

A Semi-Parametric Block Bootstrap Approach for Clustered Data

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SAE2011, Trier, Germany

12 August 2011



Overview of Presentation

- Background and Motivation
- Bootstrap Methods
- Empirical Evaluations
- Application to a Real Dataset
- Concluding Remarks

Background

- **Bootstrap technique:** a computer intensive and general way of measuring the accuracy of estimators (**Efron, 1979; Efron & Tibshirani, 1993**)
- Originally developed for parameter estimation given data values that are **independent and identically distributed (iid)**
- Random effects models for **hierarchically dependent data**, e.g. clustered data, are now widely used (e.g. in SAE)
- With such data, it is important to use bootstrap techniques that allow for the hierarchical dependence structure
- **Parametric bootstrap** based on the assumed hierarchical random effects model is widely used
 - very effective if model is **correctly specified**

Background

- If the variability assumptions of the model, e.g. the assumption that the random effects are *iid* Normal random variables, are violated, then it is hard to justify use of the parametric bootstrap
(Rasbash et al., 2000; Carpenter et al., 2003)
- A semi-parametric bootstrap for multilevel modelling is described in
Carpenter et al. (2003)
- We describe an alternative **semi-parametric block** bootstrap for clustered data
 - 'semi-parametric' because although the marginal model is bootstrapped parametrically, the dependence structure in the model residuals is non-parametrically block bootstrapped
 - 'block' because we are interested in a bootstrap procedure that is robust to within cluster heterogeneity

Focus on bootstrap confidence interval performance

Bootstrap Percentile Confidence Interval

- Upper and lower $\alpha/2$ values of the bootstrap distribution are used to construct a $100(1-\alpha)\%$ confidence interval
- Let $\hat{\theta}_{L,\alpha/2}$ denotes the value such that a fraction $\alpha/2$ of all bootstrap estimates are smaller, and likewise let $\hat{\theta}_{U,\alpha/2}$ be the value such that a fraction $\alpha/2$ of all bootstrap estimates are larger; then an approximate confidence interval for θ is $[\hat{\theta}_{L,\alpha/2}, \hat{\theta}_{U,\alpha/2}]$
- Width = $\hat{\theta}_{U,\alpha/2} - \hat{\theta}_{L,\alpha/2}$ and standardised width = $(\hat{\theta}_{U,\alpha/2} - \hat{\theta}_{L,\alpha/2})/\theta$

Random Effects Model for Clustered Data

Two-level model

$$y_{ij} = \mathbf{x}_{ij}^T \boldsymbol{\beta} + u_i + e_{ij}, \quad j = 1, \dots, n_i; i = 1, \dots, D$$

Group-specific random effects (level 2) $u_i \stackrel{IID}{\sim} N(0, \sigma_u^2)$

Individual level errors (level 1) $e_{ij} \stackrel{IID}{\sim} N(0, \sigma_e^2), \quad u_i \perp e_{ij} | x_{ij}$

Focus on bootstrap distributions for estimates $\hat{\boldsymbol{\beta}}$, $\hat{\sigma}_u^2$ and $\hat{\sigma}_e^2$

Parametric 2-Level Bootstrap (Para)

- ML/REML estimates $\hat{\beta}$, $\hat{\sigma}_u^2$ and $\hat{\sigma}_e^2$
- Simulate level 2 errors $u_i^* \stackrel{IID}{\sim} N(0, \hat{\sigma}_u^2)$, $i = 1, \dots, D$
- Simulate level 1 errors $e_{ij}^* \stackrel{IID}{\sim} N(0, \hat{\sigma}_e^2)$, $j = 1, \dots, n_i; i = 1, \dots, D$, $u_i^* \perp e_{ij}^*$
- Bootstrap Data $y_{ij}^* = x_{ij}^T \hat{\beta} + u_i^* + e_{ij}^*$
- Refit model, obtain **bootstrap parameter estimates** $\hat{\beta}^*$, $\hat{\sigma}_u^{2*}$ and $\hat{\sigma}_e^{2*}$
- Repeat B times \Rightarrow B sets of bootstrap estimates
- Generate bootstrap distributions of $\hat{\beta}$, $\hat{\sigma}_u^2$ and $\hat{\sigma}_e^2$
- Bootstrap CIs 'read off' from bootstrap distributions

Semi-Parametric 2-Level Bootstrap (CGR)

(Carpenter, Goldstein and Rasbash, 2003)

- ML/REML estimates $\hat{\beta}$, $\hat{\sigma}_u^2$ and $\hat{\sigma}_e^2$
- Level 2 residuals (EBLUPs) \hat{u}_i , $i = 1, \dots, D$
- Level 1 residuals $\hat{e}_{ij} = y_{ij} - x_{ij}^T \hat{\beta} - \hat{u}_i$, $j = 1, \dots, n_i$; $i = 1, \dots, D$
- Centre and then rescale residuals \hat{u}_i and \hat{e}_{ij}

Rescaling

- The empirical variance-covariance matrices of the level 1 and level 2 residuals can be different from their corresponding ML/REML estimates
- Rescale residuals to make these the same before bootstrapping

Rescaling (Cholesky decomposition)

- Estimate the variance-covariance matrix $\hat{\Sigma}$ of model errors $\hat{\mathbf{U}}$ (either level 2 or level 1) via ML/REML
- Cholesky decomposition $\hat{\Sigma} = \mathbf{A}\mathbf{A}^T$ calculated, where \mathbf{A} is a lower triangular matrix
- $\hat{\mathbf{V}} = \text{empirical variance/covariance matrix of } \hat{\mathbf{U}}$
- Cholesky decomposition $\hat{\mathbf{V}} = \mathbf{B}\mathbf{B}^T$ calculated, where \mathbf{B} is a lower triangular matrix
- Rescaled residuals $\hat{\mathbf{U}}^* = \hat{\mathbf{U}}\mathbf{C}$ where $\mathbf{C} = (\mathbf{AB}^{-1})^T$

- Sample **independently** with replacement from these two **new sets** of centred and rescaled residuals
- $u_i^* = srswr\left(\{\hat{u}_h; h = 1, \dots, D\}, m = 1\right)$
- $e_{ij}^* = srswr\left\{\hat{e}_{hj}, j = 1, \dots, n_i; h = 1, \dots, D\right\}$
- Bootstrap Data $y_{ij}^* = x_{ij}^T \hat{\beta} + u_i^* + e_{ij}^*$
- Refit model, obtain bootstrap parameter estimates $\hat{\beta}^*$, $\hat{\sigma}_u^{2*}$ and $\hat{\sigma}_e^{2*}$
- Repeat this process B times
- Generate bootstrap distributions for $\hat{\beta}$, $\hat{\sigma}_u^2$ and $\hat{\sigma}_e^2$
- Bootstrap CIs 'read off' from bootstrap distributions

Simple Semi-Parametric Block Bootstrap (SBB)

- Estimate $\hat{\beta}$ with residuals : $r_{ij} = y_{ij} - x_{ij}^T \hat{\beta}, j = 1, \dots, n_i; i = 1, \dots, D$
- Level 2 residuals : Group averages $\bar{r}_h = n_h^{-1} \sum_{j=1}^{n_h} r_{hj}, h = 1, \dots, D$
- Level 1 residuals : $r_{hj}^{(1)} = r_{hj} - \bar{r}_h \Rightarrow \mathbf{r}_h^{(1)}$ vector of size n_i
- Sample **independently** with replacement from these two sets of residuals
 - $\bar{r}_i^* = srswr\left(\{\bar{r}_h; h = 1, \dots, D\}, m = 1\right)$
 - $h(i) = srswr\left(\{1, \dots, D\}, m = 1\right)$
 - **Block/group structure** : $\mathbf{r}_i^{(1)*} = srswr\left(\{\mathbf{r}_{h(i)}^{(1)}\}, m = n_i\right)$
- Bootstrap Data : $\mathbf{y}_i^* = \mathbf{x}_i^T \hat{\beta} + \bar{r}_i^* \mathbf{1}_{n_i} + \mathbf{r}_i^{(1)*}$

SBB + Post Bootstrap Adjustment (SBB.Post)

- Multivariate bootstrap distribution of the variance component estimates is first transformed (**'tilted'**) in order to ensure that the bootstrap estimates of these components are uncorrelated
- All bootstrap distributions of model parameter estimates are then **'tethered'** to the original estimate values, using either a mean correction (for estimates, e.g. regression coefficients, defined on the entire real line) or a ratio correction (for estimates, e.g. variance components, that are strictly positive)

Tilting and Tethering (post-bootstrapping)

- $\left(\hat{\beta}_k^{**}\right)_B = \left[\hat{\beta}_k \mathbf{1}_B + \left(\hat{\beta}_k^*\right)_B - av_B \left(\hat{\beta}_k^*\right)\right]$
- $\left(\hat{\sigma}_u^{2**}\right)_B = \left(\hat{\sigma}_u^{*\text{mod}2}\right)_B \times \hat{\sigma}_u^2 \left\{av_B \left(\hat{\sigma}_u^{*\text{mod}2}\right)\right\}^{-1}$
- $\left(\hat{\sigma}_e^{2**}\right)_B = \left(\hat{\sigma}_e^{*\text{mod}2}\right)_B \times \hat{\sigma}_e^2 \left\{av_B \left(\hat{\sigma}_e^{*\text{mod}2}\right)\right\}^{-1}$

where

$$\begin{aligned} & \left[\left(\hat{\sigma}_u^{*\text{mod}2}\right)_B \left(\hat{\sigma}_e^{*\text{mod}2}\right)_B \right] = \exp \left\{ \mathbf{M}_B^* + \left\{ \left(\mathbf{S}_B^* - \mathbf{M}_B^*\right) \left(\mathbf{C}_B^*\right)^{-1/2} \right\} \times \mathbf{D}_B^* \right\} \\ & \mathbf{M}_B^* = \begin{bmatrix} av_B \left(\log \hat{\sigma}_u^{*2}\right) \mathbf{1}_B & av_B \left(\log \hat{\sigma}_e^{*2}\right) \mathbf{1}_B \end{bmatrix} \\ & \mathbf{S}_B^* = \begin{bmatrix} \left(\log \hat{\sigma}_u^{*2}\right)_B & \left(\log \hat{\sigma}_e^{*2}\right)_B \end{bmatrix} \\ & \mathbf{C}_B^* = \text{cov}_B \left(\mathbf{S}_B^*\right) \\ & \mathbf{D}_B^* = \begin{bmatrix} sd_B \left(\log \hat{\sigma}_u^{*2}\right) \mathbf{1}_B & sd_B \left(\log \hat{\sigma}_e^{*2}\right) \mathbf{1}_B \end{bmatrix} \end{aligned}$$

Semi-Parametric Block Bootstrap with Centred and Rescaled Residuals (SBB.Prior)

- Estimate $\hat{\beta}$ with residuals $r_{ij} = y_{ij} - x_{ij}^T \hat{\beta}, j = 1, \dots, n_i; i = 1, \dots, D$
- Level 2 residuals: Group-wise averages $\bar{r}_h = n_h^{-1} \sum_{j=1}^{n_h} r_{hj}, h = 1, \dots, D$
- Level 1 residuals: $r_{hj}^{(1)} = r_{hj} - \bar{r}_h \Rightarrow \mathbf{r}_h^{(1)}$ vector of size n_i
- **Centre and rescale** Level 1 and Level 2 residuals: \bar{r}_h and $r_{hj}^{(1)}$
- Apply SBB to these centred and rescaled residuals
- No post-bootstrap adjustment

SBB + External Calibration to Covariance Matrix of Variance Components (SBB.Prior.Adj)

- Calibrate covariance matrix of bootstrap estimates of variance components to ML/REML estimate of the covariance matrix of variance components obtained from the model - **Cholesky decomposition**
- Post-bootstrap adjustment where bootstrap distribution of variance components is tilted to recover ML/REML estimate of variance/covariance matrix of estimated variance components

Bootstrap Methods Used in Simulations

Type	Description
Para	Parametric 2-level bootstrap
CGR	Semi-Parametric 2-Level Bootstrap (Carpenter, Goldstein and Rasbash, 2003)
SBB	Simple semi-parametric Block bootstrap using empirical Level 1 and Level 2 residuals
SBB.Post	SBB with post-bootstrap tilting & tethering adjustments
SBB.Prior	SBB using internally rescaled empirical residuals
SBB.Prior.Adj	SBB using internally rescaled residuals with post-bootstrap adjustment to recover REML estimate of the variance of the estimated variance components

Simulation Design

- Total number of clusters: $D = 50, 100$
- Uniform cluster sample sizes: $n_i = 5, 20$
- $n = 250, 500, 1000, 2000$
- 1000 simulations
- 1000 Bootstrap samples per method per simulation

Model

- $y_{ij} = \beta_0 + \beta_1 x_{ij} + u_i + e_{ij}, j = 1, \dots, n_i; i = 1, \dots, D$
- $x_{ij} \sim U(0,1)$
- $u_i \stackrel{IID}{\sim} (0, \sigma_u^2), e_{ij} \stackrel{IID}{\sim} (0, \sigma_e^2) \quad u_i \perp e_{ij} | x_{ij}$
- $\beta_0 = 1, \beta_1 = 2, \sigma_u^2 = 0.04$ and $\sigma_e^2 = 0.16$
- u_i and e_{ij} generated using **four** scenarios ...

