sum_{l=1}^{D}\sum_{m=1}^{n_l}\frac{1}{D}\frac{1}{n_l}\hat{e}^2_{lm}}\sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}}\frac{1}{D}\frac{1}{n_{i'}}\hat{e}^2_{i'j'} \\
&= \hat{\sigma}^2_e.
\end{aligned}
$$

REB-1 - u_i^*

- $u_i^* = \text{SRSWR}((\hat{u}_1^{cs}, \cdots, \hat{u}_D^{cs}), 1)$ where $\hat{u}_i^{cs} = \frac{\hat{\sigma}_u}{\sqrt{D^{-1}\sum_{i'=1}^{D}(\hat{u}_i)^2}}\hat{u}_i^c$ and $\hat{u}_i^c = \hat{u}_i - D^{-1}\sum_{i'=1}^{D}\hat{u}_{i'}$

$$
\begin{aligned}
\mathrm{E}^*(u_i^*) &= \sum_{i'=1}^{D}\frac{1}{D}\hat{u}_{i'}^{cs} = \sum_{i'=1}^{D}\frac{1}{D}\frac{\hat{\sigma}_u}{\sqrt{\frac{1}{D}\sum_{l=1}^{D}\left(\hat{u}_l\right)^2}}\hat{u}_{i'}^{c} \\
&= \frac{\hat{\sigma}_u}{\sqrt{\frac{1}{D}\sum_{l=1}^{D}\left(\hat{u}_l\right)^2}}\frac{1}{D}\sum_{i'=1}^{D}\left(\hat{u}_{i'} - \frac{1}{D}\sum_{l=1}^{D}\hat{u}_l\right) = 0
\end{aligned}
$$

REB-1 - u_i^*

- $u_i^* = \text{SRSWR}((\hat{u}_1^{cs}, \cdots, \hat{u}_D^{cs}), 1)$ where $\hat{u}_i^{cs} = \frac{\hat{\sigma}_u}{\sqrt{D^{-1}\sum_{i'=1}^{D}(\hat{u}_i)^2}}\hat{u}_i^c$ and $\hat{u}_i^c = \hat{u}_i - D^{-1}\sum_{i'=1}^{D}\hat{u}_{i'}$

$$
\begin{aligned}
\mathrm{E}^*(u_i^{*2}) &= \sum_{i'=1}^{D}\frac{1}{D}(\hat{u}_{i'}^{cs})^2 = \frac{\hat{\sigma}_u^2}{\frac{1}{D}\sum_{l=1}^{D}(\hat{u}_l)^2}\frac{1}{D}\sum_{i'=1}^{D}(\hat{u}_{i'}^c)^2 \\
&= \frac{\hat{\sigma}_u^2}{\frac{1}{D}\sum_{l=1}^{D}(\hat{u}_l)^2}\frac{1}{D}\sum_{i'=1}^{D}\left(\hat{u}_{i'} - \frac{1}{D}\sum_{l=1}^{D}\hat{u}_l\right)^2 \\
&= \hat{\sigma}_u^2 \text{ only when } n_i = N/D \text{ for } i = 1, \cdots, D,
\end{aligned}
$$

since $D^{-1}\sum_{l=1}^{D}\hat{u}_l = D^{-1}\sum_{l=1}^{D}n_l^{-1}\sum_{j=1}^{n_l}(y_{lj} - \boldsymbol{x}_{lj}^\top\hat{\boldsymbol{\beta}})$ is only equal to zero when $n_i = N/D$ for $i = 1, \cdots, D$.

REB-1 - e^*_{ij}

- $d_i = \text{SRSWR}((1, \cdots, D), 1)$, then $\boldsymbol{e}^*_i = \text{SRSWR}((\hat{e}^s_{d_i 1}, \cdots, \hat{e}^s_{d_i n_{d_i}}), n_i)$, where $\hat{e}^s_{ij} = \frac{\hat{\sigma}_e}{\sqrt{N^{-1}\sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \hat{e}^2_{i'j'}}}\hat{e}_{ij}$ and $\hat{e}_{ij} = r_{ij} - n_i^{-1}\sum_{j'=1}^{n_i} r_{ij'}$

