Introduction to `BNPTSclust`

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Abstract

This document explains detailedly how to use the functions from the `BNPTSclust` package, which perform the Bayesian Nonparametric Algorithm for Time Series Clustering developed by Nieto-Barajas and Contreras-Cristan (2014). Each function implements a Gibbs Sampler to approximate the posterior distribution of the parameters that will define the final clustering. Section 1 gives a brief introduction to the problem that wants to be solved and its relevance. Section 2 outlines some theoretical results about how the clustering is obtained through the algorithm. Section 3 explains how to use each of the functions from the package and shows the results of some worked examples.

Contents

1 Introduction

Data classification is an important aspect to consider while studying a sample because it allows us to identify the heterogeneity present in the data. The explanation of such source of heterogeneity might give us more information about the data set which we might not have considered at first. Therefore, it is relevant to have data classification methods. In particular, a time series clustering algorithm would let us understand which variables have the same or different behavior through time.

Statistics has developed solutions for data classification during the course of its development. Nevertheless, many of them depend on the researcher's own criteria to determine the final groupings of the data.

The Bayesian Nonparametric Approach proposed by Nieto-Barajas and Contreras-Cristan (2014) provides an objective time series clustering scheme, because the classification mechanism is decided by the model itself. The algorithm is computer intensive, but technological development has given feasibility to the bayesian nonparametric tools it employs, which have had an acceptable performance so far.

2 Theoretical bases of the model

Bayesian analysis carries out statistical inference by combining the likelihood function of a sample with some prior information of the variable of interest. This prior information is typically modeled by assuming that the variable of interest follows a probability distribution, which is known as a *prior distribution.* This distribution is incorporated into the analysis through Bayes' Theorem to obtain the *posterior distribution* of the variable of interest. Inference is made once the *posterior distribution* is obtained.

Let $\mathbf{y_i} = \{y_{it} : t = 1, ..., T\}, i = 1, ..., n$, denote a time series and $\mathbf{y} = \{\mathbf{y_1}, ..., \mathbf{y_n}\}$ denote the sample of time series under consideration. Each observation is modeled as if it followed a dynamic linear model of the form:

$$y_{it} = F_{it}\theta_{it} + \epsilon_{it} \tag{1}$$

$$\theta_{it} = \rho\theta_{it-1} + \nu_{it} \tag{2}$$

where $\epsilon_{it} \sim N\left(0, \sigma^2_{\epsilon_i}\right)$ and $\nu_{it} \sim N\left(0, \sigma^2_{\theta}\right)$.

Equation (2) is known as the evolution equation and it represents an autoregressive process of order 1. Every θ_{it} accounts for time dependencies in the observations.

To accomodate level, trends, seasonal and temporal components, equation (1) is defined as:

$$E[y_{it}] = \mu_i + \omega_i^{'} g(t) + \upsilon_i^{'} h(t) + \theta_{it} \tag{3}$$

where μ_i denotes the level of the series; $\omega_i^{'} g(t)$ denotes a polynomial trend of the form: $\omega_{1i}t + \omega_{2i}t^2 + ... + \omega_{ni}t^n$ and $\upsilon_i^{'} h(t)$ denotes seasonal components like: $\upsilon_{1i} I(January) + ... + \upsilon_{11i} I(November)$.

The time series will be clustered according to the parameters that determine the mean level of the series, i.e. the parameters in vector $\eta_\mathbf{i} = (\mu_i, \omega_\mathbf{i}, \nu_\mathbf{i}, \theta_\mathbf{i})$. However, not all parameters might be useful for clustering, since two series that share the same trend and seasonalities may be desired to belong of the same cluster, despite their level differences.

Therefore, we can separate $\eta_\mathbf{i} = (\alpha_\mathbf{i}, \beta_\mathbf{i}, \theta_\mathbf{i})$ where $\alpha_\mathbf{i}$ will contain the parameters *not* considered for clustering and $\gamma_i = (\beta_\mathbf{i}, \theta_\mathbf{i})$ will contain the parameters used for clustering.

Given all of these specifications, the general sampling model for each time series will be defined as:

$$\mathbf{y_i} = \mathbf{Z}\alpha_\mathbf{i} + \mathbf{X}\beta_\mathbf{i} + \theta_\mathbf{i} + \epsilon_\mathbf{i}, i = 1, ..., n. \tag{4}$$

where $\mathbf{Z}$ and $\mathbf{X}$ have dimensions $T \times p$ and $T \times d$ respectively. p represents the number of parameters that will not be considered for clustering and d is the number of parameters that will be taken into account for clustering. $\alpha_\mathbf{i}$ is a $T \times 1$ vector, $\beta_\mathbf{i}$ is a $d \times 1$ dimensional vector and θ_i has dimension $T \times 1$. $\epsilon_i \sim N_T(0, \sigma^2_{\epsilon_i} I)$.

2.1 Prior specification on $\gamma_\mathbf{i}$

This prior specification is one of the most important for the model, because it defines the classification mechanism that will produce the time series clusters.

The whole vector $\gamma = \{\gamma_\mathbf{1}, ..., \gamma_\mathbf{n}\}$ is assumed to come from a *Poisson-Dirichlet* process denoted by $\mathcal{PD}(a, b, G_0)$. The parameters a and b characterize the process completely but the centering measure G_0 can be specified externally. For the model, it is assumed that $G_0 = N_d(\beta|\mathbf{0}, \mathbf{\Sigma}_\beta) \times N_T(\theta|\mathbf{0}, \mathbf{R})$ with $\mathbf{\Sigma}_\beta = \mathbf{diag}(\sigma^\mathbf{2}_{\beta_\mathbf{1}}, ..., \sigma^\mathbf{2}_{\beta_\mathbf{n}})$ and $R_{jk} = \sigma^2_\theta \rho^{|j-k|}$.

The *Poisson-Dirichlet* process is almost surely a discrete random measure and it has the property that each $\gamma_\mathbf{i}$ is a copy from an element in the vector $\gamma_\mathbf{-i} = \{\gamma_\mathbf{1}, ..., \gamma_\mathbf{i-1}, \gamma_\mathbf{i+1}, ..., \gamma_\mathbf{n}\}$ with certain probability and it is a drawing from the density g_0 associated to G_0 with another probability, i.e.:

$$f(\gamma_{\mathbf{i}}|\gamma_{-\mathbf{i}}) = \frac{b+am_i}{b+n-1} g_0(\gamma_{\mathbf{i}}) + \sum_{j=1}^{m_i} \frac{n^*_{j,i}-a}{b+n-1} I_{\gamma^*_{\mathbf{j},\mathbf{i}}}(\gamma_{\mathbf{i}}), i = 1, ..., n \tag{5}$$

where $(\gamma^*_{\mathbf{1},\mathbf{i}}, ..., \gamma^*_{\mathbf{m_i},\mathbf{i}})$ denotes the unique values in $\gamma_{-\mathbf{i}}$ which occur with frequency $n^*_{j,i}, j = 1, ..., m_i$.