Set A - Normal Scenario

- $u_i \sim N(0, \sigma_u^2 = 0.04)$ and $e_{ij} \sim N(0, \sigma_e^2 = 0.16)$

Set B - Chi-Square Scenario

- $u_i \sim 0.2 \left[(\chi_1^2 - 1) / \sqrt{2} \right]$ and $e_{ij} \sim 0.4 \left[(\chi_1^2 - 1) / \sqrt{2} \right]$

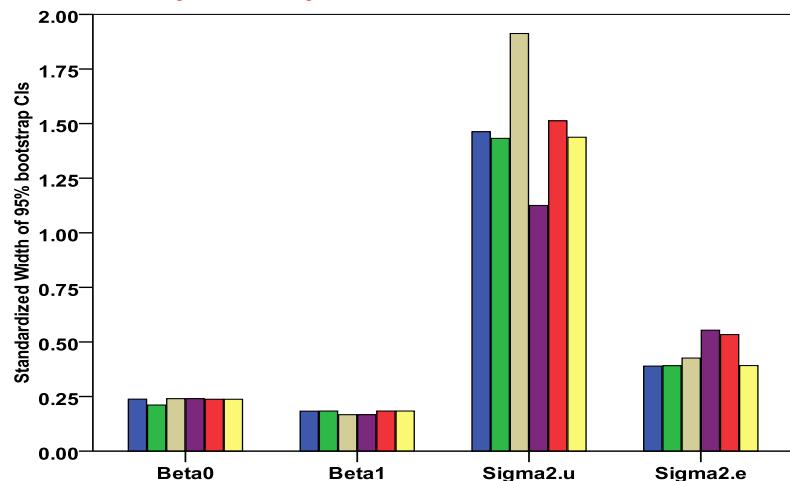
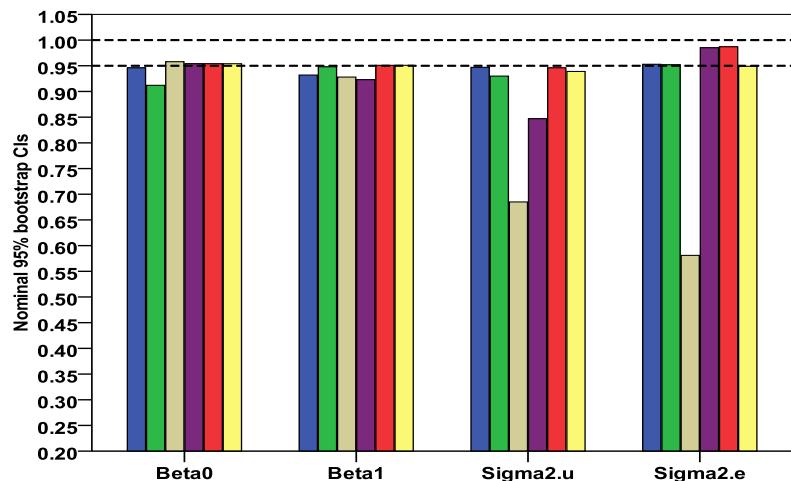
Set C - Within Cluster Auto-Correlation Scenario

- Level 2 errors normally distributed as in Set A, but Level 1 errors within each cluster independently generated as a first order auto-correlated series $e_{ij} = 0.5e_{i(j-1)} + \varepsilon_{ij}, j = 1, \dots, n_i$, with $\varepsilon_{ij} \sim N(0,1)$

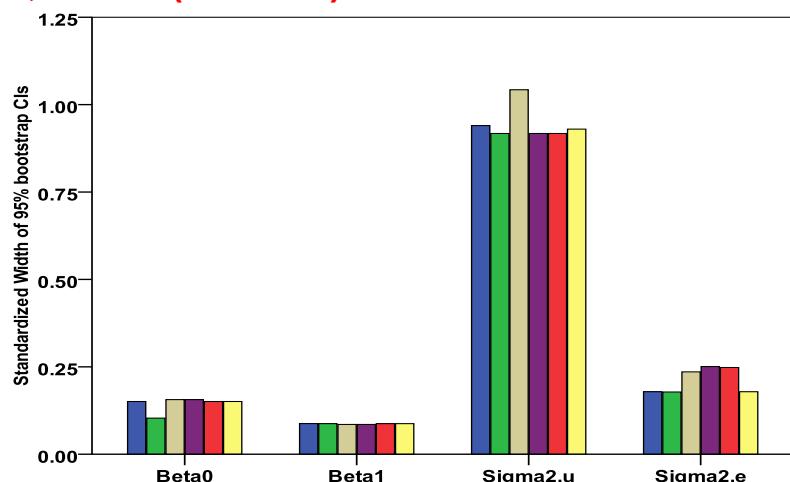
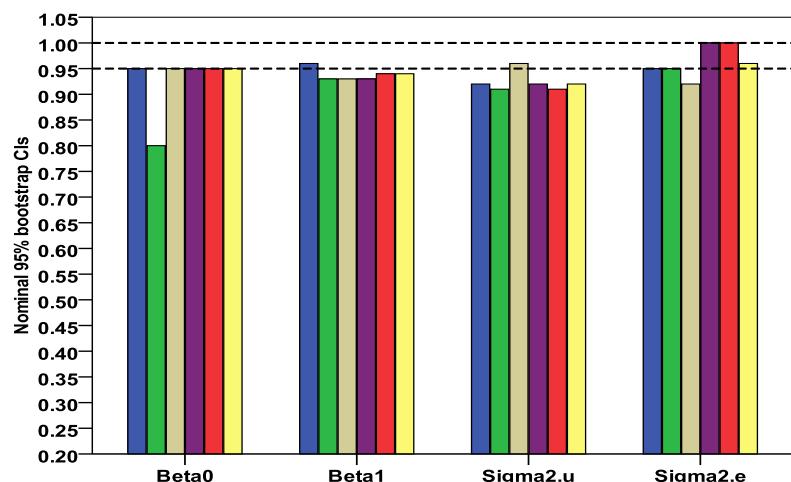
Set D - Between Cluster Auto-Correlation Scenario

- Level 2 errors normally distributed as in Set A, but Level 1 errors for entire population generated as a first order auto-correlated series $e_{ij} = 0.5e_{i(j-1)} + \varepsilon_{ij}, j = 1, \dots, n_i$, with $\varepsilon_{ij} \sim N(0,1)$, with clusters sequentially defined along the 'time' axis. This simulation approximates the type of time series problem that motivated the development of the block bootstrap

A: Normal Scenario: D=50, n_i=5 (n=250)

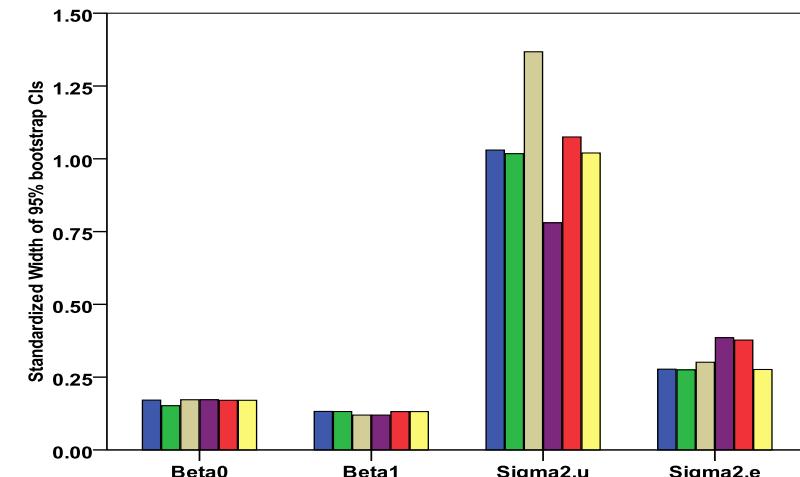
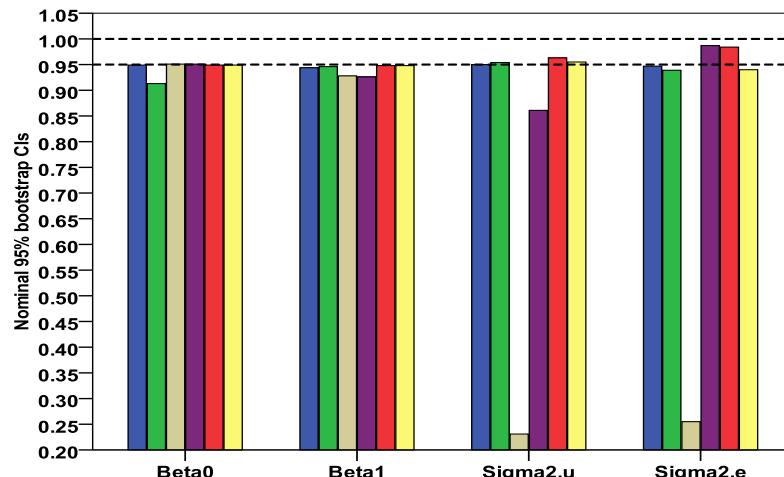


A: Normal Scenario: D=50, n_i=20 (n=1000)

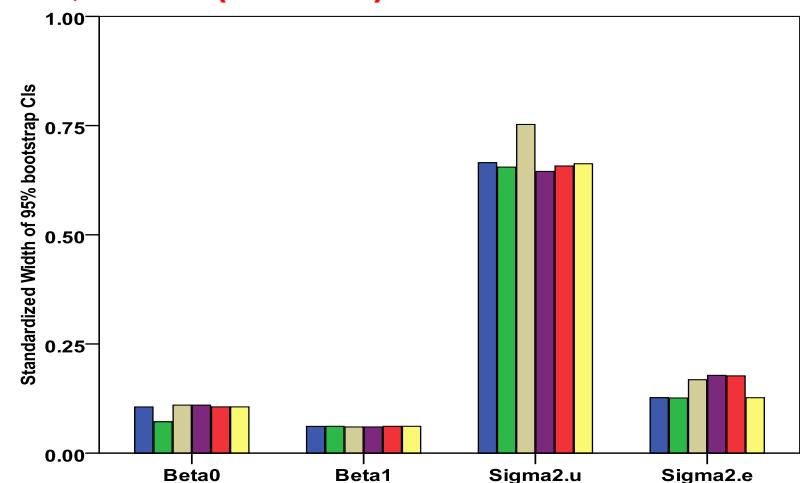
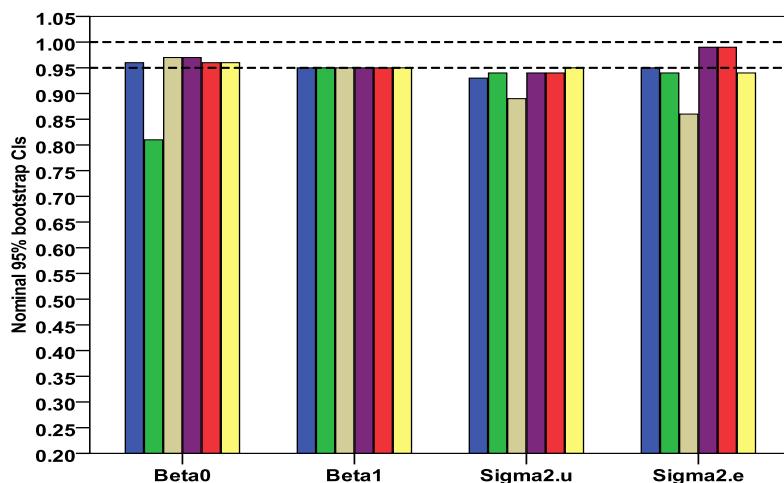


