The Impact of Bias Correction on Bootstrap Confidence Intervals for First-Order Bifurcating Autoregressive Models

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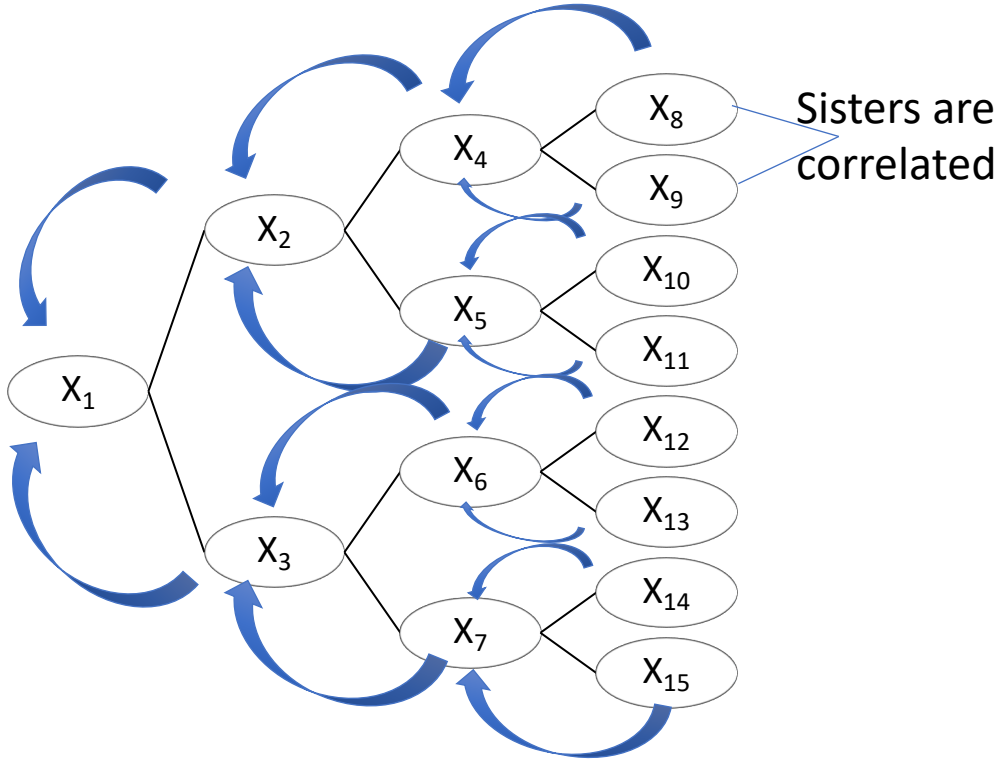
I will talk about

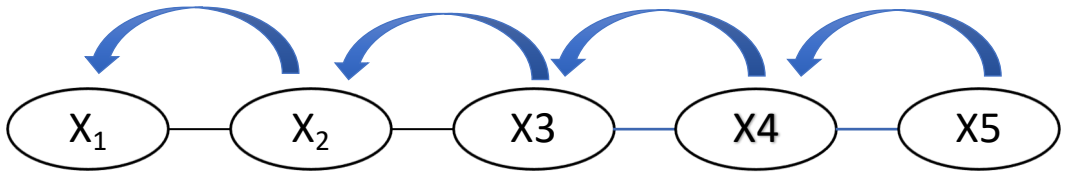
- **First Order Bifurcating Autoregressive Model**
- **Least Squares Estimation**
- **The Problem and the Goal**
- **Bias of the Least Squares Estimators**
- **The Bootstrap Bias Correction Methods**
- **The impact of Bias Correction on CI (Simulation Results)**
- **Conclusions**
- **About This Work**

First Order Bifurcating Autoregressive (BAR(1)) Model

BAR(1) Model is an adaptation of traditional first order autoregressive (AR(1)) model to binary tree structured data, where each individual observation in any generation gives rise to two offspring in the next generation.



A Binary Tree Data with the BAR(1) Structure



Serial Data with the AR(1) Structure

First Order Bifurcating Autoregressive (BAR(1)) Model

- Cowan and Staudte (1986) proposed the first-order BAR (1) model for cell lineage data and introduce the Maximum likelihood estimation under normality assumption.
- It is important to quantify inherited and environmental effects to explain the progression of the quantitative characteristic of the cells (cell lifetime or cell volume at the time of division).

The BAR (1) Model

The traditional AR(1) model is given by

$$X_t = \phi_0 + \phi_1 X_{t-1} + \varepsilon_t, \qquad \text{for all } t \geq 2$$

where,

- X_t is the observed value at time t.
- X_{t-1} is the observed value at time (t-1).
- ϕ_0 and ϕ_1 are the parameters that needs to be estimated, where ϕ_0 is the intercept and ϕ_1 denotes the autoregressive parameter.

The BAR (1) Model

The BAR(1) model is given by

$$X_t = \phi_0 + \phi_1 X_{\left[\frac{t}{2}\right]} + \varepsilon_t, \qquad \text{for all } t \geq 2$$

where

- X_t is an observed value at time t.
- $X_{\left[\frac{t}{2}\right]}$ is the mother of X_t for all $t \geq 1$, where $[u]$ defines the largest integer $\leq u$.
- ϕ_0 and ϕ_1 are the parameters that need to be estimated, where ϕ_1 denotes the maternal correlation or the inherited effect.

The BAR (1) Model

The BAR(1) model can be written

Daughters Mother

$$X_{2t} = \phi_0 + \phi_1 X_t + \varepsilon_{2t},$$
$$X_{2t+1} = \phi_0 + \phi_1 X_t + \varepsilon_{2t+1}, \qquad \text{for all } t \geq 1$$

where,

- X_{2t} *and* X_{2t+1} are an observed sister cells lifetime at time t.
- X_t denotes the mother of X_t for all $t \geq 1$.
- ϕ_0 *and* ϕ_1 are the parameters that needs to be estimated, where ϕ_0 is the intercept and ϕ_1 denotes the maternal correlation or the inherited effect.

The BAR (1) Model

- $\{(\varepsilon_{2t}, \varepsilon_{2t+1}),\ \mathrm{t} \geq 1\}$ are independently and identically distributed (iid) bivariate random variables with mean zero and a variance–covariance structure,

$$\begin{pmatrix} 1 & \theta \\ \theta & 1 \end{pmatrix} \sigma^2,$$

where,

- θ is the correlation between $(\varepsilon_{2t}, \varepsilon_{2t+1})$ or the environmental effect.
- σ^2 is the variance of ε_{2t} and ε_{2t+1}.
- It is assumed that $\phi_t \in (-1, 1), t = 1, .., p$. This implies the process is stationary.
- The correlation coefficient between the sisters (X_{2t}, X_{2t+1}) is defined as ρ and it is given by

$$\rho = \phi_1^2 + (1 - \phi_1^2)\theta.$$

The idea came from

Zhou and Basawa (2005) “Least-squares estimation for bifurcating autoregressive processes” Statistics and Probability Letters, Volume 74(1), 77-88.

- They introduced the least squares estimates for the BAR(p) models including the BAR(1) model and derived the asymptotic distribution for the LS estimators.
- They did not investigate the finite sample properties of these estimators.

Least Squares Estimation

<u>The LS estimators of BAR(1) are given by</u>

$$\hat{\phi}_1 = \frac{\sum_{t=1}^{m} X_t (U_t - \bar{U}_t)}{\sum_{t=1}^{m} (X_t - \bar{X})^2}, \qquad \hat{\phi}_0 = \bar{U}_t - \hat{\phi}_1 \bar{X},$$

where,

$$U_t = \frac{X_{2t} + X_{2t+1}}{2}, \; \bar{X} = \frac{1}{m} \sum_{t=1}^{m} X_t \,, \; \bar{U}_t = \frac{1}{m} \sum_{t=1}^{m} U_t \,, \; m = \frac{n-1}{2},$$

and m the number of triplets (X_t, X_{2t}, X_{2t+1}).

Least Squares Estimation

When substituting U_t in the $\hat{\phi}_1$ and $\hat{\phi}_0$ equations, it gives the common LS equations of the autoregressive process of order one

$$\hat{\phi}_1 = \frac{\sum_{t=1}^{n} X_t \left(X_{\left[\frac{t}{2}\right]} - \bar{X}_t \right)}{\sum_{t=1}^{n} (X_t - \bar{X}_t)^2}$$

$$\hat{\phi}_0 = \left(1 - \hat{\phi}_1\right) \bar{X}_t$$

where, $\bar{X}_t = \frac{1}{n} \sum_{t=1}^{n} \bar{X}_t$.