If for two series i, j it is the case that $\gamma_{\mathbf{i}} = \gamma_{\mathbf{j}}$, then it will be considered that both belong to the same group. However, we need the posterior distribution of every $\gamma_{\mathbf{i}}$ to be able to determine the final clustering.

Such posterior distribution cannot be expressed analytically and it must be calculated numerically as explained by Nieto-Barajas, L.E. and Contreras-Cristan, A. (2014) through a process called *Gibbs sampling*. This is the objective of the functions from this package. The user supplements the path to where the file is kept in his computer and the functions carry out the Gibbs sampling to approximate the posterior distribution of γ.

2.2 Prior specification of the rest of the parameters

To approximate correctly the posterior distribution of γ we need to compute the posterior distribution of the rest of the parameters in the model too. These distributions are approximated through *Gibbs sampling* as well in the functions of the package. The prior distributions assigned to the rest of the parameters are the following:

- $\alpha_{\mathbf{i}} \overset{iid}{\sim} N_p(\mathbf{0}, \mathbf{\Sigma}_\alpha), i = 1, ..., n$
- $\sigma^2_{\epsilon_i} \sim IGa(c^\epsilon_0, c^\epsilon_1), i = 1, ..., n$
- $\sigma^2_{\beta_j} \sim IGa(c^\beta_0, c^\beta_1), j = 1, ..., d$
- $\sigma^2_{\alpha_k} \sim IGa(c^\alpha_0, c^\alpha_1), k = 1, ..., p$
- $f(\sigma^2_\theta, \rho) \propto (\sigma^2_\theta)^{-1} \frac{\sqrt{1+\rho^2}}{1-\rho^2}$
- $f(a) = \pi I_0(a) + (1-\pi) Be(a|q^a_0, q^a_1)$
- $f(b|a) = Ga(b + a|q^b_0, q^b_1)$

3 Functions' description and examples

As explained before, the functions of these package implement a Gibbs sampler to approximate the posterior distribution of the model parameters. The functions `tseriescm`, `tseriescq` and `tseriesca` perform time series clustering for monthly, quarterly and annual data respectively.

3.1 Functions' arguments

- `filedir.` This is a string with the directory of where the file is saved in the user's computer. For example, the variable could be defined as: `filedir <- "C:/Users/MyName/Documents/mydata.csv"`. It is assumed that the file is in csv (comma-separated values) format and that the time series are ordered by columns. A name for each time series must appear in the first row of the file. The observation periods for the time series must appear in the first column of the file.

- `maxiter.` *Gibbs sampling* is an iterative process and it requires a several number of repetitions to achieve convergence and approximate correctly the posterior distribution of the model parameters. `maxiter` is the maximum number of iterations that the Gibbs sampling carries out. The default is 2000 and the user can increase the number of iterations under the consideration that it will also take more time for the program to finish, since it is computer intensive. However, the number of iterations must be greater than 1000 always, since the first 1000 iterations are discarded.

- `p` and `d.` As stated in the previous section, `p` and `d` represent the number of parameters that will and will not be considered for clustering respectively. The default values for each function are:

  - `tseriescm:  p = 1` and `d = 13`. This means that only the level is omitted for clustering and the parameters considered are the indicator functions for 11 months, a linear and a quadratic trend.
  - `tseriescq:  p = 1` and `d = 5`. This means that only the level is omitted for clustering and the parameters considered are the indicator functions for 3 quarters, a linear and a quadratic trend.
  - `tseriesca:  p = 1` and `d = 2`. This means that only the level is omitted for clustering and the parameters considered are only a linear and a quadratic trend, since there is no way to establish a periodicity with annual time series data.

  There are a several number of values that these parameters can take. For example:

  - If the user does not want the polynomial trends to appear and the level is to be omitted, then: `p = 1` and d = 11,3 for the `tseriescm` and `tseriescq` functions respectively. The trends should not be omitted in the `tseriesca` function.
  - If the user only wants a linear trend to be considered for clustering and the the level is to be omitted, then: `p = 1` and d = 12,4,1 for the `tseriescm, tseriescq` and `tseriesca` functions respectively.
  - If the user wants the linear trend and the level to be omitted for clustering then: `p = 2` and d = 11,3 for the `tseriescm` and `tseriescq` functions respectively.

- If the user wants the linear trend and the level to be omitted for clustering, but the quadratic term is to be considered, then: `p = 2` and d = 12,4,1 for the `tseriescm, tseriescq` and `tseriesca` functions respectively.

Note that the seasonal components for months and quarters are always considered for clustering in the `tseriescm` and `tseriescq` functions.

- `c0eps,c1eps,c0beta,c1beta,c0alpha,c1alpha`. These are the parameters of the inverse gamma prior on $\sigma^2_\epsilon, \sigma^2_\beta, \sigma^2_\alpha$. Their value must be always positive and they affect the number of groups that will be in the final clustering. The default values are: `c0eps = c0beta = c0alpha = 2` and `c1eps = c1beta = c1alpha = 1` which tend to generate a small number of clusters. If the number of groups wants to be increased, then these parameters should be given values close to zero, e.g. `c0eps = c0beta = c0alpha = 0.001` and `c1eps = c1beta = c1alpha = 0.001`.

- `priora` and `priorb`. These arguments indicate whether a prior distribution on parameters `a` and `b` should be assigned or not. If their value is zero, then no prior is assigned on the parameters and their value is fixed throughout the algorithm. If their value is one, then the posterior distribution of these parameters is approximated by the functions. The default value is `priora = priorb = 0`. Of course, both arguments need not take the same value.

Please note that if `priora` or `priorb` are set to one, the functions will require the user to enter certain values to run:

- If `priora` is set to one, the following messages will come up:

```
> Enter the value of the mixing proportion of the prior
distribution on 'a':

> Enter the value for the shape parameters of the prior
distribution on 'a':
```

The first message asks the user to enter a number between zero and one and the second message asks the user to enter two positive numbers. According to Nieto-Barajas and Contreras-Cristan (2014) the recommended values for these parameters are: `0.5,1,1`.

  – If `priorb` is set to one, the following message will come up:

    ```
    > Enter the value for the shape parameters of the prior
    distribution on 'b':
    ```

    This asks the user to enter two positive numbers necessary for the function to run. According to Nieto-Barajas and Contreras-Cristan (2014) the recommended values for these parameters are: `1,1`.

- `a` and `b`. If `priora` or `priorb` are zero, `a` and `b` are the fixed values the parameters take throughout the algorithm. If `priora` or `priorb` are one, then `a` and `b` are the initial values that the parameters take for the algorithm. Please note that `a` and `b` must always satisfy that: $0 \leq \mathtt{a} < 1$ and $\mathtt{a} + \mathtt{b} > 0$.

- `indlpml`. This argument indicates if the LPML (Logarithm of Pseudo-Marginal Likelihood) for the model is to be computed. This is a goodness of fit measure and larger positive values indicate a better fit. If `indlpml` is zero, then LPML is not calculated. If `indlpml` is one, then the LPML is computed, but this will make the functions run slower. The default value is `indlpml = 0`, since the LPML value is not essential for the clustering outcome.