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A: Normal Scenario: D=100, n_i=5 (n=500)

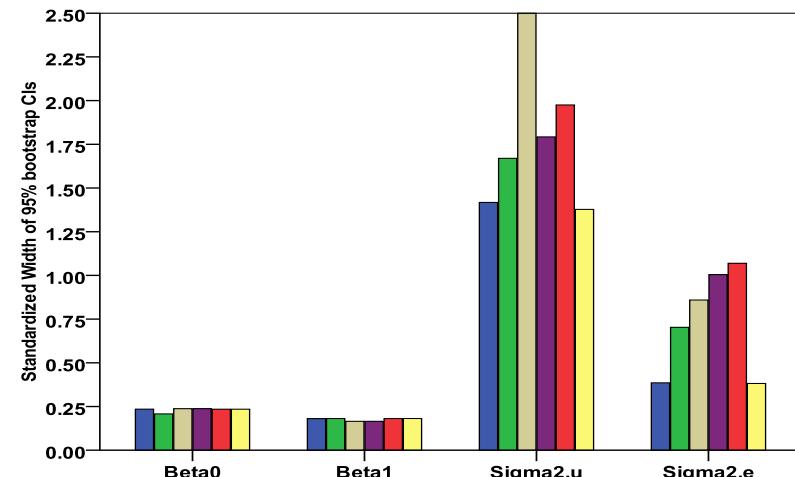
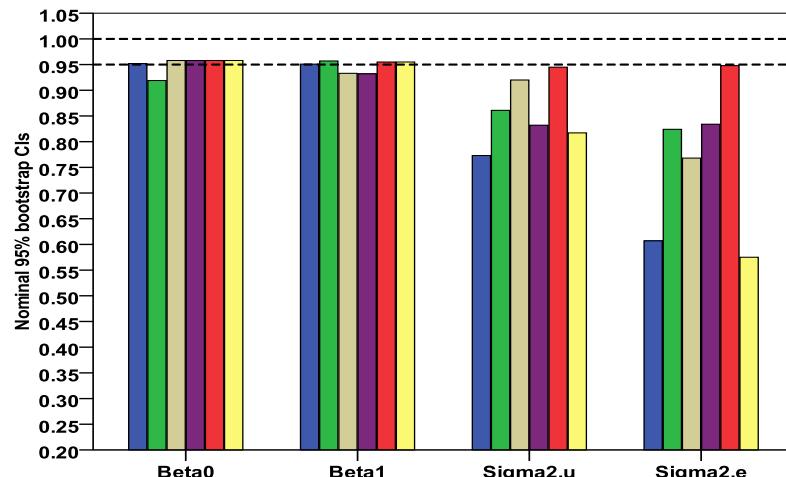


A: Normal Scenario: D=100, n_i=20 (n=2000)

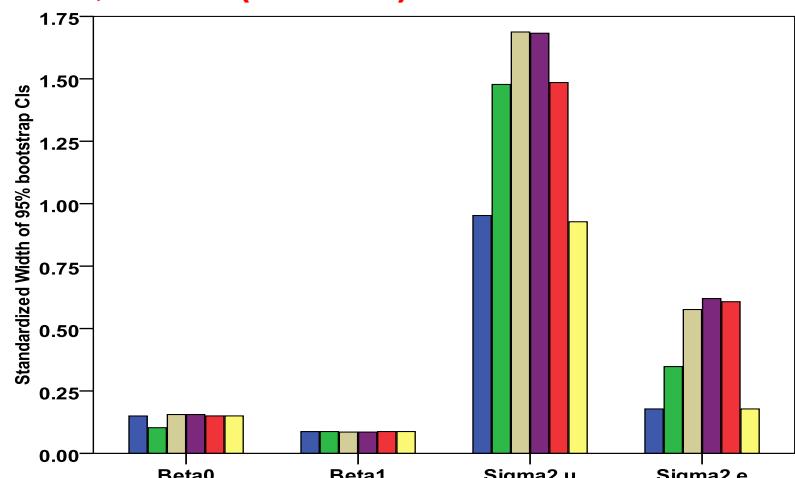
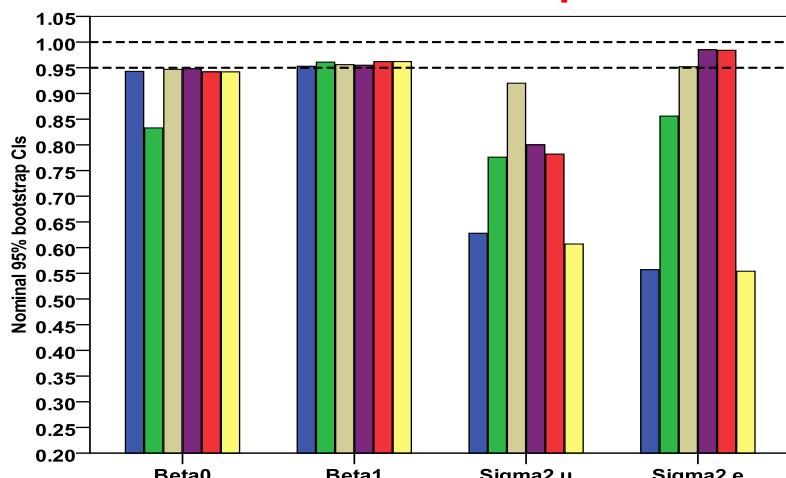


█ Para
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B: Chi-Square Scenario: D=50, n_i=5 (n=250)

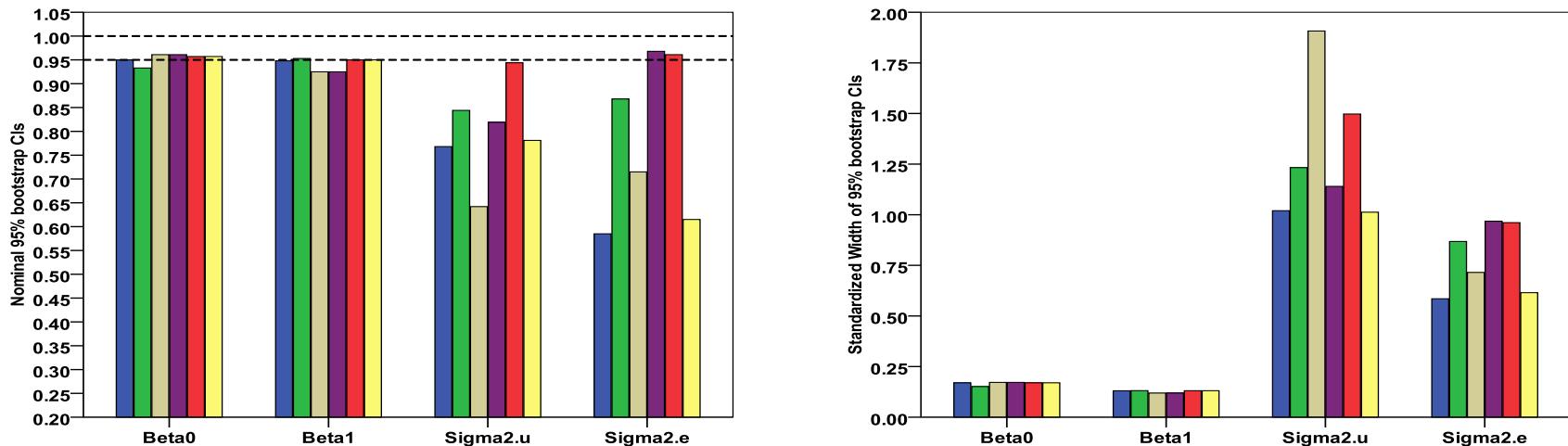


B: Chi-Square Scenario: D=50, n_i=20 (n=1000)

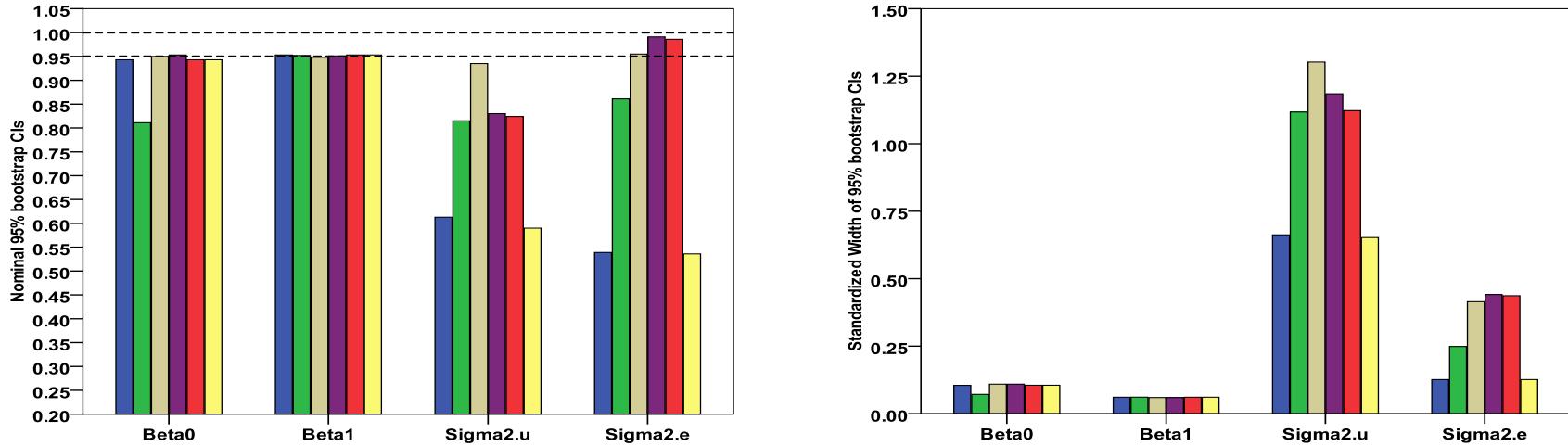


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B: Chi-Square Scenario: D=100, n_i=5 (n=500)