The Problem

- Although the LS estimators of the BAR model coefficients are asymptotically unbiased, this study shows that the finite sample bias of these estimators can be quite large, which might make inferences based on these estimators to be inaccurate.

- This should not be surprising as it is well-known that the LS estimators for the AR(1) model tend to have significant biases, especially when the autoregressive parameter is close to the boundaries (see Hurwicz (1950)).

The Goal

- Study the bias of LS estimates for BAR(1).
- Propose a bias correction method for the LS estimators of the BAR(1) model.
- Study the Confidence Interval coverage before and after bias correction.

Bias of the Least Squares Estimators

- Monte Carlo Study is used for demonstrating empirically the bias of the LS estimator of the BAR(1) autoregressive coefficient ϕ_1.

- The Monte Carlo Setting:
  - Perfect binary trees of size n = 31, 63, 127, 255 (accounting for varying number of generations; g = 4, 5, 6, 7, respectively)
  - Combination of $\phi_1 = \pm 0.15(\pm 0.15) \pm 0.90$ and $\theta = \pm 0.15(\pm 0.15) \pm 0.90$
  - The model intercept $\phi_1 = 10$
  - All generated trees are assumed stationary
  - The initial observation in the tree, X_1, is randomly selected from a large simulated binary tree of size 127
  - Under each of these settings, N = 50,000 trees are generated and the LS estimator ϕ_1^{LS} is obtained for each tree

Bias of the Least Squares Estimators

- The empirical bias and absolute relative bias (ARB) of ϕ_1^{LS} are calculated as follows:

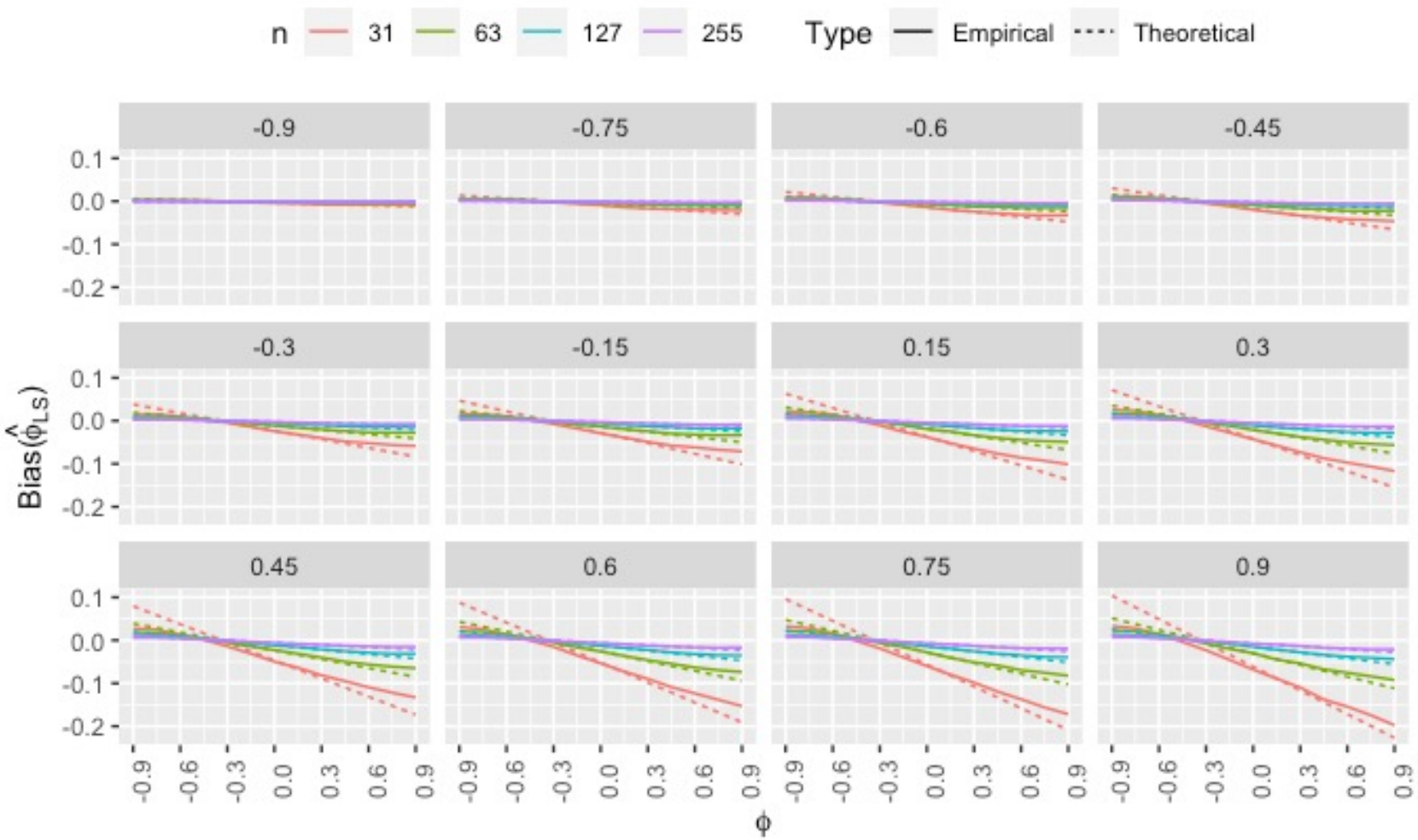
$$\widehat{\mathrm{BIAS}}(\hat{\phi}_1^{\mathrm{LS}}) = \frac{1}{N}\sum_{j=1}^{N}\left(\hat{\phi}_1^{\mathrm{LS},(j)} - \phi_1\right),$$

$$\widehat{\mathrm{ARB}}(\hat{\phi}_1^{\mathrm{LS}}) = \left|\widehat{\mathrm{BIAS}}(\hat{\phi}_1^{\mathrm{LS}})/\phi_1\right|,$$

where, $\phi_1^{\mathrm{LS},(j)}$ is the LS estimator from iteration $j = 1,2,\ldots,N$.

Bias of the Least Squares Estimators

The Monte Carlo results are summarized in the following graphs

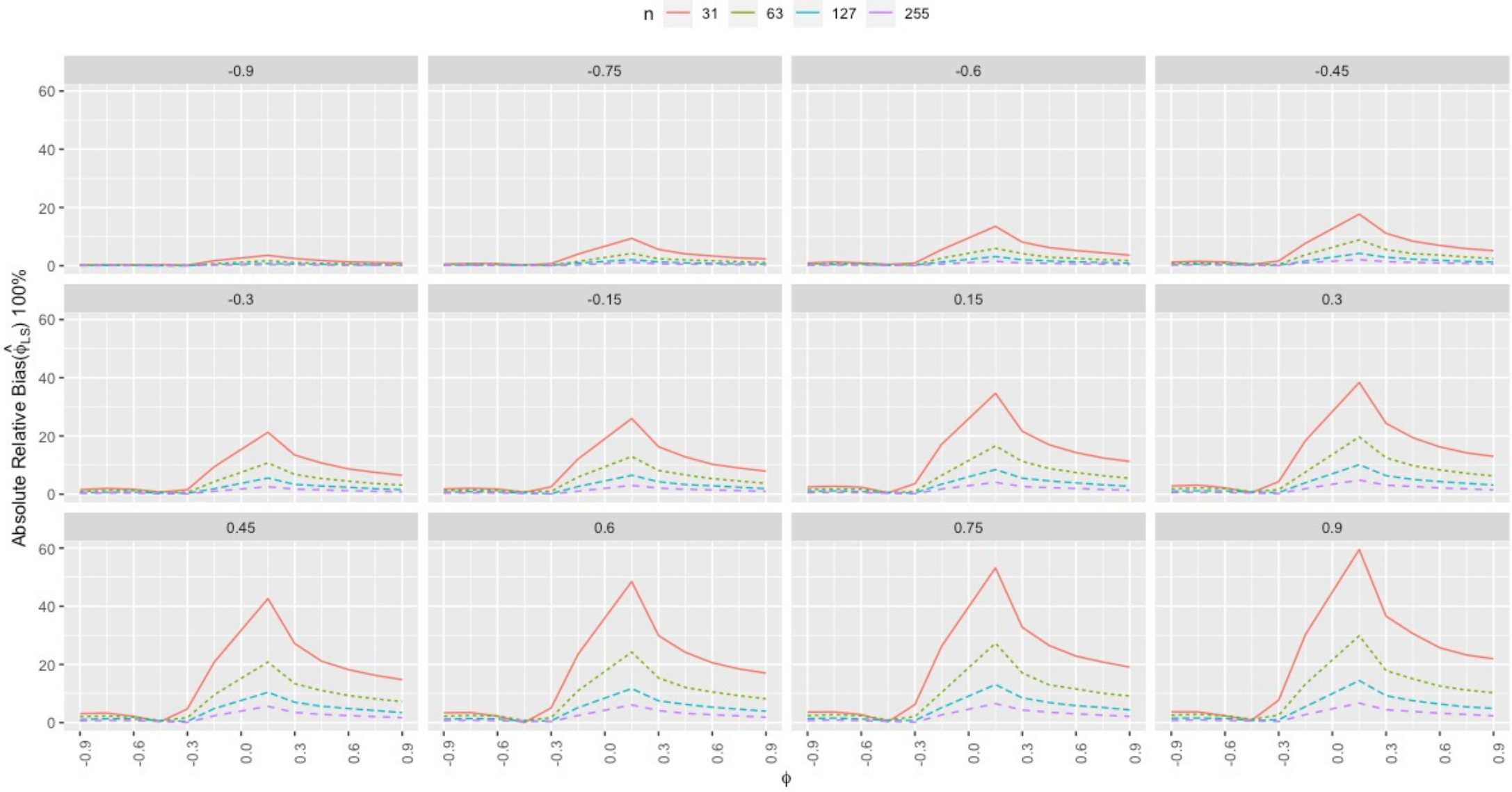


Bias of the Least Squares Estimators

Comments on the results:

- The bias of ϕ_1^{LS} can be quite significant for many combinations of ϕ_1 and θ, especially for small sample sizes.
- the magnitude of bias is considerable when θ is positive and ϕ_1 is larger than -0.45.
- In general, it is clear that ϕ_1^{LS} tends to slightly overestimate large negative value of ϕ_1 < -0.45 and underestimates all values of ϕ_1 with the magnitude of overestimation increasing as we move towards +1.
- the bias appears to be linear in ϕ_1 over the major part of its domain.

Bias of the Least Squares Estimators



Bias of the Least Squares Estimators

Comments on the results:

- In general, the pattern of relative bias is the same for all ϕ_1 and θ combinations but with different relative bias levels. The relative bias level increases as the value of θ goes from the -1 to +1.
- Also, the relative bias decreases as the sample size increases.
- The relative bias continues to be considerably large for values of ϕ_1 that are larger than -0.30 as long as remains θ away from +1.
- For small sample sizes (n = 31) and when ϕ_1 is near zero (-0.15 to 0.15), the bias of ϕ_1^{LS} can be as large as 5% to 60% (as moves from -1 to +1) of the true value of ϕ_1.

Bias-Correction Methods for the LS Estimators

Two Methods:

Elbayoumi and Mostafa (2020), showed that the following two methods for correcting the bias of the LS estimates for the BAR(1) model:

1. Bootstrap Bias Correction
    - Single Bootstrap
    - Fast Double Bootstrap

2. Bias Correction with Linear Bias Function

The Bootstrap Bias Correction Methods

Single Bootstrap Bias Correction Algorithm

Given the original sample X_t^n, compute the LS estimates $\hat{\phi}_0$ and $\hat{\phi}_1$, and the estimated errors $\hat{e}_{2t}$ and $\hat{e}_{2t+1}$ for all $t \geq 1$. From the estimated errors, draw B bootstrap samples each of size $m = (n-1)/2$ by sampling with replacement from among the pairs $(\hat{e}_{2t}, \hat{e}_{2t+1})$ and form X_t^{n*}, $b = 1, \dots, B$ by

$$X_{2t,b}^{n*} = \hat{\phi}_0^{LS} + \hat{\phi}_1^{LS} X_t^n + \hat{e}_{2t,b}, \text{ and } X_{2t+1,b}^{n*} = \hat{\phi}_0^{LS} + \hat{\phi}_1^{LS} X_t^n + \hat{e}_{2t+1,b}$$

The initial value $X_1^* = X_1$ in all trees. Next, for each bootstrap binary tree sample, compute the $\hat{\phi}_{1,b}^*$, $b = 1, \dots, B$. Then, obtain the estimated bias $\beta_{\hat{\phi}_1}$ as,

$$\hat{\beta}_{\hat{\phi}_1^{LS}} = \frac{1}{B} \sum_{b=1}^{B} \left(\hat{\phi}_{1,b}^* - \hat{\phi}_1^{LS} \right).$$

Finally, The bootstrap bias corrected LS estimator is $\hat{\phi}_1^{SBC} = \hat{\phi}_1^{LS} - \hat{\beta}_{\hat{\phi}_1^{LS}}$.

The Bootstrap Bias Correction Methods

Fast Double Bootstrap Bias Correction Algorithm

Given the original sample X_t^n, apply the single bootstrap algorithm to generate B_1 bootstrap replicates of the tree, X_t^{n*}, $b = 1, \dots, B_1$. Using the LS estimates $\hat{\phi}_0^*$, $\hat{\phi}_1^*$ and the errors $(\hat{e}_{2t}^*, \hat{e}_{2t+1}^*)$ computed from each of B_1 the bootstrap samples X_t^{n*}, draw $B_2 = 1$ bootstrap sample by sampling with replacement m pairs errors and forming X_t^{n**} as follows

$$X_{2t,b}^{n**} = \hat{\phi}_0^* + \hat{\phi}_1^* X_t^* + \hat{e}_{2t,b}^{**}, \text{ and } X_{2t+1,b}^{n**} = \hat{\phi}_0^* + \hat{\phi}_1^* X_t^* + \hat{e}_{2t+1,b}^{**}$$

We keep the initial value $X_1^{**n} = X_1^{n*}$ in all second phase trees. Next, for each second phase bootstrap samples, compute $\hat{\phi}_{1,b}^{**}$. This results in two series of bootstrap iterates $\hat{\phi}_{1,b}^*$ and $\hat{\phi}_{1,b}^{**}$, for $b = 1, \dots, B_1$. Define the Monte Carlo estimate of the second phase bias adjustment factor $\gamma_{\hat{\phi}_1}^{LS}$ as,

$$\gamma_{\hat{\phi}_1}^{LS} = \hat{\beta}_{\hat{\phi}_1^{LS}} - \frac{1}{B_1} \sum_{b=1}^{B_1} \left(\hat{\phi}_{1,b}^{**} - \hat{\phi}_{1,b}^* \right)$$

Finally, The fast double bootstrap bias corrected LS estimator is $\hat{\phi}_1^{FDBC} = \hat{\phi}_1^{LS} - \hat{\beta}_{\hat{\phi}_1^{LS}} - \gamma_{\hat{\phi}_1}^{LS}$, where $\hat{\beta}_{\hat{\phi}_1^{LS}}$ is the estimated bias from the single bootstrap bias correction algorithm .

The Bootstrap Bias Correction Methods

Bias Correction with Linear Bias Function

Theorem: Consider the stationary BAR(1) model (i.e.,$|\phi_1|<1$) and suppose the model errors have finite fourth-order moments (i.e ., $E(\varepsilon_t^4) < \infty\ \forall t$). Then, the bias of the LS estimator ϕ_1^{LS} is given by

$$E\left(\phi_1^{\mathrm{LS}} - \phi_1\right) = -\frac{1}{n}(1+\theta)(1+3\phi_1) + O(n^{-2}).$$

Therefore, the corrected LS estimator for the autoregressive parameter ϕ_1 is

$$\hat{\phi}_1^{LBC} = \frac{1}{n - 3(1+\hat{\theta})}\left(n\hat{\phi}_1^{LS} + (1+\hat{\theta})\right),$$

where, $\hat{\theta} = \frac{1}{m\hat{\sigma}^2}\sum_{t=1}^{m}\hat{e}_{2t}\hat{e}_{2t+1}$ and $\hat{\sigma}^2 = \frac{1}{(n-3)}\sum_{t=1}^{n}\hat{e}^2$.

The proof of this theorem can be found on Page 4 of Elbayoumi T. M. and Mostafa S. A. (2020), On the Estimation Bias in First-Order Bifurcating Autoregressive Models, Stat Journal., 17;00:1-6.
https://doi.org/10.1002/sta4.342

The Bias Correction methods

- All proposed bias-correcting estimators reduce the bias of the LS estimator for nearly all combinations of ϕ_1 and θ even when the sample size is small.
- The success of the linear-bias-correction method in reducing the bias is not surprising since the bias of the LS estimator is indeed, approximately, linear as a function of ϕ_1.
- While both the single and fast double bootstrap bias-corrected estimators, produce significance reductions in the bias, the fast double bootstrap estimator has better performance than the single bootstrap estimator for small samples.
- For moderate to large samples, both methods perform similarly.

The Bias Correction methods

- The bootstrap estimators have better performance for values of ϕ_1 near the boundaries (-1,+1).
- There is no clear winner among the two methods for values of ϕ_1 that are away from the boundaries.
- The large bias improvement observed for the corrected estimator comes, in some cases, at the cost of increasing the RMSE compared to the LS estimator for small samples.