3.2 Functions' output

While the function is running, every 50 iterations a message like this will be displayed:

```
                    ⋮
 Iteration Number:  1500.  Progress:  75%
Iteration Number:  1550.  Progress:  77.5%
 Iteration Number:  1600.  Progress:  80%
                    ⋮
```

Clearly, progress percentage depends on the maximum number of iterations desired. When it finishes, the function will return the following variables as a list:

- `mstar`. This variable contains the number of groups in the chosen cluster configuration.

- `gnstar`. Each time series is identified by a number according to its column in the file provided by the user. `gnstar` will contain the group number to which each time series belongs in the final cluster configuration. For example, if the file contains 10 time series and group 1 consists of the series 1, 4, 7 and 10, group 2 consists of the series 2, 3, 5, 6 and 8 and group 3 consists only of series 9, then `gnstar` would be defined as:

```
> gnstar
[1] 1 2 2 1 2 2 1 2 3 1
```

- `HM.` This is the *Heterogeneity Measure* of the final cluster configuration. The larger the value of HM, the more heterogeneous a clustering is. A clustering with small HM and a small number of groups is preferable.

- `arrho, ara` and `arb.` At each iteration, *Gibbs sampling* produces a simulation of the posterior distribution of the model parameters. However, the parameters ρ, a and b, require an extra step in which the simulated values are not always accepted as a sample of their posterior distribution. Hence, the variables `arrho, ara` and `arb` contain the *Acceptance Rate* of the simulations for each parameter. The *Acceptance Rate* is simply the number times a simulation was accepted over the total number of iterations.

- `sig2epssample, sig2alphasample, sig2betasample, sig2thesample, rhosample, asample, bsample` and `msample.` The first three variables are matrices that contain in their columns the posterior distribution sample of parameters $\sigma^2_{\epsilon_i}$, $\sigma^2_{\alpha_j}$ and $\sigma^2_{\beta_k}$, $\forall i, j, k$. The rest of the variables are vectors with the posterior distribution sample of $\sigma^2_\theta, \rho, a, b$ and the sample of the number groups at each Gibbs sampling iteration saved.

- `lpml.` The variable contains the value of LPML calculated for the model if the argument `indlpml` was given the value of one.

When the function is done with the process, several plots will also be returned:

- *Trace plots.* These are the first eight plots returned by the functions and they assess the convergence of the Gibbs sampler. They are simply the plot of the simulated values of the posterior distribution of each parameter at every iteration. If the plots are stationary, then the Gibbs sampler achieved convergence and the final clustering configuration is acceptable.

- *Histograms.* These are the following eight plots returned by the functions and they give and idea of the frequency in which each simulated value appears as a sample of the posterior distribution of each parameter.

- *Ergodic mean plots.* The next eight plots are the ergodic mean of the samples of the posterior distributions of the model parameters at every iteration. The ergodic mean is just the sum of the simulated values up to a certain iteration divided by the total number of iterations at that point. If the plot converges to a value as the iterations increase, then it can be considered that the Gibbs sampler achieved convergence and the final clustering configuration is acceptable.

- *Cluster plots.* The last graphs provided by the functions plot the time series that belong to each cluster, for all clusters. This makes it easier to visualize and to interpret the reason for which the algorithm determined the final cluster configuration.

These are some examples of the output that each function produces. Please note that the examples might have slight differences from what you get, due to the probabilistic nature of the functions.

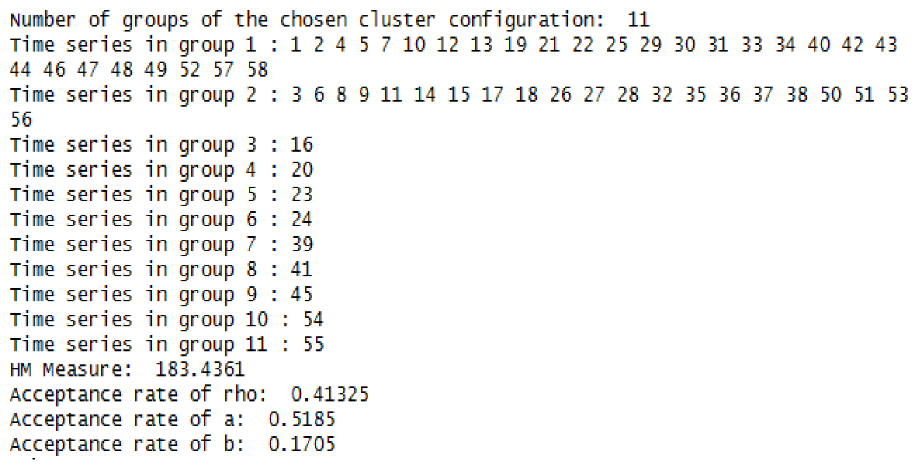
3.2.1 `tseriescm` example.

This function performs the clustering algorithm for monthly time series data. This example comes from the monthly adjusted closing prices of 58 shares from the Mexican stock exchange market. This is the database used by Nieto-Barajas, L.E. and Contreras-Cristan, A. (2014). The following output was obtained by running the following code:

```
> data(stocks)
> write.csv(stocks,file="stocks.csv")
> ts <- tseriescm("stocks.csv",maxiter = 4000,priora = 1,priorb = 1)
# When the program asks for values, enter 0.5,1,1,1 and 1 in that order.
```

These arguments imply that the prior on γ will be a Poisson-Dirichlet Process. The ouput is the following:

- *Console output*



```
Number of groups of the chosen cluster configuration:  11
Time series in group 1 : 1 2 4 5 7 10 12 13 19 21 22 25 29 30 31 33 34 40 42 43
44 46 47 48 49 52 57 58
Time series in group 2 : 3 6 8 9 11 14 15 17 18 26 27 28 32 35 36 37 38 50 51 53
56
Time series in group 3 : 16
Time series in group 4 : 20
Time series in group 5 : 23
Time series in group 6 : 24
Time series in group 7 : 39
Time series in group 8 : 41
Time series in group 9 : 45
Time series in group 10 : 54
Time series in group 11 : 55
HM Measure:  183.4361
Acceptance rate of rho:  0.41325
Acceptance rate of a:  0.5185
Acceptance rate of b:  0.1705
```

Figure 1: Console output for the function `tseriescm`.

- *Trace plots*

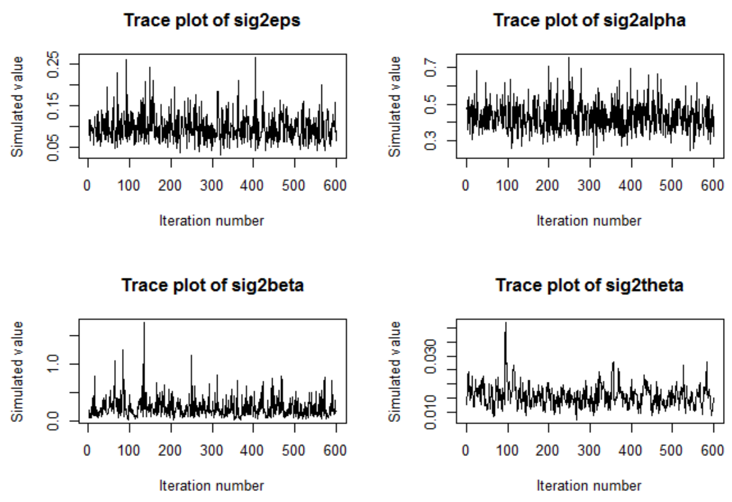


Figure 2: Trace plots for the function `tseriescm`.