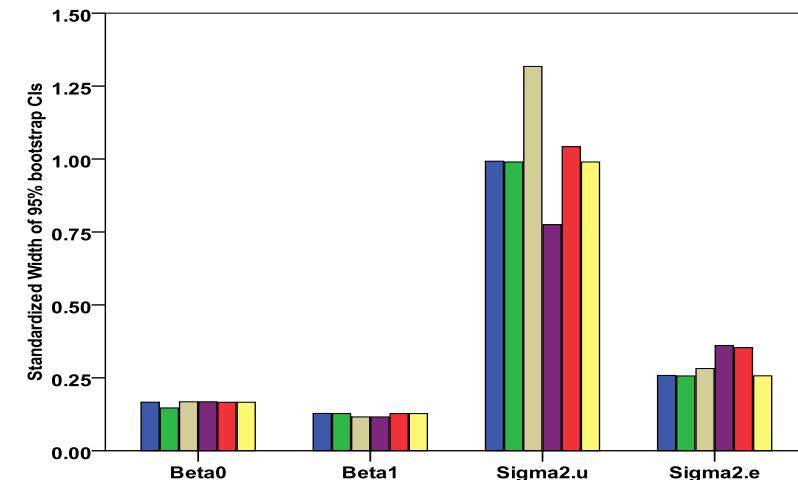
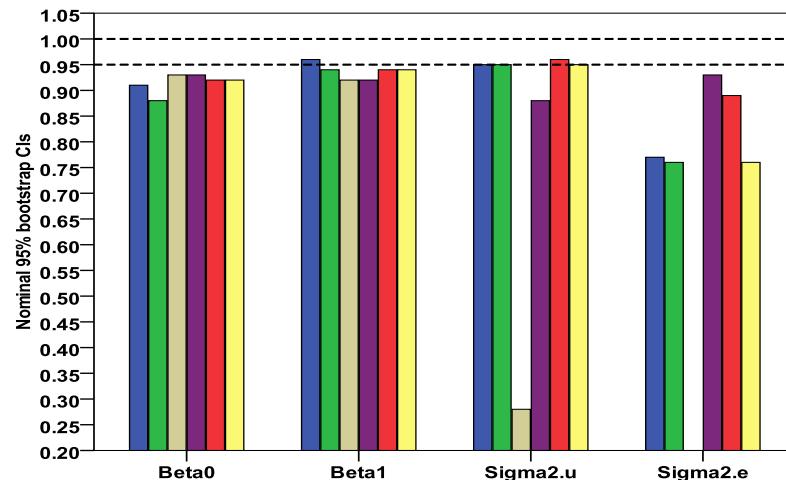


B: Chi-Square Scenario: D=100, n_i=20 (n=2000)

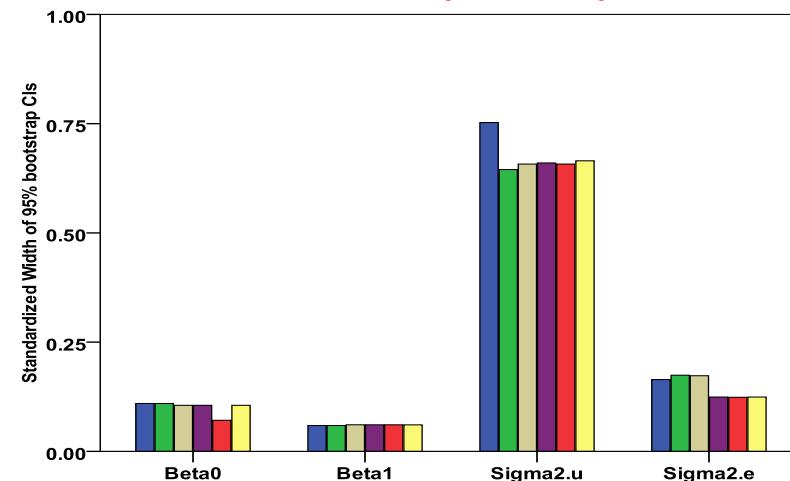
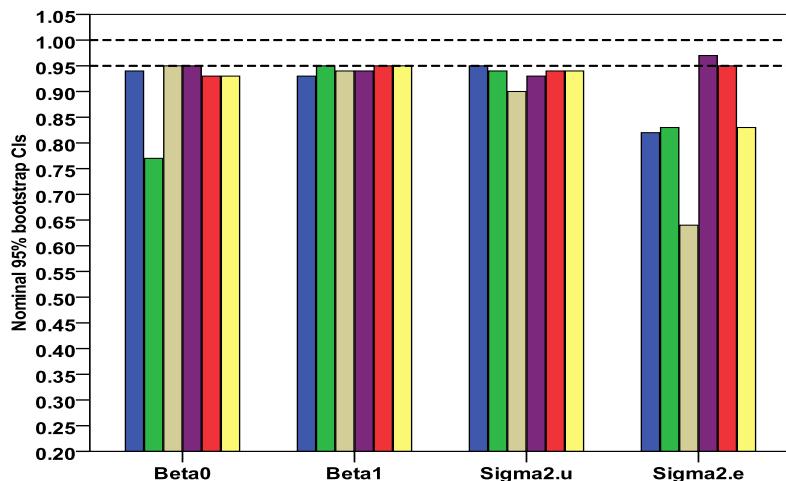


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█ SBB.Prior.Adj

C: Within Cluster Auto-Correlation Scenario: D=100, n_i=5 (n=500)

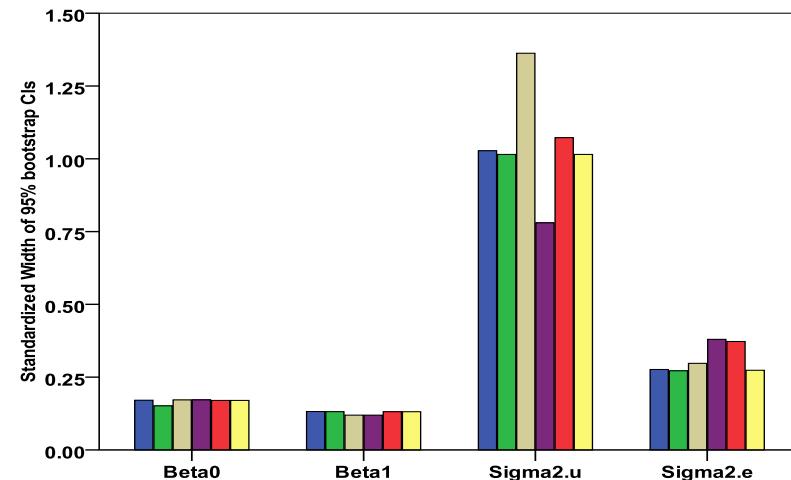
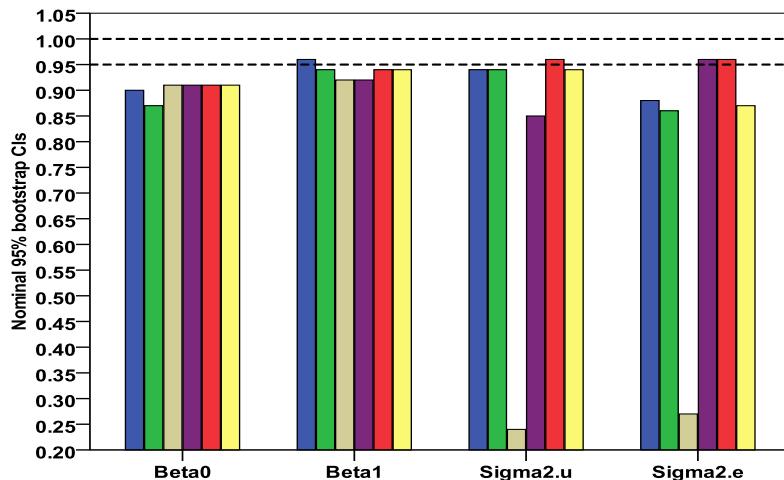


C: Within Cluster Auto-Correlation Scenario: D=100, n_i=20 (n=2000)

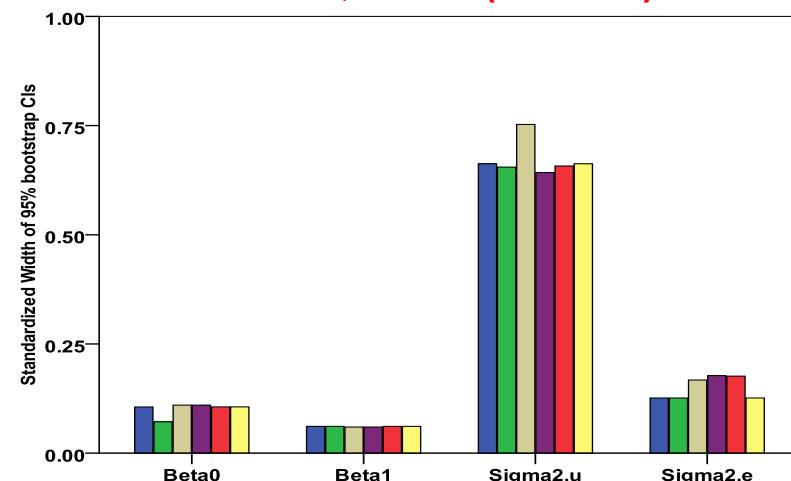
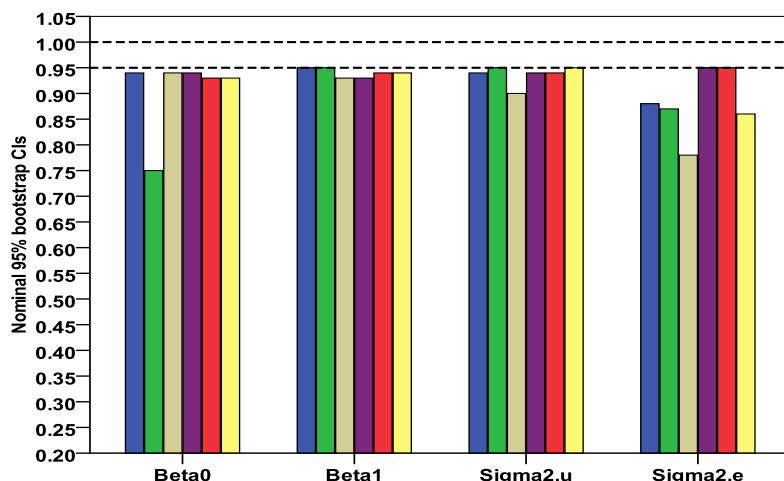


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D: Between Cluster Auto-Correlation Scenario: D=100, n_i=5 (n=500)



D: Between Cluster Auto-Correlation Scenario: D=100, n_i=20 (n=1000)



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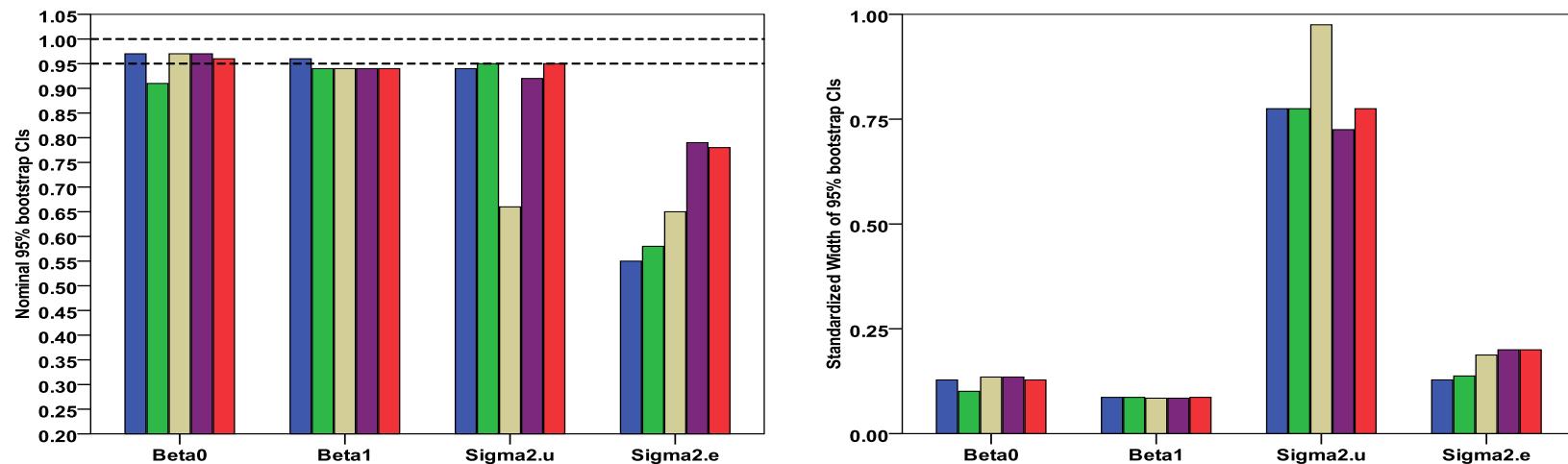
Simulation Results for Spatially Correlated Data