The impact of Bias Correction on CI

- The asymptotic normal CI using the variance formula, $\hat{\phi}_1^{LS} \pm z_\alpha \text{ se}\left(\hat{\phi}_1^{LS}\right)$
- the asymptotic normal CI using bootstrap standard deviation, $\hat{\phi}_1^{LS} \pm z_\alpha \, se_{boot}$
- the percentile CI, $\left(\hat{\phi}^*_{1(\alpha N)}, \hat{\phi}^*_{1((1-\alpha)N)}\right)$
- the asymptotic CI based on single bootstrap bias correction, $\hat{\phi}_1^{SBC} \pm z_\alpha \text{ se}\left(\hat{\phi}_1^{SBC}\right)$
- the asymptotic CI based on fast double bootstrap bias correction, $\hat{\phi}_1^{FDBC} \pm z_\alpha \text{ se}\left(\hat{\phi}_1^{FDBC}\right)$
- the percentile CI based on single bootstrap, $\left(\hat{\phi}^{SBC}_{1(\alpha N)}, \hat{\phi}^{SBC}_{1((1-\alpha)N)}\right)$
- the percentile CI based on fast double bootstrap, $\left(\hat{\phi}^{FDBC}_{1(\alpha N)}, \hat{\phi}^{FDBC}_{1((1-\alpha)N)}\right)$
- the Bias Corrected and accelerated CI, $\left(\hat{\phi}^*_{1(\alpha_1)}, \hat{\phi}^*_{1(\alpha_2)}\right)$, where $\alpha_1 = \Phi(2\hat{z}_0 + z_\alpha)$, $\alpha_2 = \Phi(2\hat{z}_0 + z_{1-\alpha})$, and $\hat{z}_0 = \Phi^{-1}\left(\frac{1}{N}\sum_{b=1}^{N} I\left(\hat{\phi}^*_{1b} < \hat{\phi}_1^{LS}\right)\right)$.

The impact of Bias Correction on CI

Monte Carlo Study:

The simulation experiments are designed to:

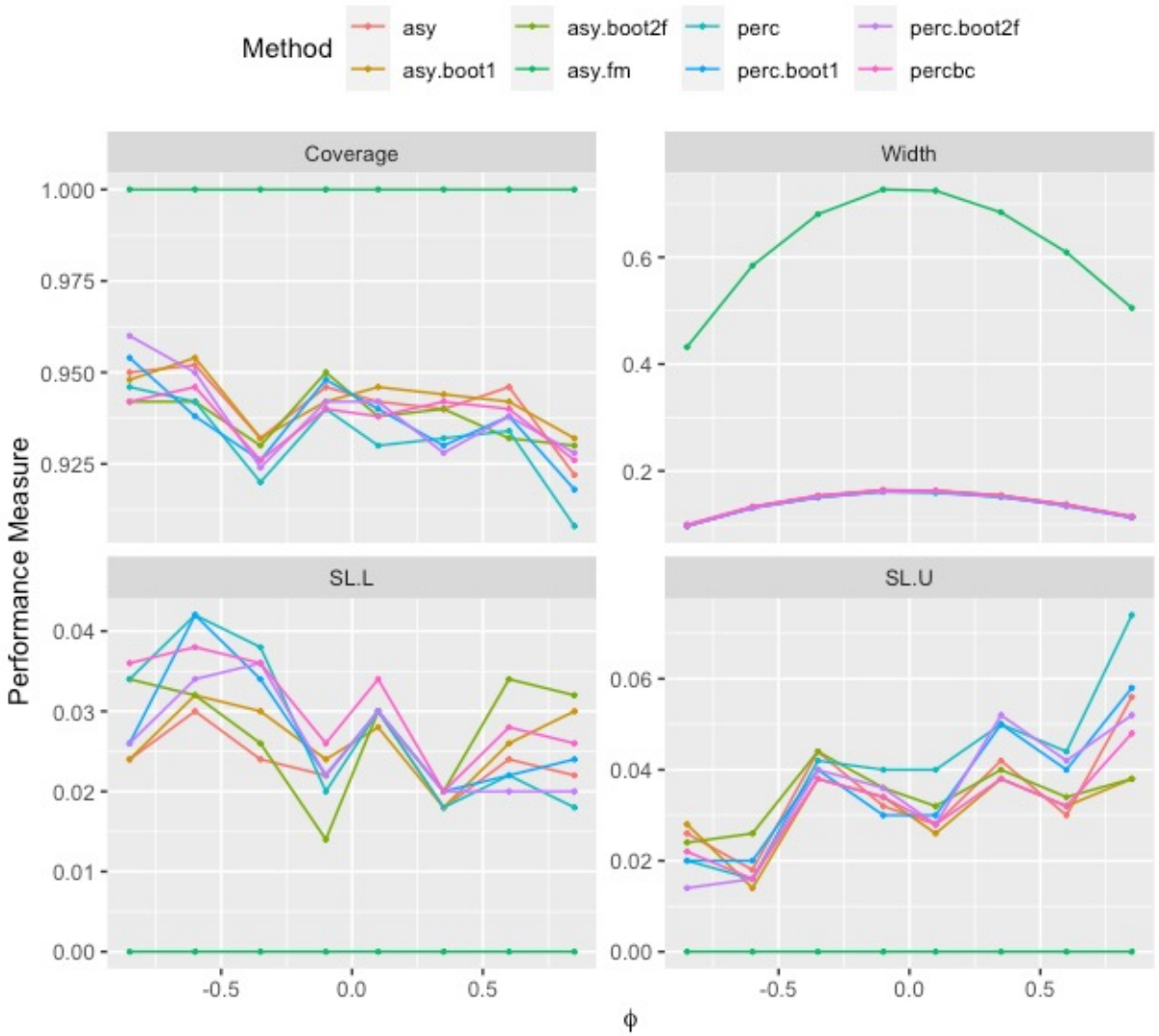
1. evaluate the coverage of several confidence intervals before and after bias correction of the LS estimator of the autoregressive coefficient in the BAR(1) model
2. compare the performance of proposed bias correction methods on the confidence intervals converge

Simulation Settings

- Under each of these settings, $N = 500$ trees are generated and the LS estimator ϕ_1^{LS} is obtained for each tree.
- Five confidence interval for the coefficient ϕ_1 are obtained. Namely, the asymptotic normal CI using the variance formula, the asymptotic normal CI using bootstrap standard deviation, the percentile CI, the asymptotic CI based on single bootstrap bias correction, the asymptotic CI based on fast double bootstrap bias correction, the percentile CI based on single bootstrap, the percentile CI based on fast double bootstrap, and the Bias Corrected percentile CI.
- In both single bootstrap and fast double bootstrap methods, the number of resamples is $B = 199$.
- For each estimated CI, the nominal CI coverage is 95%.