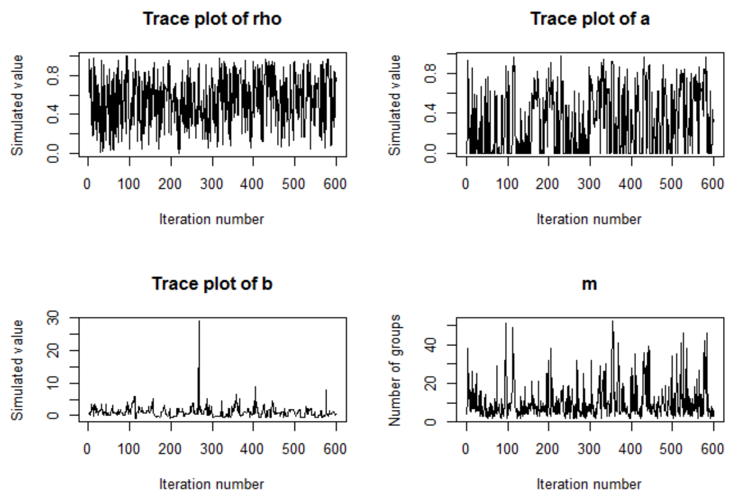


Figure 3: Trace plots for the function `tseriescm`.

- *Histograms*

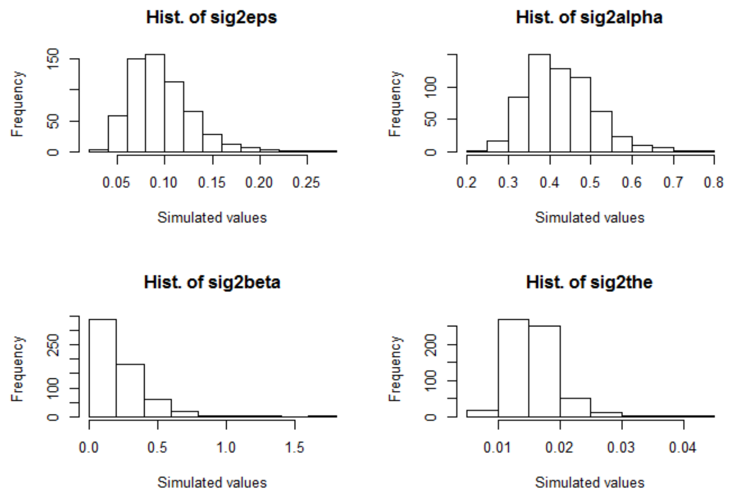


Figure 4: Histograms for the function `tseriescm`.

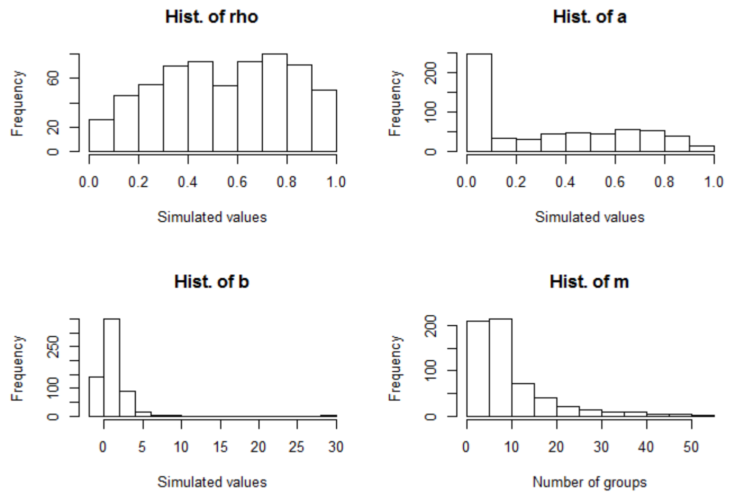


Figure 5: Histograms for the function `tseriescm`.

- *Ergodic Mean Plots*

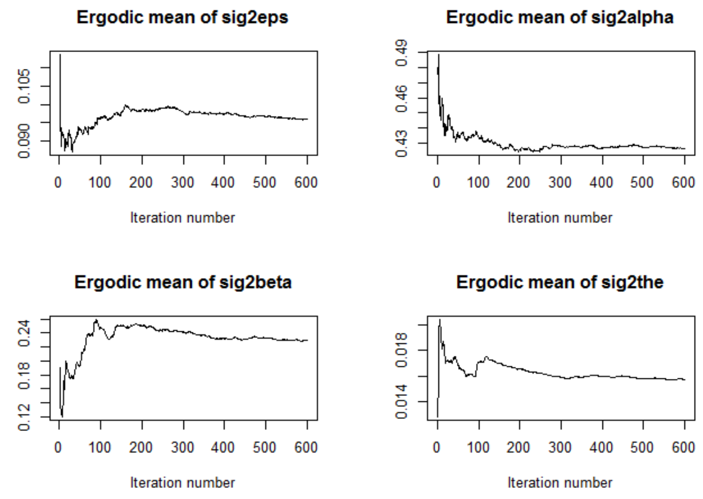


Figure 6: Ergodic Mean plots for the function `tseriescm`.

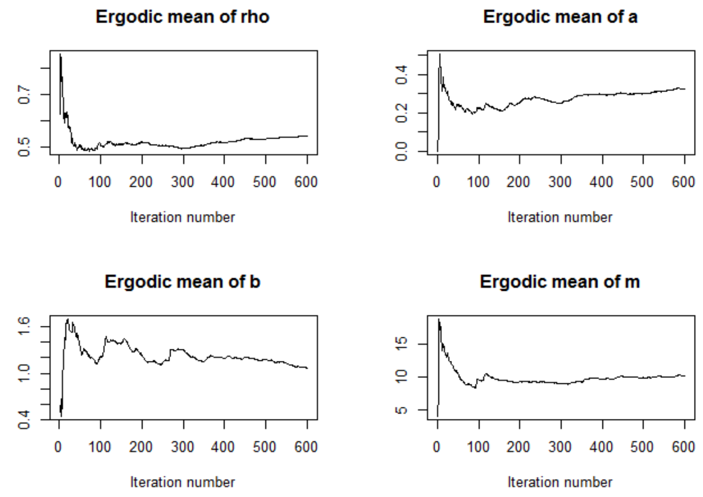


Figure 7: Ergodic Mean plots for the function `tseriescm`.