- Total number of clusters: $D = 100$
- Uniform cluster sample sizes: $n_i = 20$
- $y_{ij} = 1 + 2x_{ij} + u_i + e_{ij}, j = 1, \dots, n_i; i = 1, \dots, D$
- $u_i \sim (0, \sigma_u^2)$, $\mathbf{e}_i = 0.45\mathbf{W}\mathbf{e}_i + \mathbf{z}_i$ (SAR specification)
- $\sigma_u^2 = 0.04$ (WA) & 0.005 (WB) and $\sigma_e^2 = 0.3205$ (WA) & 0.0177 (WB)

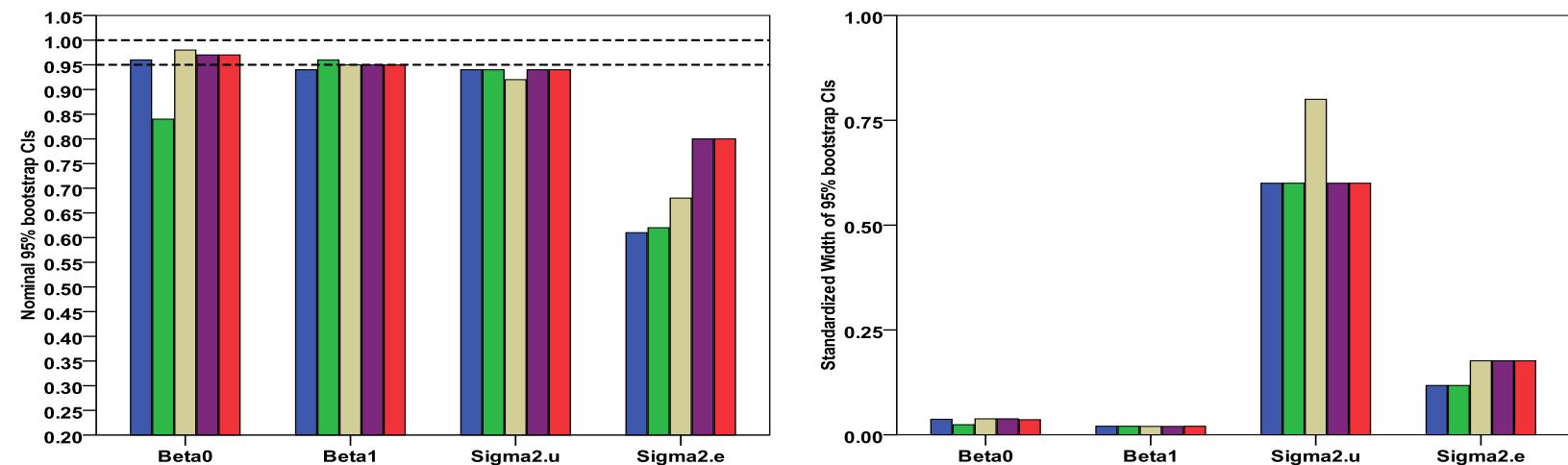
WA																			
0	4	3	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	4	3	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	4	0	4	3	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	3	4	0	4	3	2	1	0	0	0	0	0	0	0	0	0	0	0	0
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0	0	0	0	0	0	0	0	0	0	0	0	1	2	3	4	0	4	3	2

WB																			
0	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1
19	0	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2
18	19	0	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3
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15	16	17	18	19	0	19	18	17	16	15	14	13	12	11	10	9	8	7	6
14	15	16	17	18	19	0	19	18	17	16	15	14	13	12	11	10	9	8	7
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2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	0	19
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WA



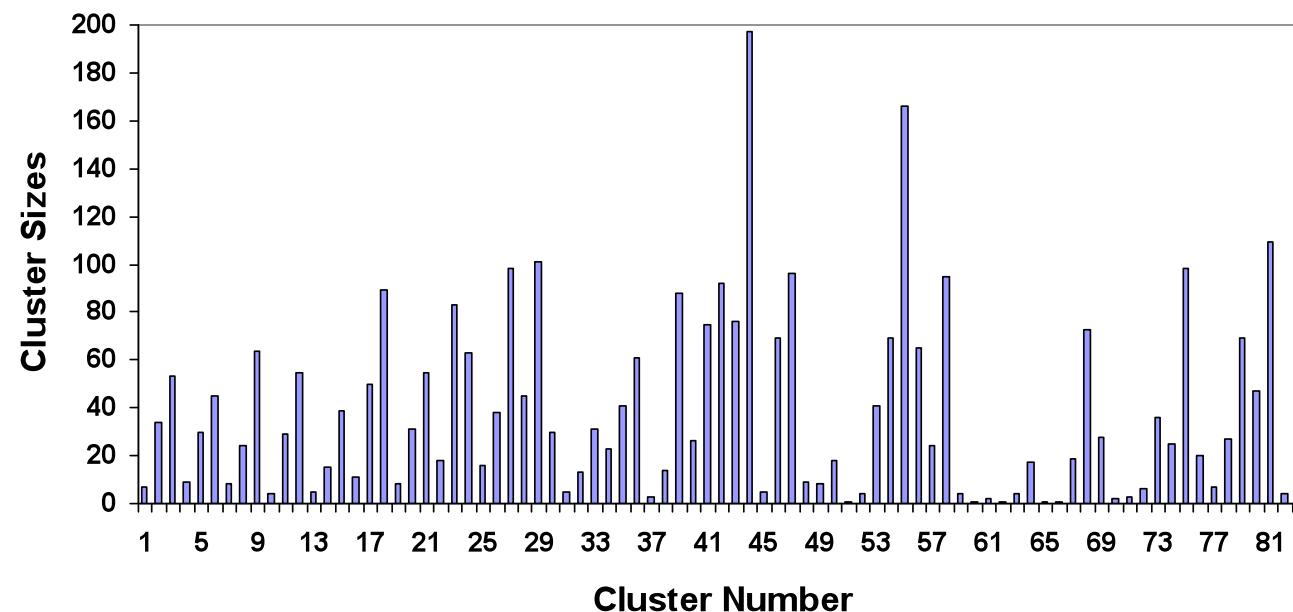
WB



█ Para █ SBB █ SBB.Prior
█ CGR █ SBB.Post

Atlant (Australian Rain Technology) Data (Beare et al. 2010)

Response Variable	: Daily rainfall or log (Daily rainfall)
Explanatory Variables	: 37
Cluster	: 4 Day Downwind Cluster
No of Clusters	: 83
Total sample size	: 3177 (Min=1, Max=197, Average=38)

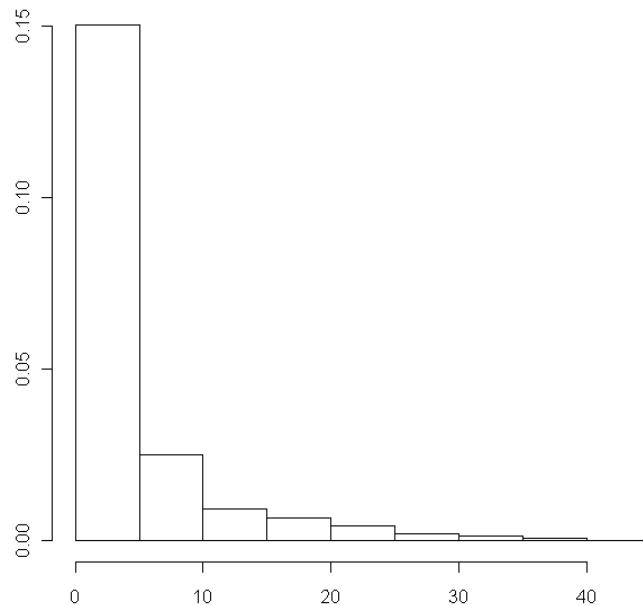


Explanatory Variables

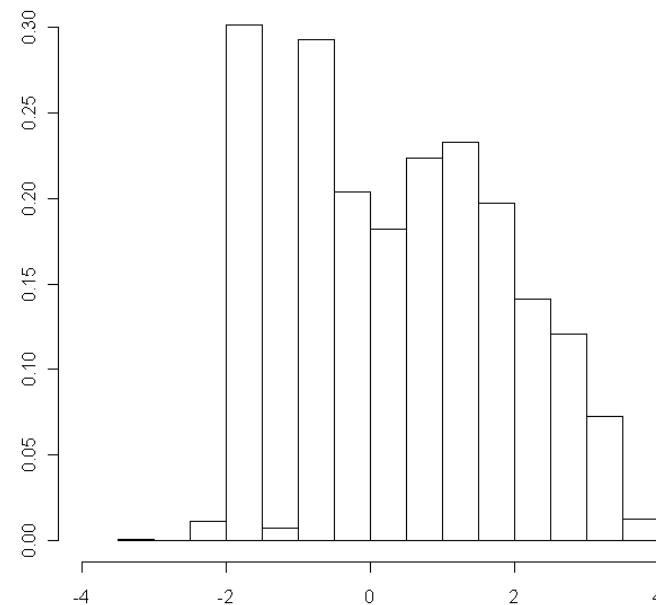
No.	Variable	No.	Variable
1	Intercept	20	Elevation (100m)
2	August/September	21	Distance from C2
3	WRE	22	C2 Theta
4	Upwind Rain 0.1mm and over	23	Lagged C2 Theta
5	Wind Speed 700	24	C2 Theta * C2 Distance
6	Lagged Wind Speed 700	25	Lag C2 Theta * C2 Distance
7	Wind Speed 850	26	Distance from C3
8	Lagged Wind Speed 850	27	C3 Theta
9	Wind Speed 925	28	Lagged C3 Theta
10	Lagged Wind Speed 925	29	C3 Theta * C3 Distance
11	SWD 700	30	Lag C3 Theta * C3 Distance
12	SLWD 700	31	C2 On 1
13	SWD 850	32	C2 On 2
14	SLWD 850	33	C2 On 1 * C2 Distance
15	SWD 925	34	C2 On 2 * C2 Distance
16	SLWD 925	35	C3 On 1
17	Air Temp	36	C3 On 2
18	Dew Point Difference	37	C3 On 1 * C3 Distance
19	Sea Level Pressure	38	C3 On 2 * C3 Distance

Response Variable

Daily Rainfall



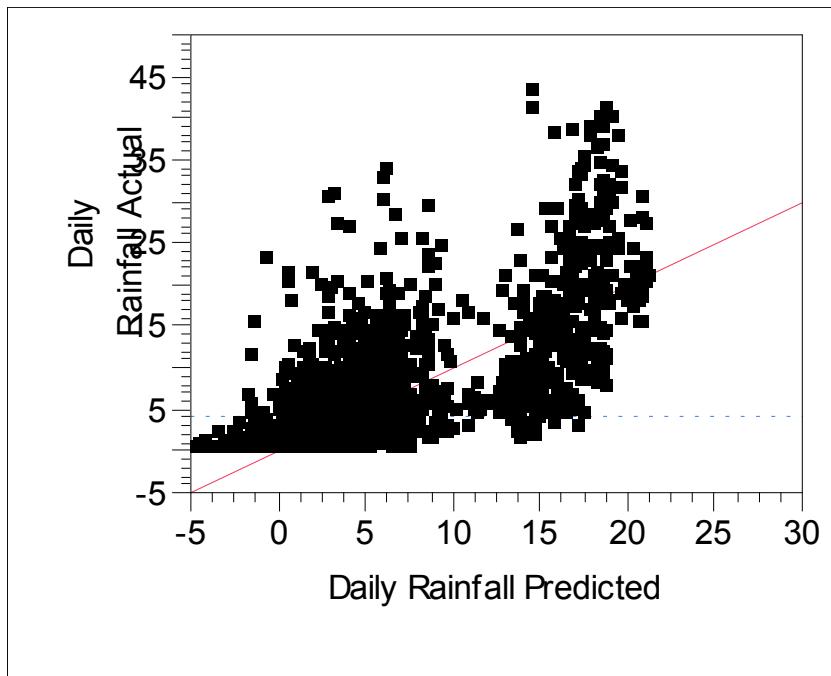
log (Daily Rainfall)