$$
\begin{aligned}
\mathrm{E}^*(e^*_{ij}) &= \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{1}{D}\frac{1}{n_{i'}}\hat{e}^s_{i'j'} \\
&= \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{1}{D}\frac{1}{n_{i'}} \frac{\hat{\sigma}_e}{\sqrt{\frac{1}{N}\sum_{l=1}^{D}\sum_{m=1}^{n_l}\hat{e}^2_{lm}}}\hat{e}_{i'j'} \\
&= \frac{\hat{\sigma}_e}{\sqrt{\frac{1}{N}\sum_{l=1}^{D}\sum_{m=1}^{n_l}\hat{e}^2_{lm}}} \sum_{i'=1}^{D}\frac{1}{D}\frac{1}{n_{i'}}\sum_{j'=1}^{n_{i'}}\left(r_{i'j'} - \frac{1}{n'_i}\sum_{m=1}^{n_{i'}} r_{i'm}\right) \\
&= 0
\end{aligned}
$$

REB-1 - e_{ij}^*

- $d_i = \text{SRSWR}((1, \cdots, D), 1)$, then $\boldsymbol{e}_i^* = \text{SRSWR}((\hat{e}^s_{d_i 1}, \cdots, \hat{e}^s_{d_i n_{d_i}}), n_i)$, where $\hat{e}^s_{ij} = \frac{\hat{\sigma}_e}{\sqrt{N^{-1} \sum_{i'=1}^{D} \sum_{j'=1}^{n_{i'}} \hat{e}^2_{i'j'}}} \hat{e}_{ij}$ and $\hat{e}_{ij} = r_{ij} - n_i^{-1} \sum_{j'=1}^{n_i} r_{ij'}$

$$
\begin{aligned}
\mathrm{E}^*(e_{ij}^{*2}) &= \sum_{i'=1}^{D} \sum_{j'=1}^{n_{i'}} \frac{1}{D} \frac{1}{n_{i'}} \left(\hat{e}^s_{i'j'}\right)^2 \\
&= \frac{\hat{\sigma}_e^2}{\frac{1}{N} \sum_{l=1}^{D} \sum_{m=1}^{n_l} \hat{e}^2_{lm}} \sum_{i'=1}^{D} \sum_{j'=1}^{n_{i'}} \frac{1}{D} \frac{1}{n_{i'}} \hat{e}^2_{i'j'} \\
&= \hat{\sigma}_e^2, \text{ only when } n_i = N/D \text{ for } i = 1, \cdots, D
\end{aligned}
$$

PREB-0 - u_i^*

- $u_i^* = \text{SRSWR}((\hat{u}_1, \cdots, \hat{u}_D), 1)$ where
  $\hat{u}_i = n_i^{-1} \sum_{j=1}^{n_i} r_{ij} = n_i^{-1} \sum_{j=1}^{n_i} (y_{ij} - \boldsymbol{x}_{ij}^\top \hat{\boldsymbol{\beta}})$

$$
\begin{aligned}
\mathrm{E}^*(u_i^*) &= \sum_{i'=1}^{D} \frac{1}{D} \hat{u}_{i'} = \sum_{i'=1}^{D} \frac{1}{D} \frac{1}{n_{i'}} \sum_{j'=1}^{n_i'} r_{i'j'} \\
&= \sum_{i'=1}^{D} \frac{1}{D} \frac{1}{n_{i'}} \sum_{j'=1}^{n_{i'}} \left(y_{i'j'} - \boldsymbol{x}_{i'j'}^\top \hat{\boldsymbol{\beta}} \right) = 0, \text{ only when } n_i = N/D \; \forall i
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{E}^*(u_i^{*2}) &= \sum_{i'=1}^{D} \frac{1}{D} \hat{u}_{i'}^2 = \sum_{i'=1}^{D} \frac{1}{D} \left(\frac{1}{n_{i'}} \sum_{j'=1}^{n_{i'}} r_{i'j'} \right)^2 \\
&= \sum_{i'=1}^{D} \frac{1}{D} \frac{1}{n_{i'}^2} \left\{ \sum_{j'=1}^{n_{i'}} \left(y_{i'j'} - \boldsymbol{x}_{i'j'}^\top \hat{\boldsymbol{\beta}} \right) \right\}^2 \neq \hat{\sigma}_u^2.
\end{aligned}
$$