- *Cluster plots*

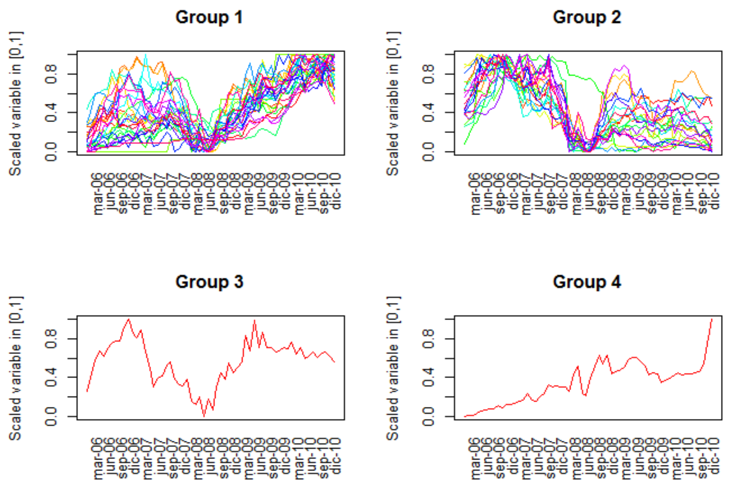


Figure 8: Cluster plots for the function `tseriescm`.

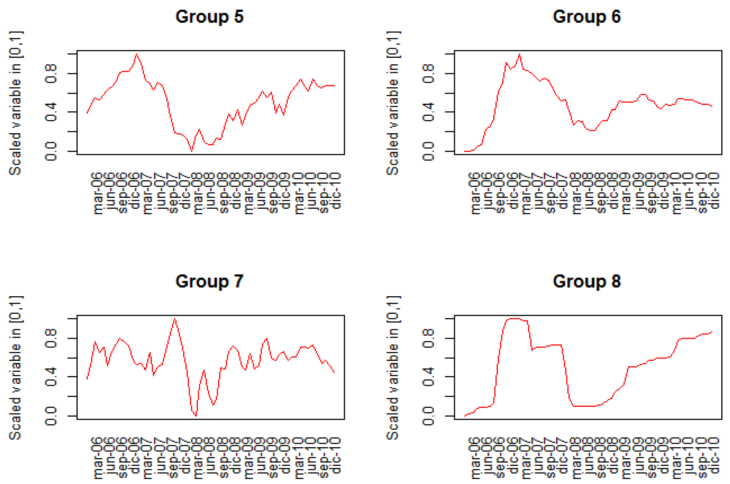


Figure 9: Cluster plots for the function `tseriescm`.

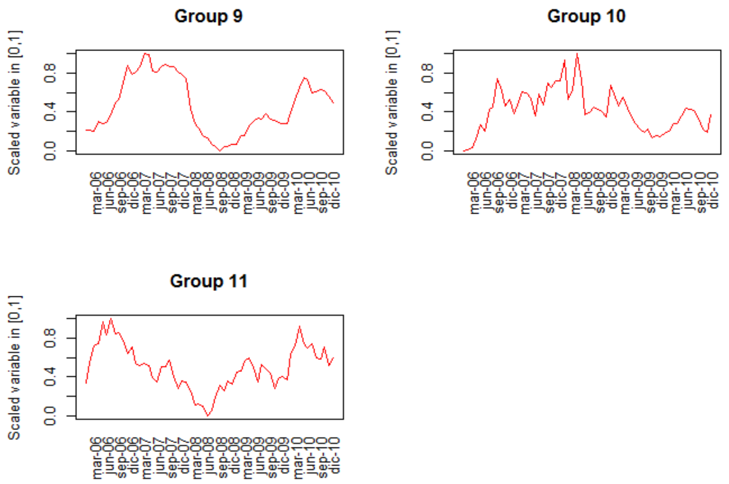


Figure 10: Cluster plots for the function `tseriescm`.

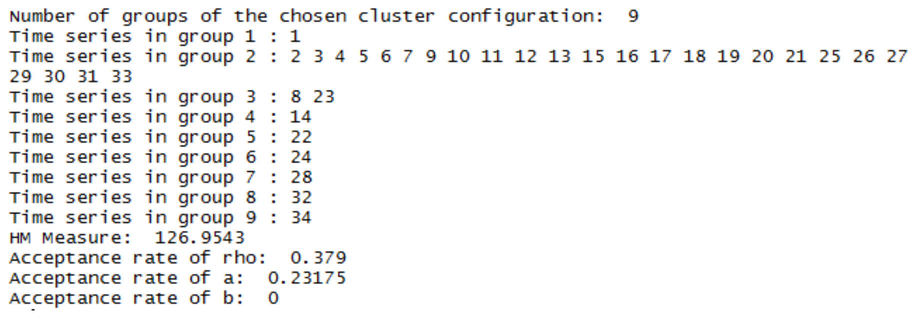
3.2.2 `tseriescq` example.

This function performs the clustering algorithm for quarterly time series data. This example comes from quarterly average house price data in Scotland from 2003 to 2014. The output was obtained by running the following code:

```
> data(houses)
> write.csv(houses,file="houses.csv")
> ts <- tseriescq("houses.csv",maxiter = 4000,priora = 1)
# When the program asks for values, enter 0.5,1 and 1 in that order.
```

These arguments imply that the prior on γ will be a Normalized Stable Process. The ouput is the following:

- *Console output*



```
Number of groups of the chosen cluster configuration:  9
Time series in group 1 : 1
Time series in group 2 : 2 3 4 5 6 7 9 10 11 12 13 15 16 17 18 19 20 21 25 26 27
29 30 31 33
Time series in group 3 : 8 23
Time series in group 4 : 14
Time series in group 5 : 22
Time series in group 6 : 24
Time series in group 7 : 28
Time series in group 8 : 32
Time series in group 9 : 34
HM Measure:  126.9543
Acceptance rate of rho:  0.379
Acceptance rate of a:  0.23175
Acceptance rate of b:  0
```

Figure 11: Console output for the function `tseriescq`.

- *Trace plots*

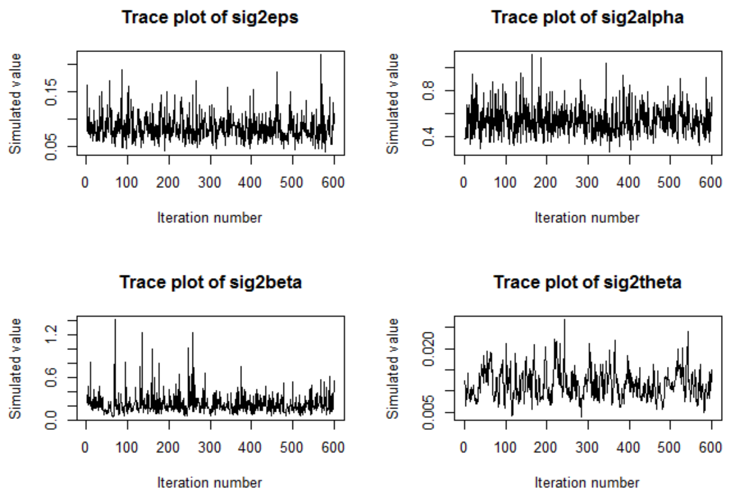


Figure 12: Trace plots for the function `tseriescq`.