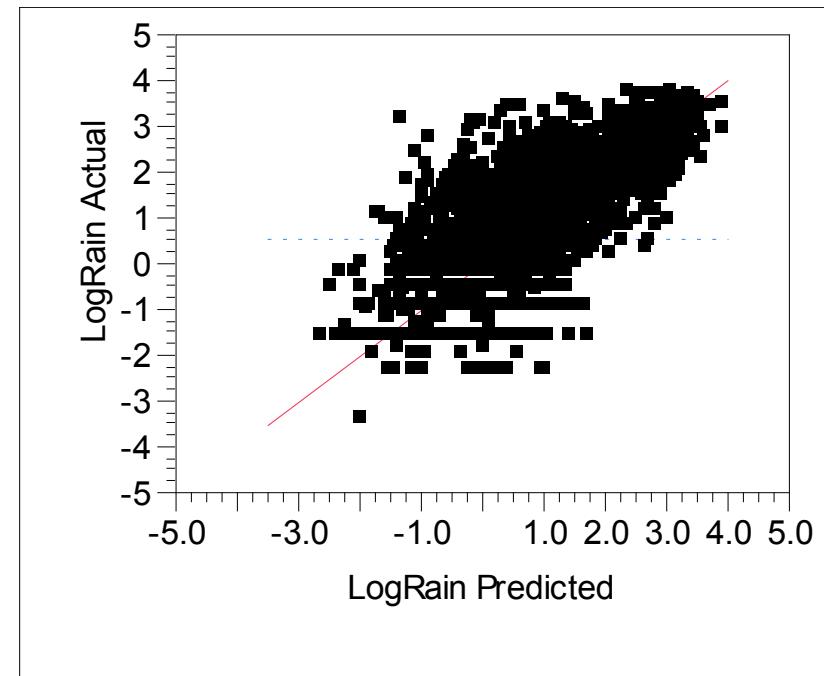
	Mean	Std Dev	Median
Rain	4.29	6.39	1.67
LogRain	0.51	1.44	0.51

Model Fit: Actual by Predicted Plot

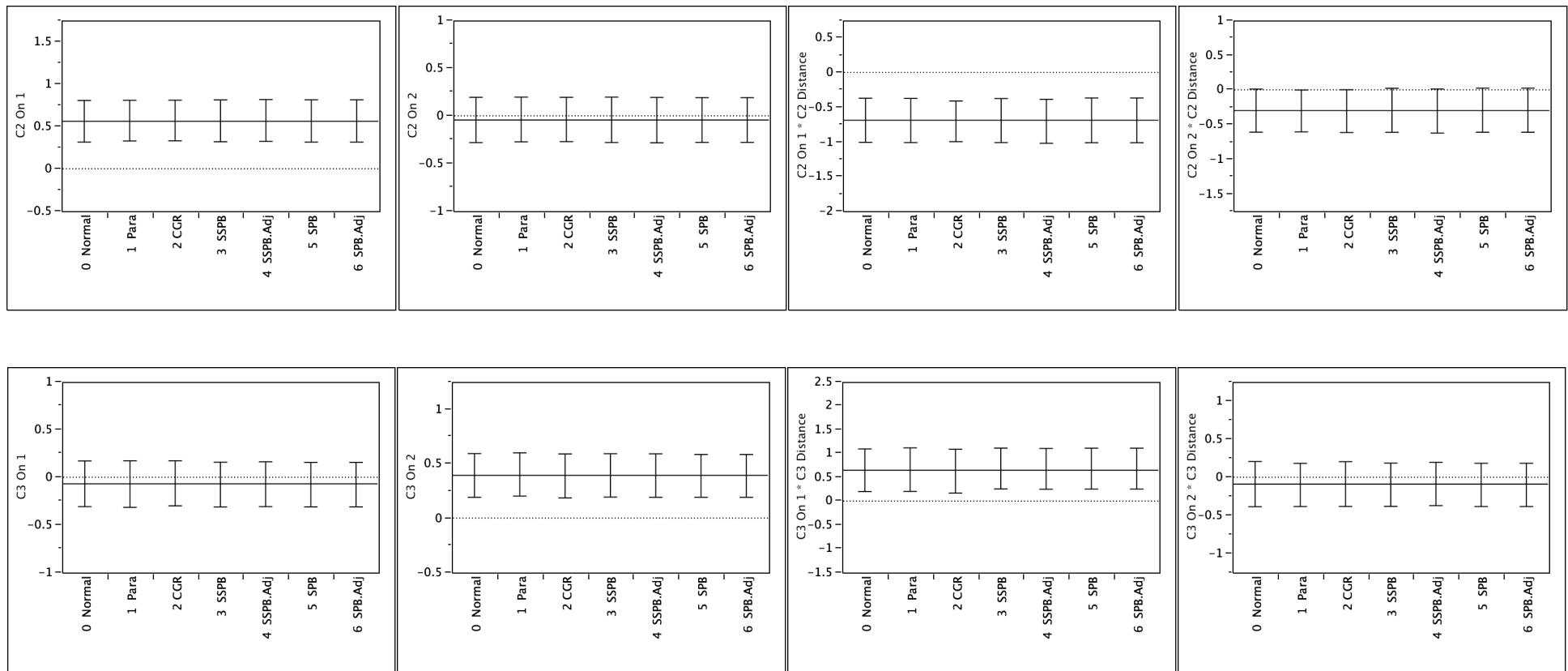
Daily Rainfall



log (Daily Rainfall)



Log (Daily Rainfall): 95% CIs for 8 Effect Variables

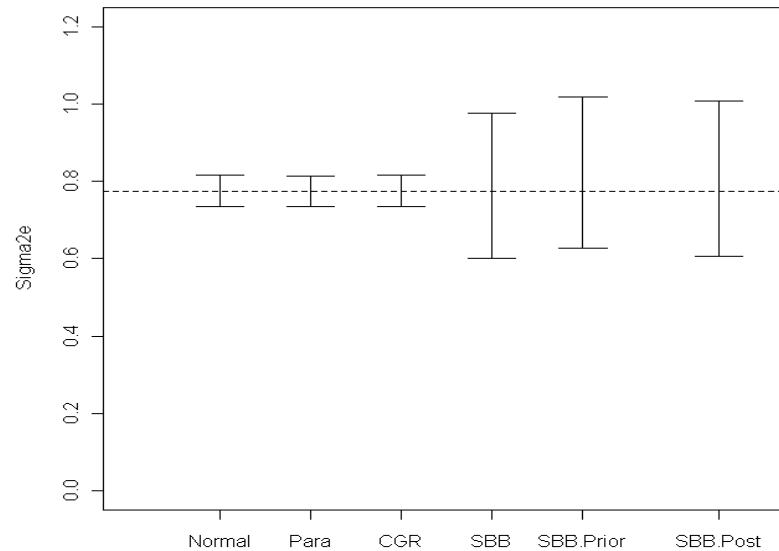
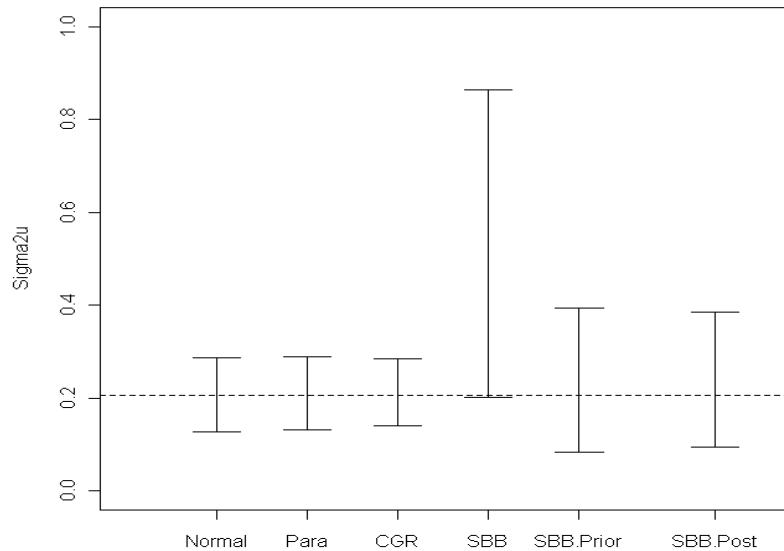


- If the bootstrap confidence interval **fails** to include 0, then the p-value is deemed to be less than or equal to 0.05, and the effect is **significant**
- Bootstrap does not change conclusions about fixed effects parameters

Log (Daily Rainfall): 95% CIs for Variance Components

$$\hat{\sigma}_u^2 = 0.206$$

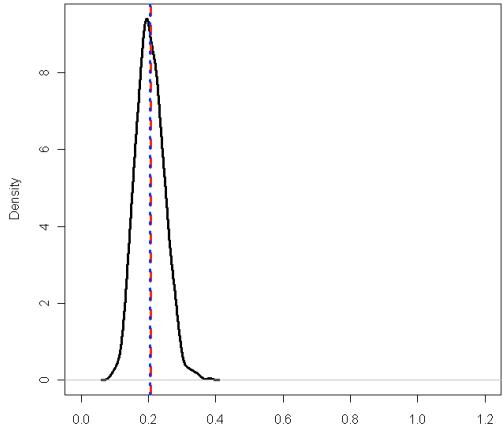
$$\hat{\sigma}_e^2 = 0.775$$



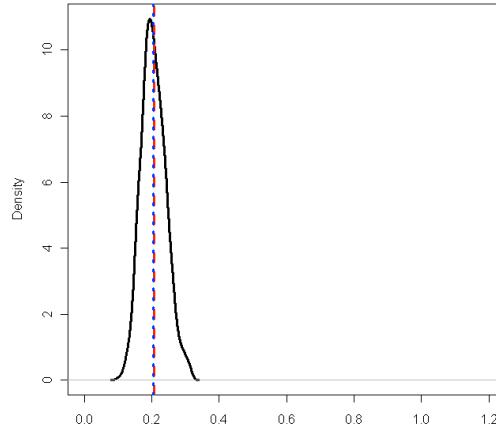
- Semiparametric block bootstrap results seem more believable

$$\text{Red} : \hat{\sigma}_u^2 = 0.206$$

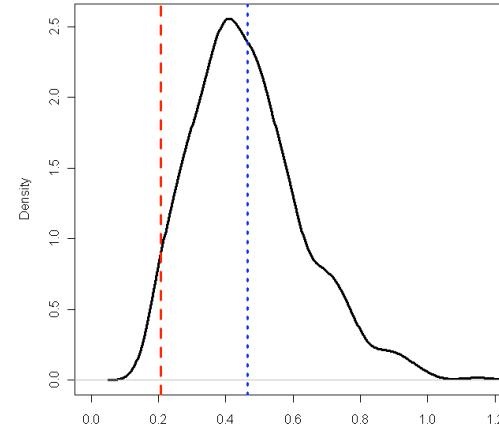
$$\text{Blue} : \bar{\hat{\sigma}}_u^{2*} = B^{-1} \sum_{b=1}^B \hat{\sigma}_u^{2*(b)}$$