PREB-0 - e^*_{ij}

- $d_i = \text{PPSWR}((1,\cdots,D),(n_1/N,\cdots,n_D/N),1)$, then
  $\boldsymbol{e}^*_i = \text{SRSWR}((\hat{e}_{d_i 1},\cdots,\hat{e}_{d_i n_{d_i}}), n_i)$, where $\hat{e}_{ij} = r_{ij} - \hat{u}_i = r_{ij} - n_i^{-1}\sum_{j'=1}^{n_i} r_{ij'}$

$$
\begin{aligned}
\mathrm{E}^*(e^*_{ij}) &= \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{1}{D}\frac{1}{n_{i'}}\hat{e}_{i'j'} = \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{1}{D}\frac{1}{n_{i'}}\left(r_{i'j'} - \hat{u}_{i'}\right) \\
&= \sum_{i'=1}^{D}\frac{1}{D}\frac{1}{n_{i'}}\sum_{j'=1}^{n_{i'}}\left(r_{i'j'} - \frac{1}{n_{i'}}\sum_{l=1}^{n_{i'}} r_{i'l}\right) = 0, \ \text{ and} \\
\mathrm{E}^*(e^{*2}_{ij}) &= \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{1}{D}\frac{1}{n_{i'}}\hat{e}^2_{i'j'} = \sum_{i'=1}^{D}\sum_{j'=1}^{n_{i'}} \frac{1}{D}\frac{1}{n_{i'}}\left(r_{i'j'} - \hat{u}_{i'}\right)^2 \\
&= \sum_{i'=1}^{D}\frac{1}{D}\frac{1}{n_{i'}}\sum_{j'=1}^{n_{i'}}\left\{y_{i'j'} - \boldsymbol{x}^\top_{i'j'}\hat{\boldsymbol{\beta}} - \frac{1}{n_{i'}}\sum_{l=1}^{n_{i'}}\left(y_{i'l} - \boldsymbol{x}^\top_{i'l}\hat{\boldsymbol{\beta}}\right)\right\}^2 \neq \hat{\sigma}^2_e.
\end{aligned}
$$

PREB-2

- Modification of the PREB-0 bootstrap distributions $\{\hat{\boldsymbol{\theta}}^{*(b)} : b = 1, \cdots, B\}$ ensures that they are centered at the ML estimate $\hat{\boldsymbol{\theta}}$:

$$\frac{1}{B}\sum_{b=1}^{B}\hat{\boldsymbol{\beta}}^{**(b)} = \frac{1}{B}\sum_{b=1}^{B}\hat{\boldsymbol{\beta}}^{*(b)} - \sum_{l=1}^{B}\hat{\boldsymbol{\beta}}^{*(l)} + \hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}},$$

$$\frac{1}{B}\sum_{b=1}^{B}\hat{\sigma}_u^{2**(b)} = \frac{1}{B}\sum_{b=1}^{B}\hat{\sigma}_u^{2*(b)} \times \frac{\hat{\sigma}_u^2}{\frac{1}{B}\sum_{l=1}^{B}\hat{\sigma}_u^{2*(l)}} = \hat{\sigma}_u^2, \quad \text{and}$$

$$\frac{1}{B}\sum_{b=1}^{B}\hat{\sigma}_e^{2**(b)} = \frac{1}{B}\sum_{b=1}^{B}\hat{\sigma}_e^{2*(b)} \times \frac{\hat{\sigma}_e^2}{\frac{1}{B}\sum_{l=1}^{B}\hat{\sigma}_e^{2*(l)}} = \hat{\sigma}_e^2.$$

PREB-2

- However, these modifications do not necessarily provide valid estimators of the sampling variability of $\hat{\boldsymbol{\theta}}$.
- For example, the bootstrap variance of the k-th fixed effect coefficient $\{\hat{\beta}_k^{**(b)} : b = 1, \cdots, B\}$ under PREB-2 is given as

$$\begin{aligned}\frac{1}{B}\sum_{b=1}^{B}\left(\hat{\beta}_k^{**(b)} - \frac{1}{B}\sum_{l=1}^{B}\hat{\beta}_k^{**(l)}\right)^2 &= \frac{1}{B}\sum_{b=1}^{B}\left(\hat{\beta}_k^{**(b)} - \hat{\beta}_k\right)^2 \\ &= \frac{1}{B}\sum_{b=1}^{B}\left(\hat{\beta}_k^{*(b)} - \frac{1}{B}\sum_{l=1}^{B}\hat{\beta}_k^{*(l)}\right)^2,\end{aligned}$$

which coincides with the bootstrap variance under PREB-0.