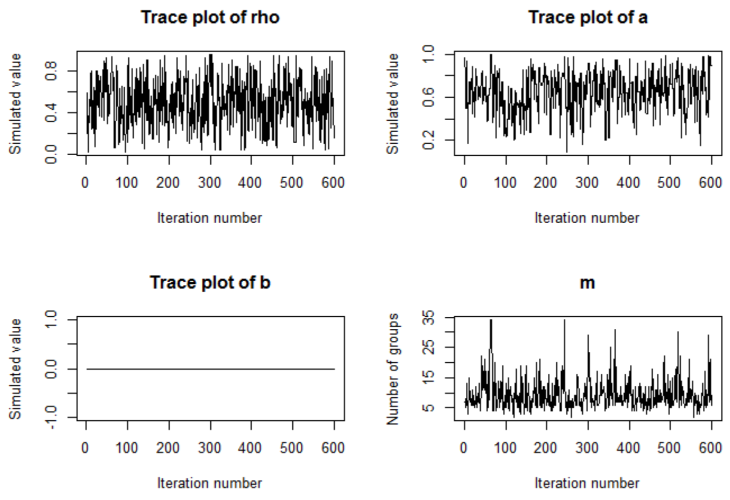


Figure 13: Trace plots for the function `tseriescq`.

- *Histograms*

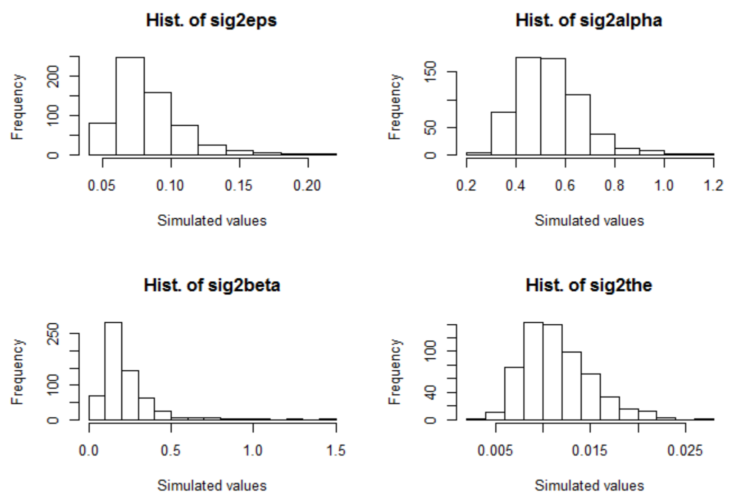


Figure 14: Histograms for the function `tseriescq`.

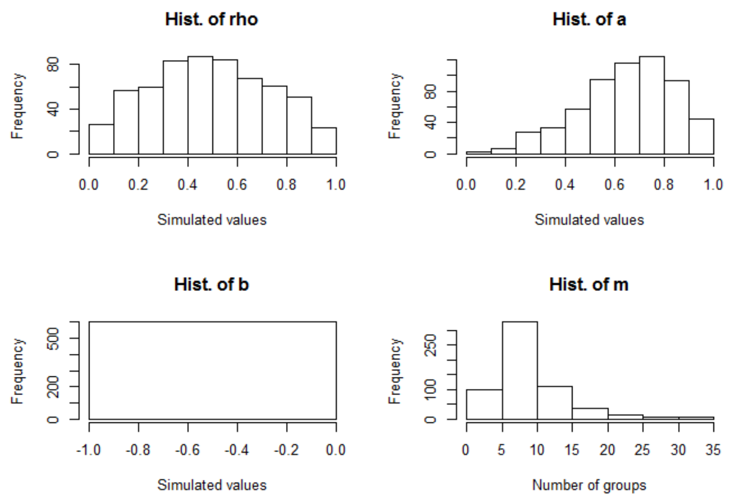


Figure 15: Histograms for the function `tseriescq`.

- *Ergodic Mean Plots*

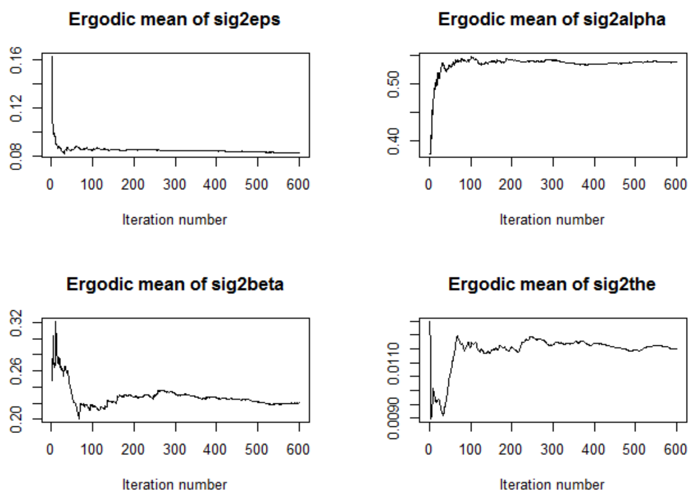


Figure 16: Ergodic Mean plots for the function `tseriescq`.

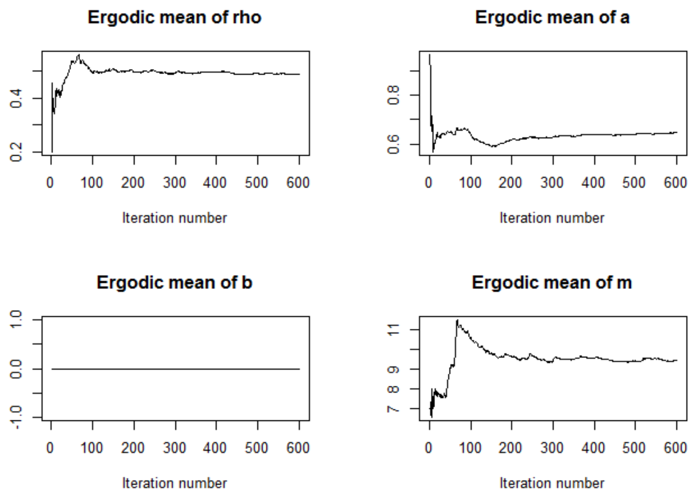


Figure 17: Ergodic Mean plots for the function `tseriescq`.

- *Cluster plots*

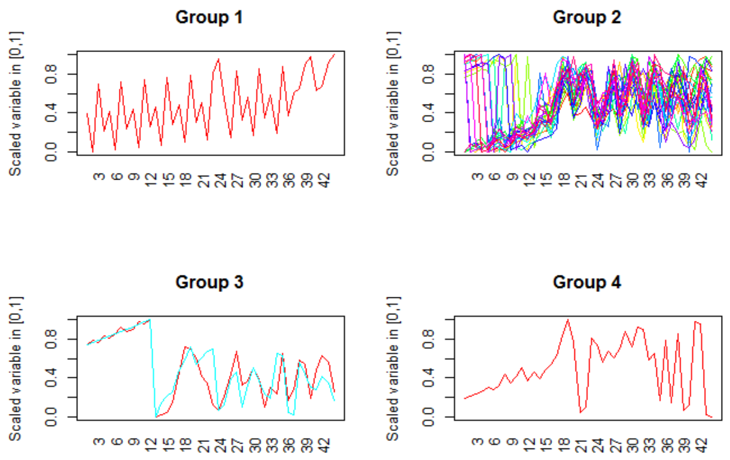


Figure 18: Cluster plots for the function `tseriescq`.