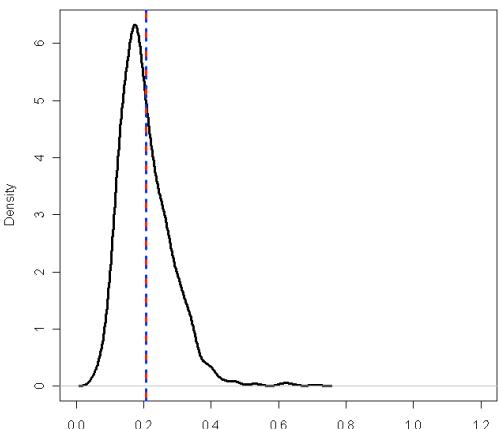
Para



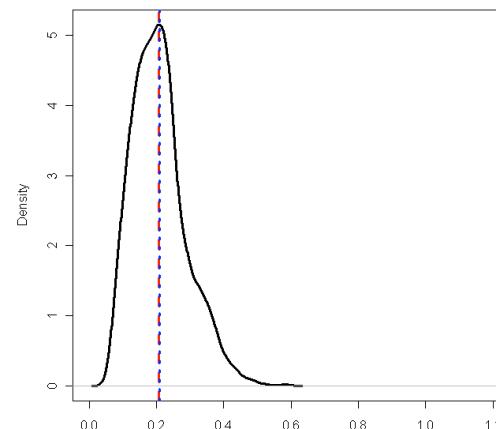
CGR



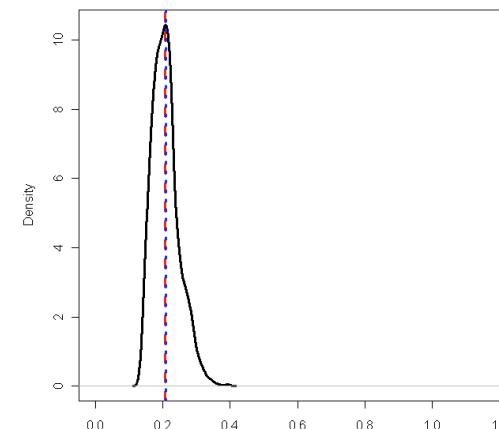
SBB



SBB.Post



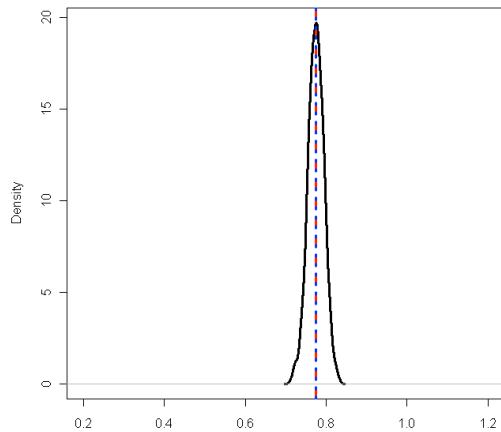
SBB.Prior



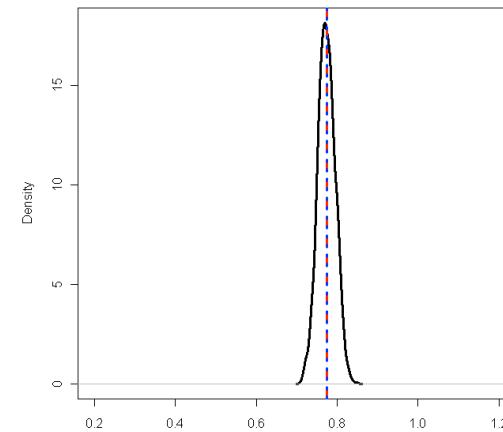
SBB.Prior.Adj

$$\text{Red: } \hat{\sigma}_e^2 = 0.775$$

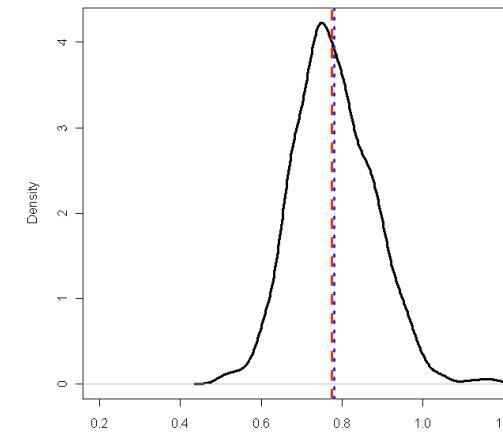
$$\text{Blue: } \bar{\hat{\sigma}}_e^{2*} = B^{-1} \sum_{b=1}^B \hat{\sigma}_e^{2*(b)}$$



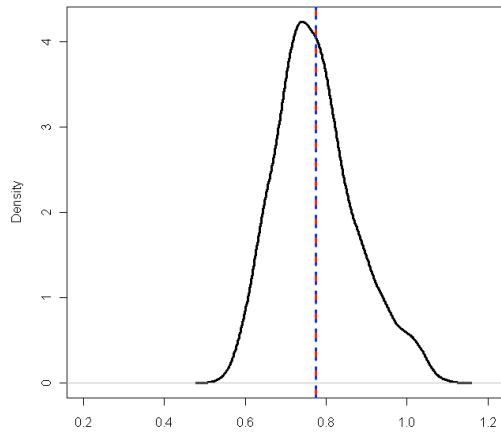
Para



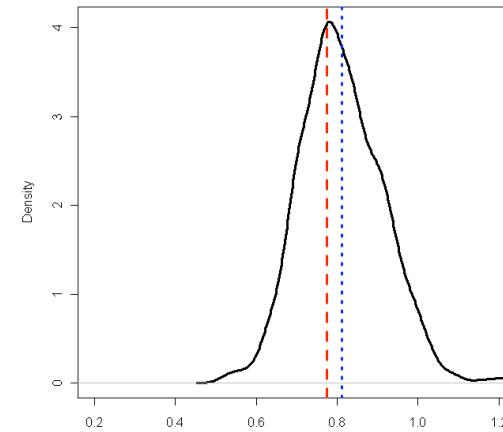
CGR



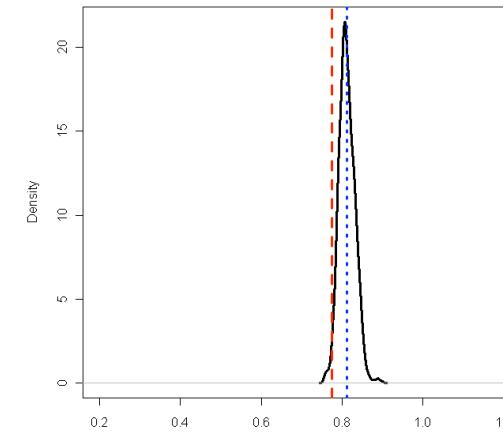
SBB



SBB.Post

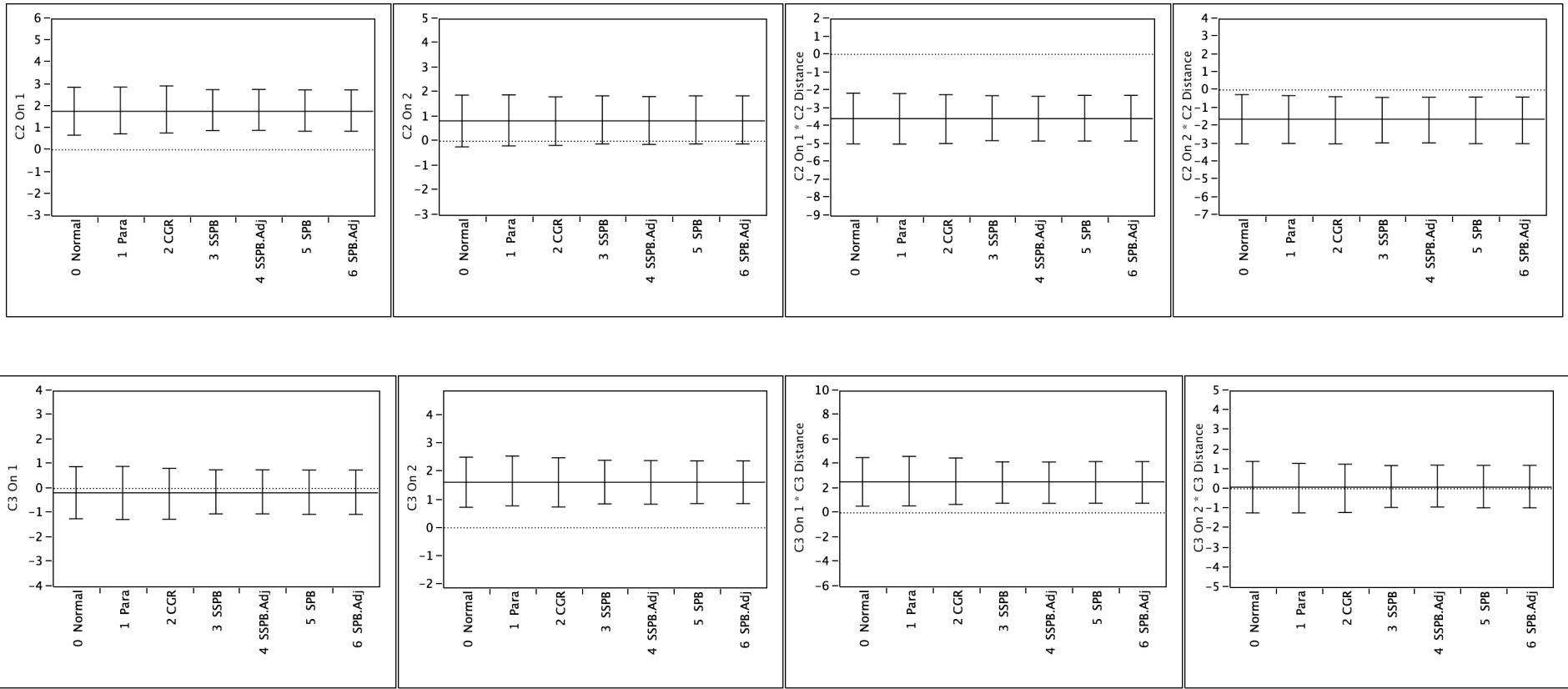


SBB.Prior



SBB.Prior.Adj

Daily Rainfall: 95% CIs for 8 Effect Variables

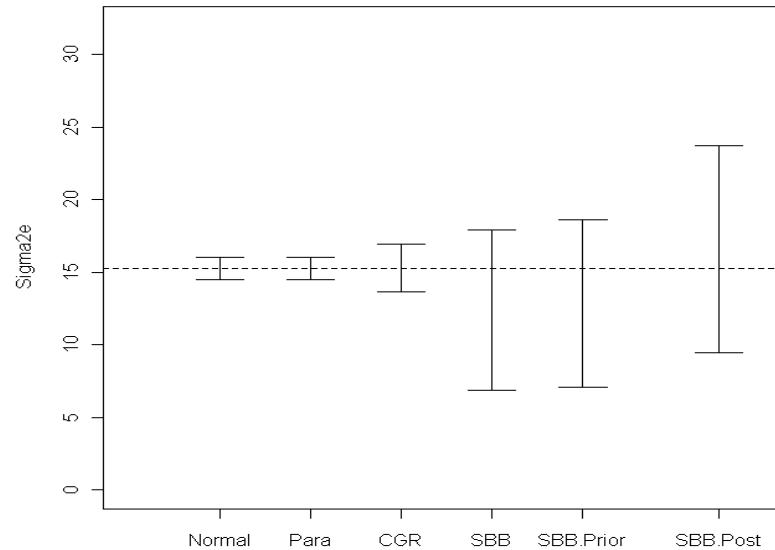
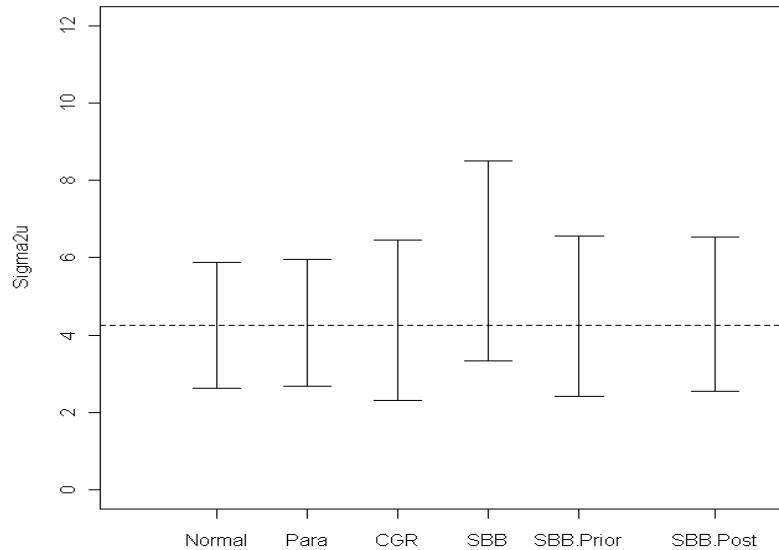