The impact of Bias Correction on CI

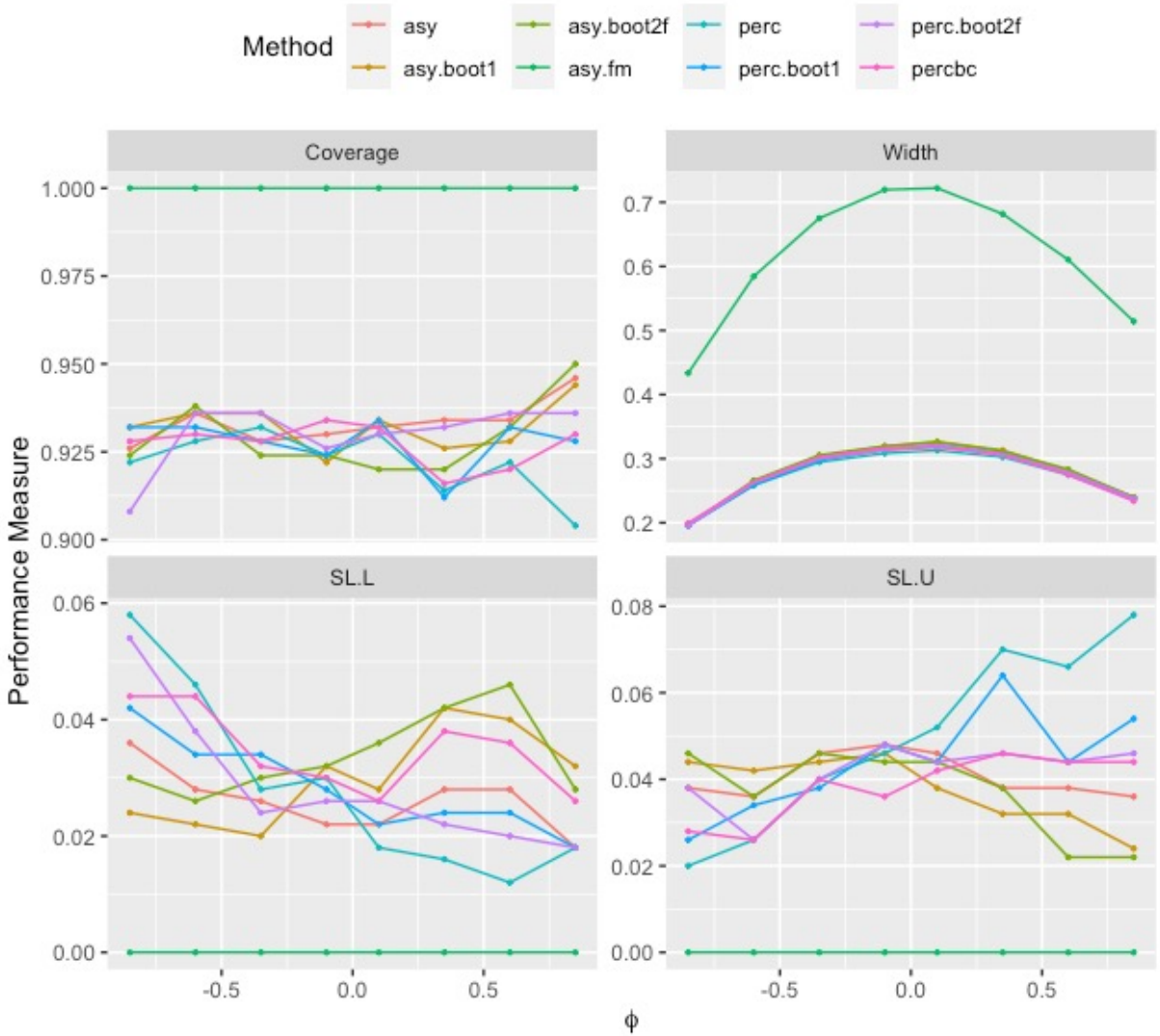
Simulation Results:



The coverage, width, symmetry of CIs of ϕ_1 at $\theta = -0.9$ and n = 63.

The impact of Bias Correction on CI

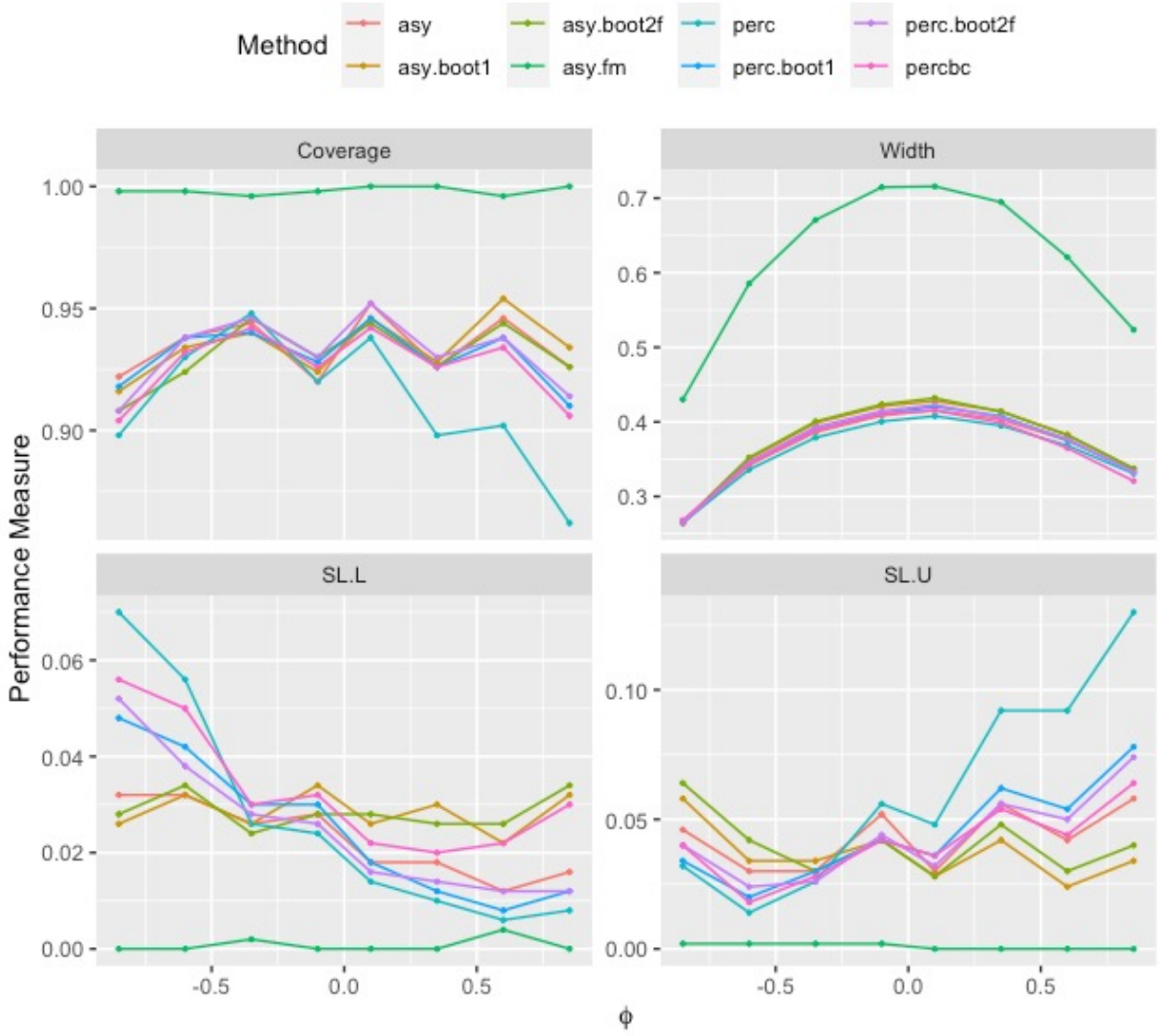
Simulation Results:



The coverage, width, symmetry of CIs of ϕ_1 at $\theta = -0.6$ and n = 63.

The impact of Bias Correction on CI

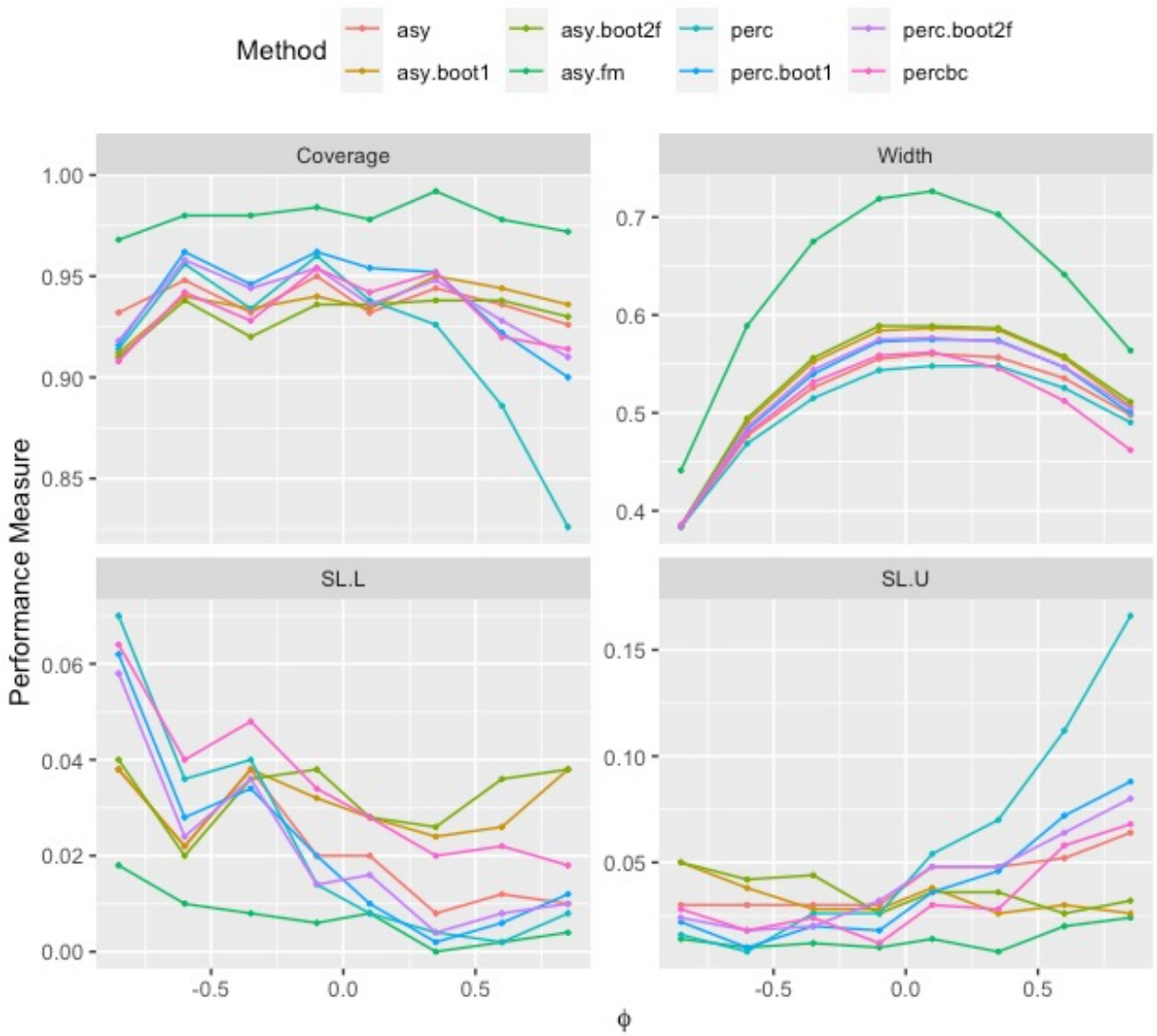
Simulation Results:



The coverage, width, symmetry of CIs of ϕ_1 at $\theta = -0.3$ and n = 63.

The impact of Bias Correction on CI

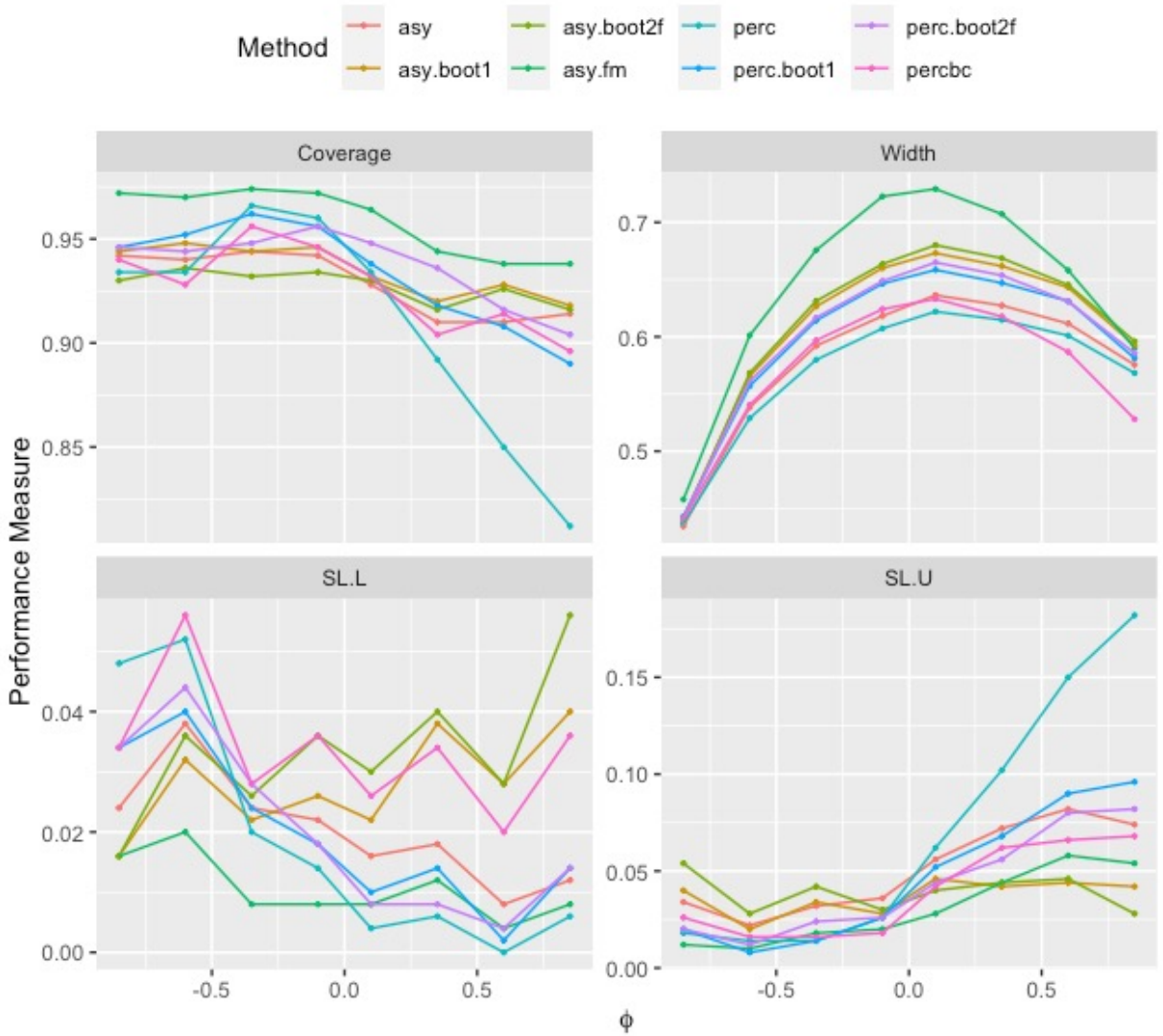
Simulation Results:



The coverage, width, symmetry of CIs of ϕ_1 at $\theta = 0.3$ and n = 63.

The impact of Bias Correction on CI

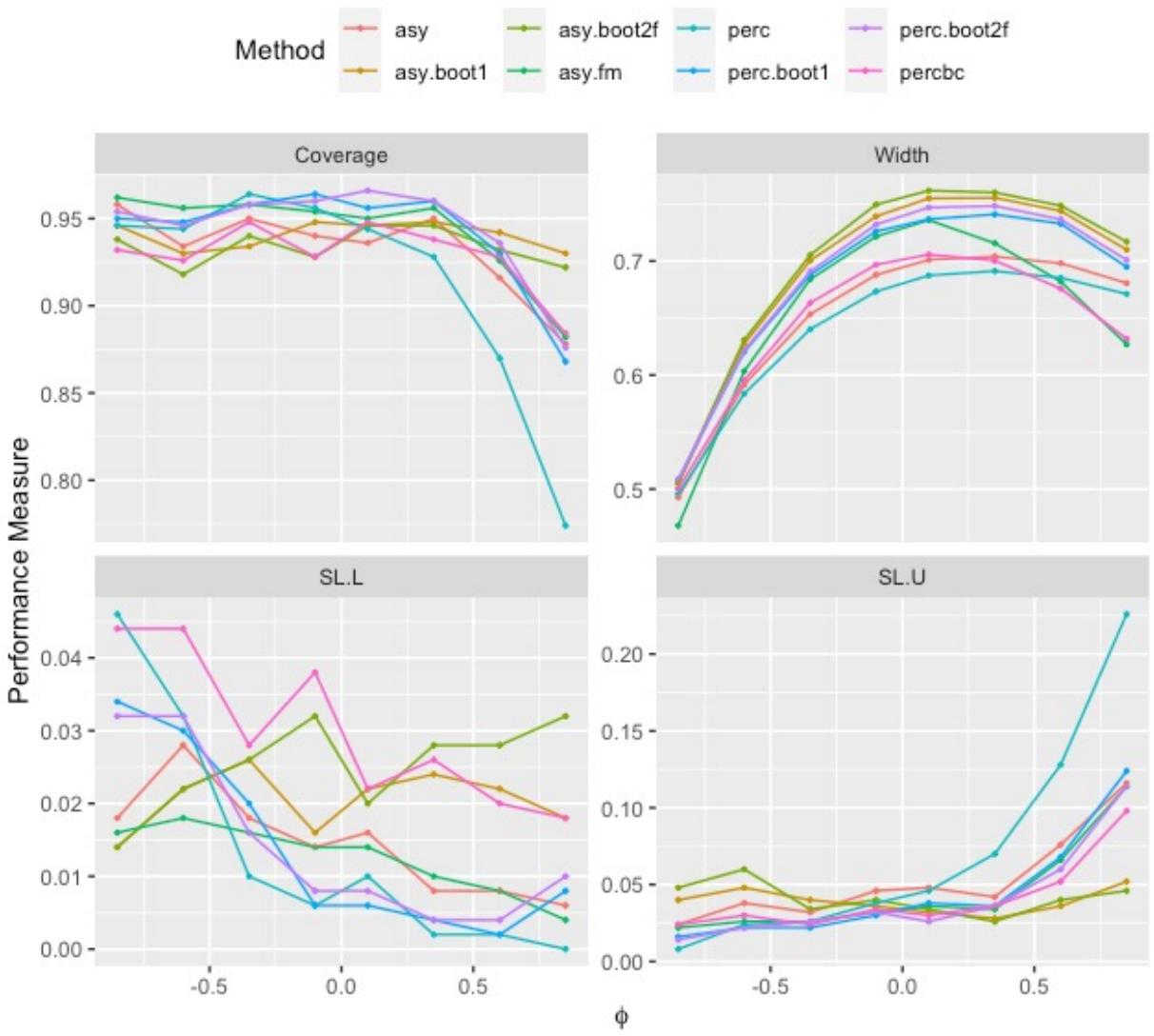
Simulation Results:



The coverage, width, symmetry of CIs of ϕ_1 at $\theta = 0.6$ and n = 63.