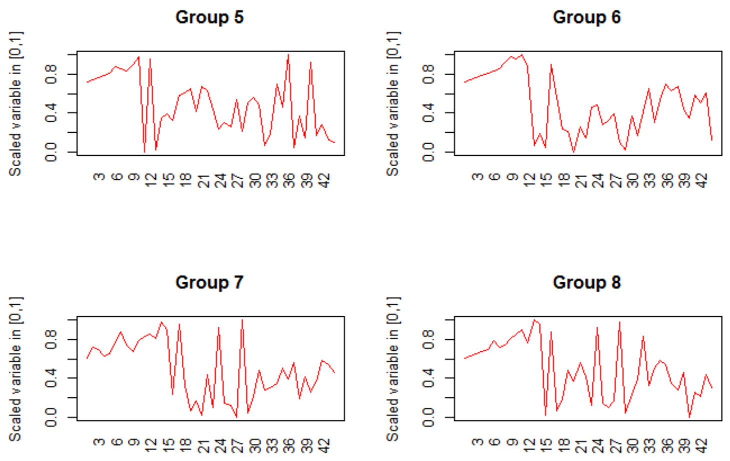


Figure 19: Cluster plots for the function `tseriescq`.

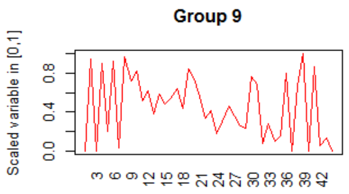


Figure 20: Cluster plots for the function `tseriescq`.

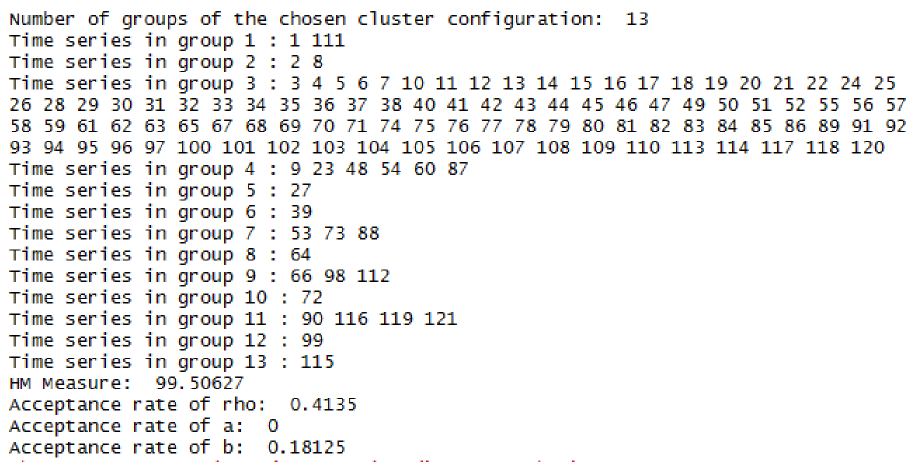
3.2.3 `tseriesca` example.

This function performs the clustering algorithm for annual time series data. This example comes from the yearly GDP per worker for 121 countries from 1993 to 2012. The output was obtained by running the following code:

```
> data(gdp)
> write.csv(gdp,file="gdp.csv")
> ts <- tseriesca("gdp.csv",maxiter = 4000,c0eps = 0.001,c1eps = 0.001,
c0beta = 0.001,c1beta = 0.001,c0alpha = 0.001,c1alpha = 0.001,priorb
= 1,a = 0,b = 0.1)
# When the program asks for values, enter 1 and 1 in that order.
```

These arguments imply that the prior on γ will be a Dirichlet Process. The ouput is the following:

- *Console output*



```
Number of groups of the chosen cluster configuration:  13
Time series in group 1 : 1 111
Time series in group 2 : 2 8
Time series in group 3 : 3 4 5 6 7 10 11 12 13 14 15 16 17 18 19 20 21 22 24 25
26 28 29 30 31 32 33 34 35 36 37 38 40 41 42 43 44 45 46 47 49 50 51 52 55 56 57
58 59 61 62 63 65 67 68 69 70 71 74 75 76 77 78 79 80 81 82 83 84 85 86 89 91 92
93 94 95 96 97 100 101 102 103 104 105 106 107 108 109 110 113 114 117 118 120
Time series in group 4 : 9 23 48 54 60 87
Time series in group 5 : 27
Time series in group 6 : 39
Time series in group 7 : 53 73 88
Time series in group 8 : 64
Time series in group 9 : 66 98 112
Time series in group 10 : 72
Time series in group 11 : 90 116 119 121
Time series in group 12 : 99
Time series in group 13 : 115
HM Measure:  99.50627
Acceptance rate of rho:  0.4135
Acceptance rate of a:  0
Acceptance rate of b:  0.18125
```

Figure 21: Console output for the function `tseriesca`.

- *Trace plots*

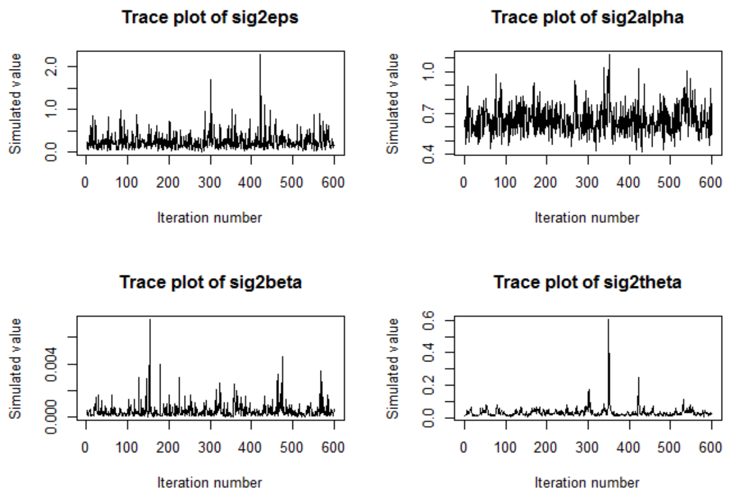


Figure 22: Trace plots for the function `tseriesca`.