- Again, bootstrap does not change conclusions about fixed effects parameters

Daily Rainfall: 95% CIs for Variance Components

$$\hat{\sigma}_u^2 = 4.246$$

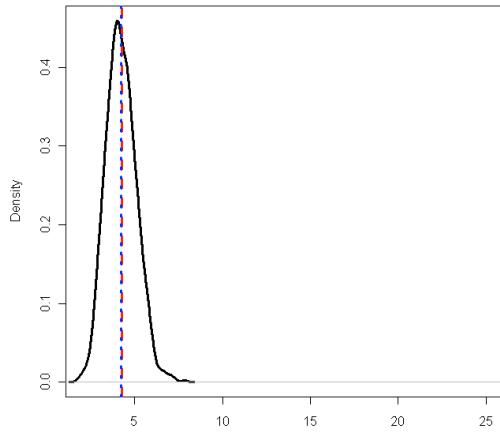
$$\hat{\sigma}_e^2 = 15.269$$



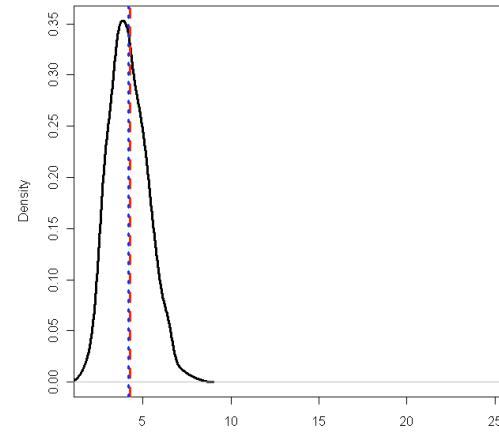
- Normal, Para and CGR CIs for σ_e^2 seem overly optimistic ...

Red: $\hat{\sigma}_u^2 = 4.246$

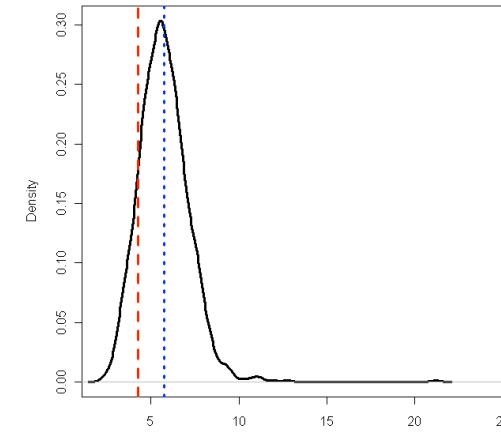
Blue: $\bar{\hat{\sigma}}_u^{2*} = B^{-1} \sum_{b=1}^B \hat{\sigma}_u^{2*(b)}$



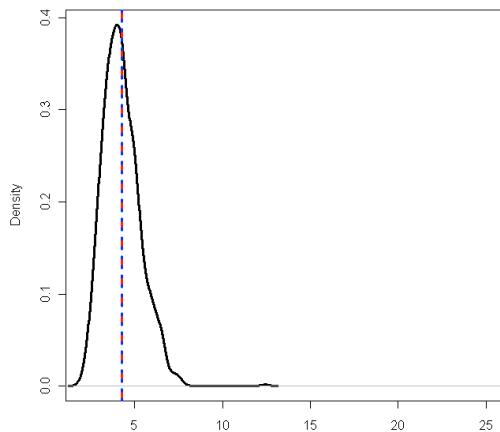
Para



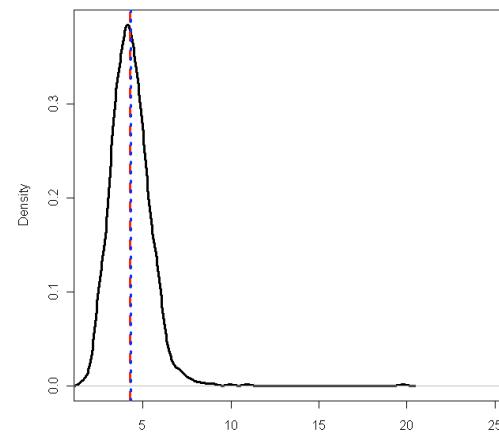
CGR



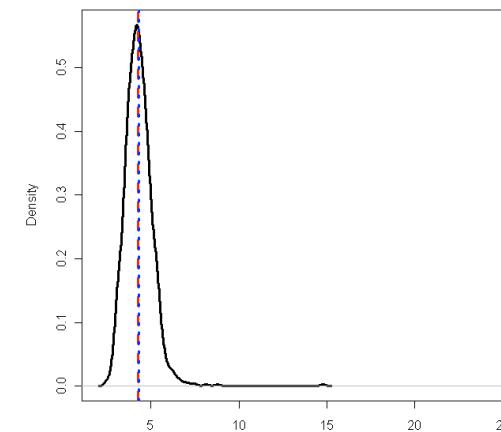
SBB



SBB.Post



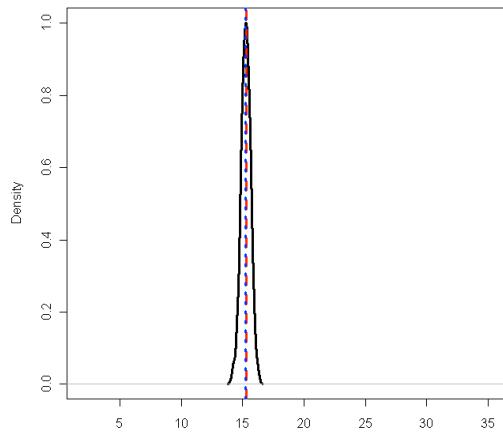
SBB.Prior



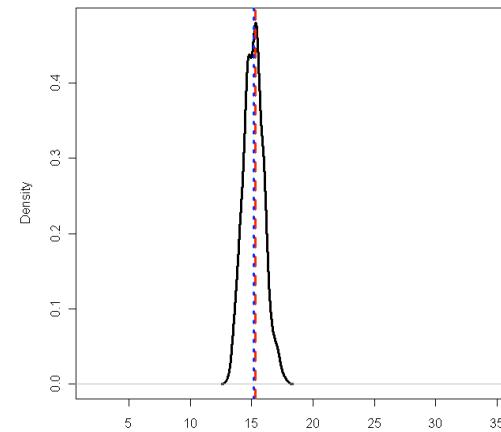
SBB.Prior.Adj

Red: $\hat{\sigma}_e^2 = 15.269$

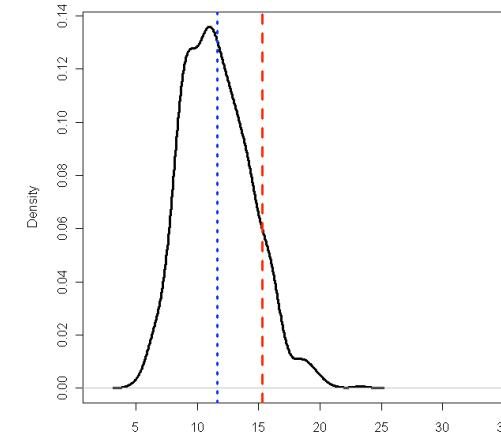
Blue: $\bar{\hat{\sigma}}_e^{2*} = B^{-1} \sum_{b=1}^B \hat{\sigma}_e^{2*(b)}$



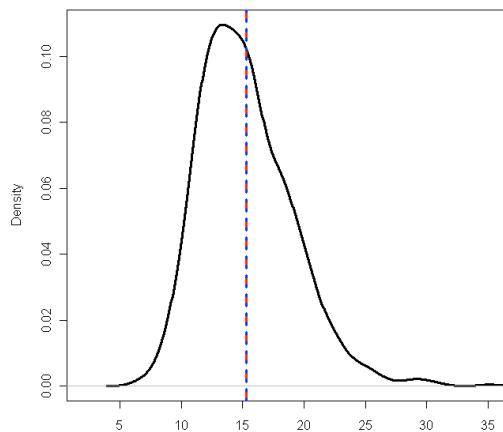
Para



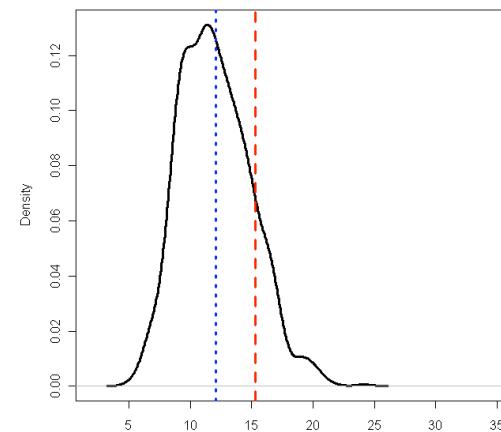
CGR



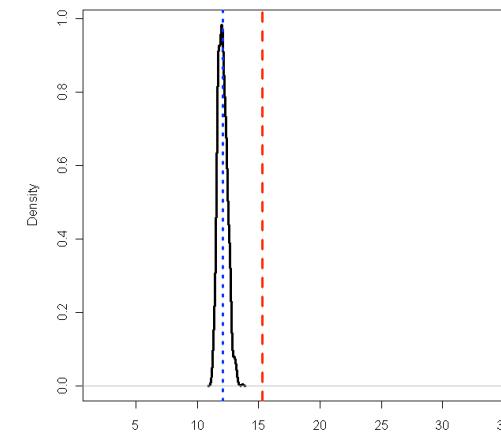
SBB



SBB.Post



SBB.Prior



SBB.Prior.Adj

Concluding Remarks

- The semiparametric block bootstrap methods are simple to implement and are free of both the distribution and the dependence assumptions of the parametric bootstrap
- Their main assumption is that the marginal model is correct
- They lead to **consistent** estimators of confidence intervals (theoretical results are not shown here)
- **A robust alternative:** Protection against within group heterogeneity
- Empirical evaluations confirm these conclusions
- Satisfactory performance when applied to real data

References

1. Beare, S., Chambers, R., Peak, S. and Ring, J.M. (2010). Accounting for Spatiotemporal Variation of Rainfall Measurements when Evaluating Ground-Based Methods of Weather Modification. Working Papers Series 17-10, Centre for Statistical and Survey Methodology, The University of Wollongong, Australia. Available from: <http://cssm.uow.edu.au/publications>
2. Carpenter, J.R., Goldstein, H., Rasbash, J. (2003). A Novel Bootstrap Procedure for Assessing the Relationship between Class Size and Achievement. *Journal of the Royal Statistical Society. Series C (Applied Statistics)*, **52 (4)**, pp. 431-443.
3. Efron, B. (1979). Bootstrap Methods: Another Look at the Jackknife. *The Annals of Statistics*, **7 (1)**, 1 – 26.
4. Efron, B. and Tibshirani, R.J. (1993): *An introduction to the bootstrap*. Chapman & Hall.
5. Rasbash, J., Browne, W, Goldstein, H., Yang, M., Plewis, I., Healy, M., Woodhouse, G., Draper, D., Langford, I. and Lewis, T. (2000) A User's Guide to MLwiN. London: Institute of Education.