The impact of Bias Correction on CI

Simulation Results:



The coverage, width, symmetry of CIs of ϕ_1 at $\theta = 0.9$ and n = 63.

The impact of Bias Correction on CI

- The asymptotic normal CI using the variance formula of Zhue and Basawa (2005) has a large coverage (100%) for all ϕ_1 and θ is negative. The coverage is less than 100% but still above the 95% when θ moves to +1 and the coverage drops to less than 95% significantly when the bias gets its highest level when ϕ_1 and θ are close to +1.
- There is no winner CI method when for all values of ϕ_1 and θ is negative except when $\phi_1 > 0$ and $\theta = -0.3$.
- When the bias gets its higher levels for each value of θ and $\phi_1 > 0$, the asymptotic CIs based on single bootstrap bias correction and based on fast double bootstrap bias correction converges still robust against the bias.

Conclusions

The above results suggest that

- Either the single or fast double bootstrap bias correction estimators are recommended for correcting the LS estimation bias for the BAR(1) model.
- If the practitioner is concerned with the computational cost associated with the bootstrap estimators, the linear bias correcting estimator can serve as a good alternative that can significantly reduce the bias.
- It is recommended to use the asymptotic CIs based on single bootstrap bias correction and based on fast double bootstrap bias correction.

About This Work

- This work can be extended to the higher order BAR models. For more details please see (Elbayoumi T. M. and Mostafa S. A. (2021), On the Estimation Bias in First-Order Bifurcating Autoregressive Models, Stat Journal., 17;00:16.

  https://doi.org/10.1002/sta4.342)

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SPECIAL ISSUE PAPER

On the estimation bias in first-order bifurcating autoregressive models

Tamer M. Elbayoumi, Sayed A. Mostafa

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About This Work

The authors of this article created R Package. The package name is bifurcatingr. It can be download from CRAN (**The Comprehensive R Archive Network**).

https://cran.r-project.org/web/packages/bifurcatingr/index.html

bifurcatingr: Bifurcating Autoregressive Models

Estimation of bifurcating autoregressive models of any order, p, BAR(p) as well as several types of bias correction for the least squares estimators of the autoregressive parameters as described in Zhou and Basawa (2005) <doi:10.1016/j.spl.2005.04.024> and Elbayoumi and Mostafa (2020) <doi:10.1002/sta4.342>. Currently, the bias correction methods supported include bootstrap (single, double and fast-double) bias correction and linear-bias-function-based bias correction. Functions for generating and plotting bifurcating autoregressive data from any BAR(p) model are also included.

Version:	1.0.0
Depends:	R (≥ 2.10)
Imports:	graphics (≥ 4.0.0), igraph (≥ 1.2.5), MASS (≥ 7.3.0)
Suggests:	knitr, rmarkdown
Published:	2021-02-15
Author:	Tamer Elbayoumi [aut, cre], Sayed Mostafa [aut]
Maintainer:	Tamer Elbayoumi <tmelbayoumi at ncat.edu>
License:	GPL-3
NeedsCompilation:	no
Materials:	README
CRAN checks:	bifurcatingr results

Downloads:

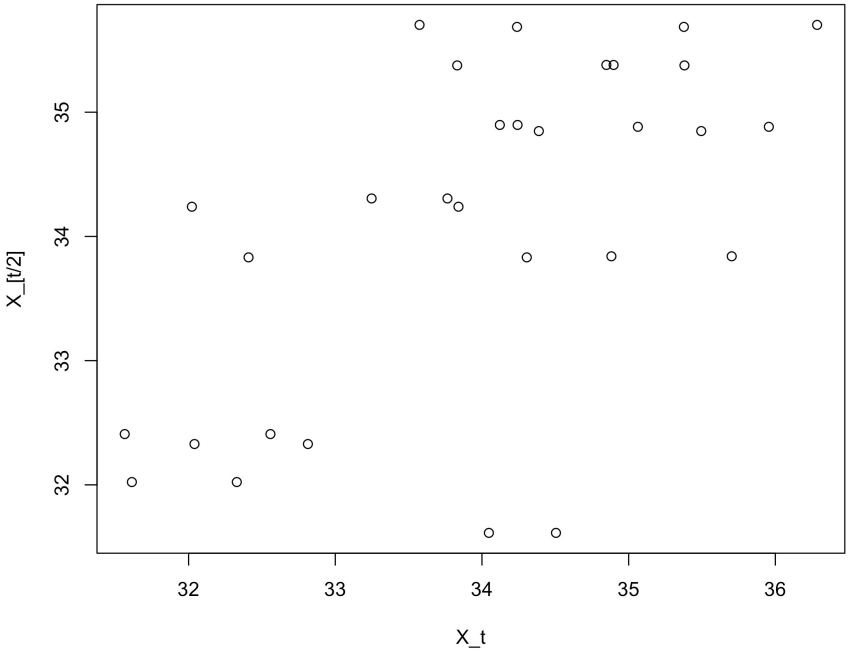
Reference manual:	bifurcatingr.pdf
Package source:	bifurcatingr_1.0.0.tar.gz
Windows binaries:	r-devel: bifurcatingr_1.0.0.zip, r-release: bifurcatingr_1.0.0.zip, r-oldrel: not available
macOS binaries:	r-release: bifurcatingr_1.0.0.tgz, r-oldrel: not available

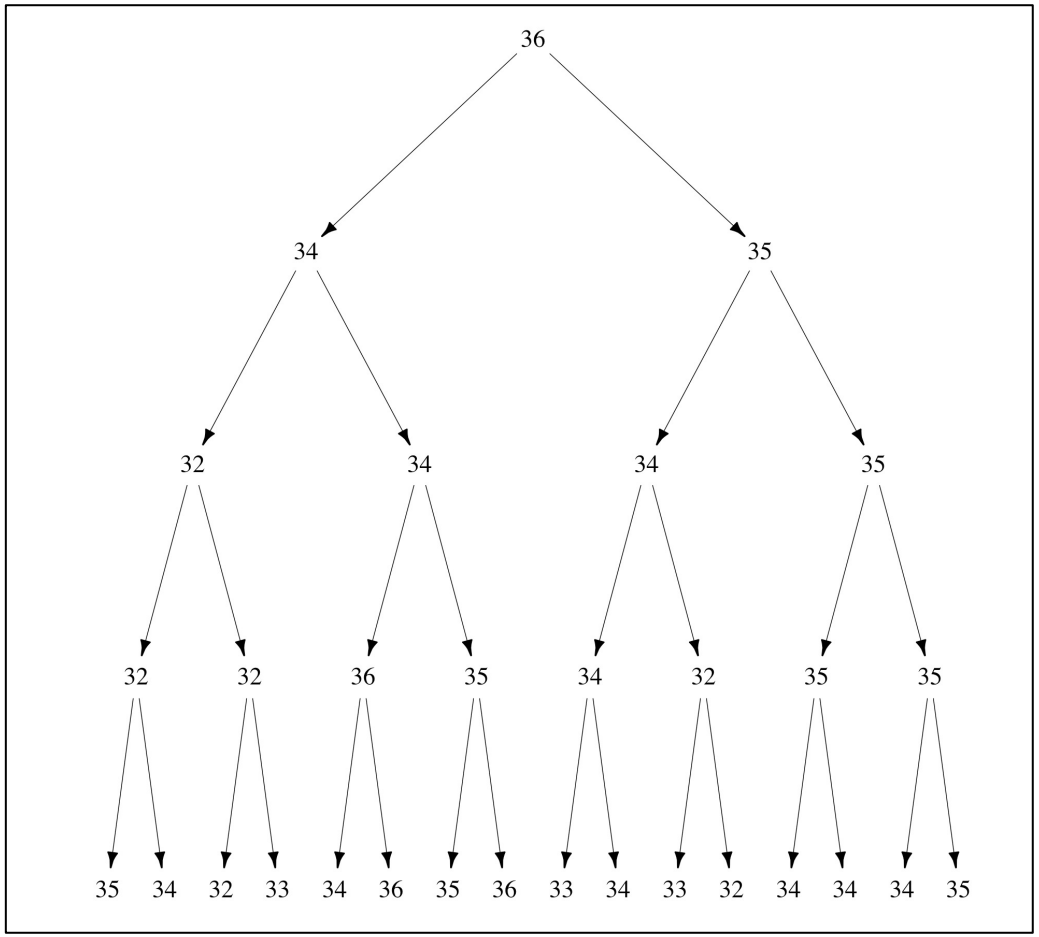
Linking:

Please use the canonical form `https://CRAN.R-project.org/package=bifurcatingr` to link to this page.

About This Work

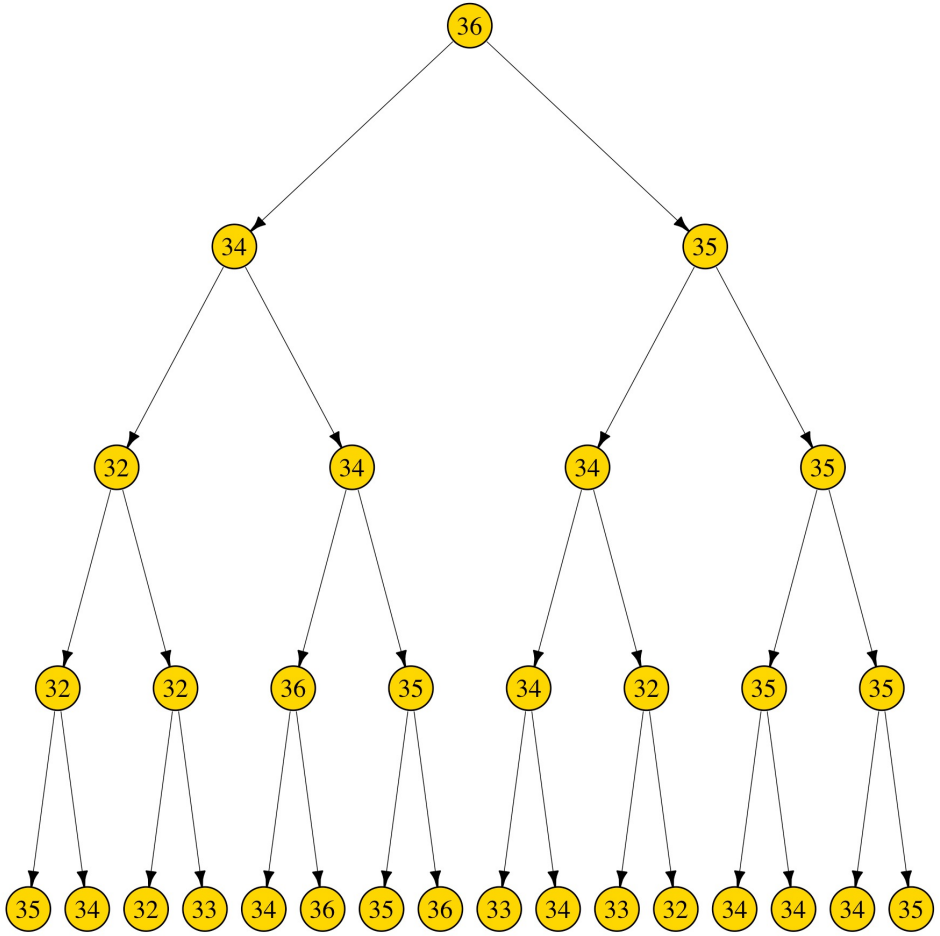
```
> library(bifurcatingr)
> z<-bfa.tree.gen(31,1,1,1,0.5,0.5,0,10,c(0.7))
> bfa.tree.plot(z)
> bfa.scatterplot(z,1)
```





About This Work

bfa.tree.plot(z, shape = "circle", vertex.color="gold")



About This Work

```
> z<-bfa.tree.gen(127,1,1,1,-0.9,-0.9,0,10,c(0.6))
> bfa.ls(z,1)
$coef
     Intercept   X_[t/2]
[1,]  9.183517 0.6333091

$error.cor
[1] -0.9192077

>
```

About This Work

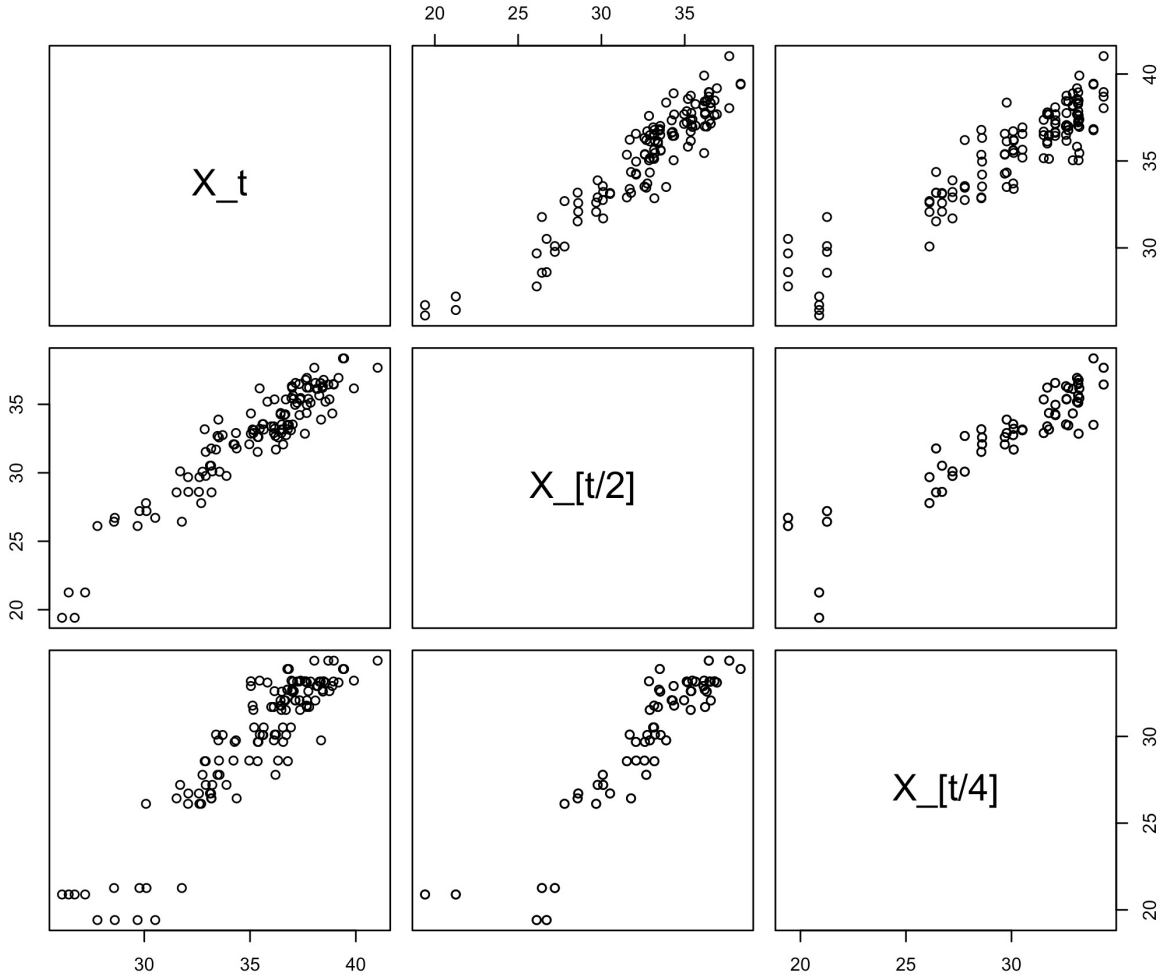
```
> z<-bfa.tree.gen(127,2,1,1,-0.9,-0.9,0,10,c(0.5,0.3))
> bfa.ls(z,2)
$coef
     Intercept   X_[t/2]   X_[t/4]
[1,]  10.28216 0.4941249 0.2967057

$error.cor
[1] -0.8181084

>
```

About This Work

```
> bfa.scatterplot(z,2)
>
```



About This Work

```
> bfa.ls.bc(z,2,method="boot2fast")
[1] 0.4956211 0.2941134
>
```

In Progress

- **A continuation of this work, the bifurcatingr package will be updated and we will add to it the Confidence Intervals methods.**

References

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Thank you!