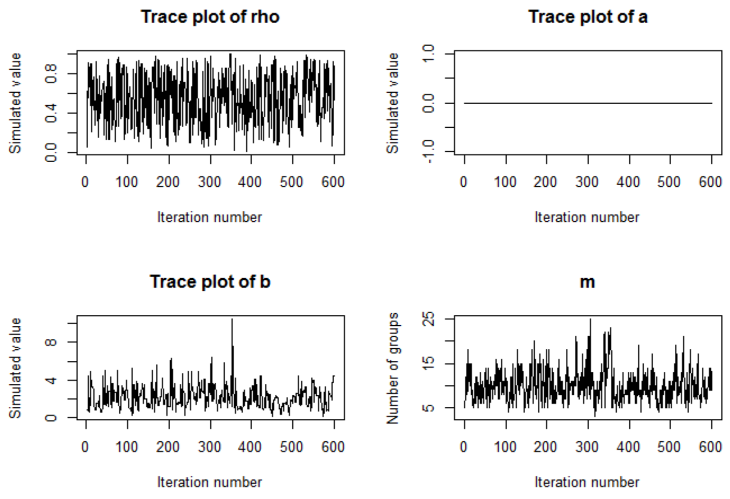


Figure 23: Trace plots for the function `tseriesca`.

- *Histograms*

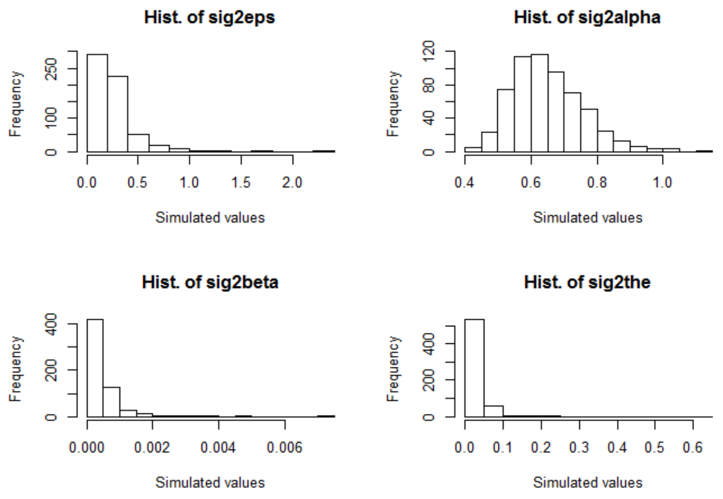


Figure 24: Histograms for the function `tseriesca`.

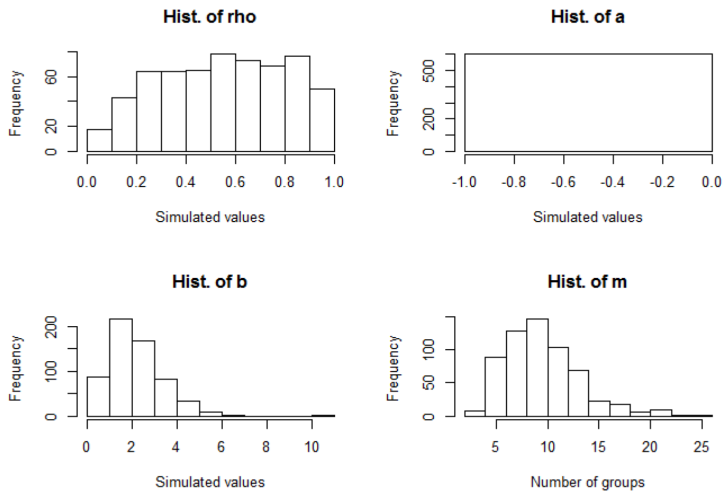


Figure 25: Histograms for the function `tseriesca`.

- *Ergodic Mean Plots*

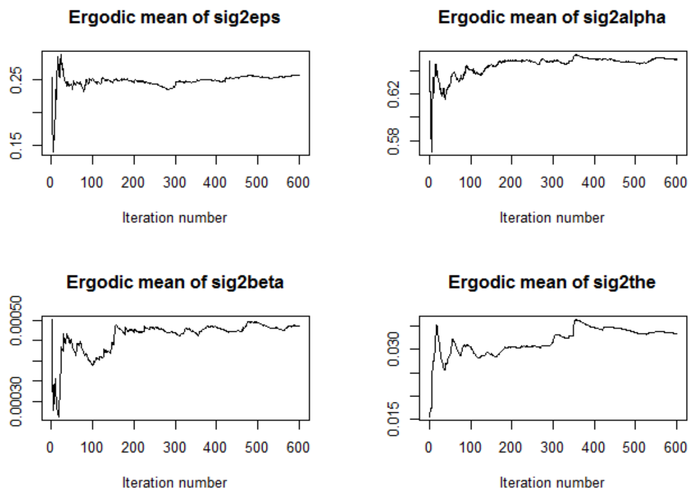


Figure 26: Ergodic Mean plots for the function `tseriescq`.

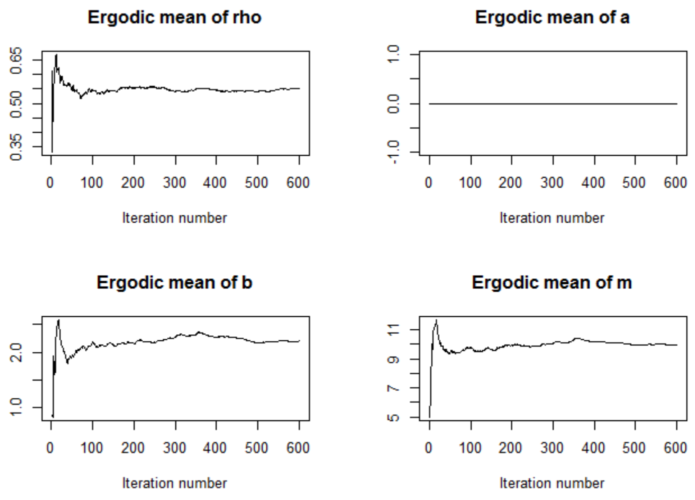


Figure 27: Ergodic Mean plots for the function `tseriescq`.

- *Cluster plots*

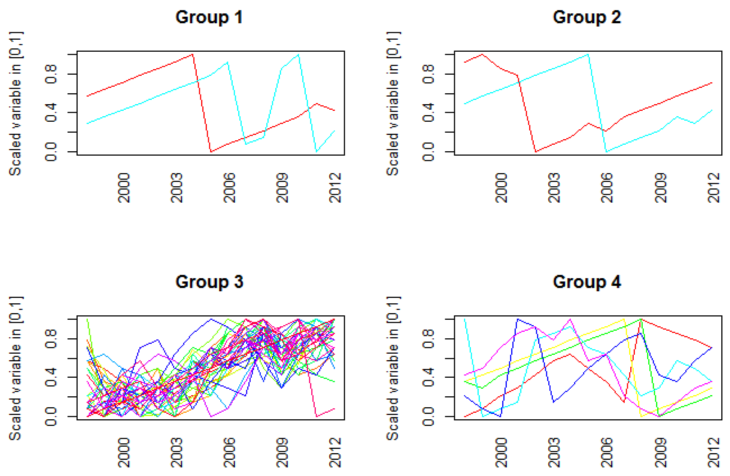


Figure 28: Cluster plots for the function `tseriesca`.

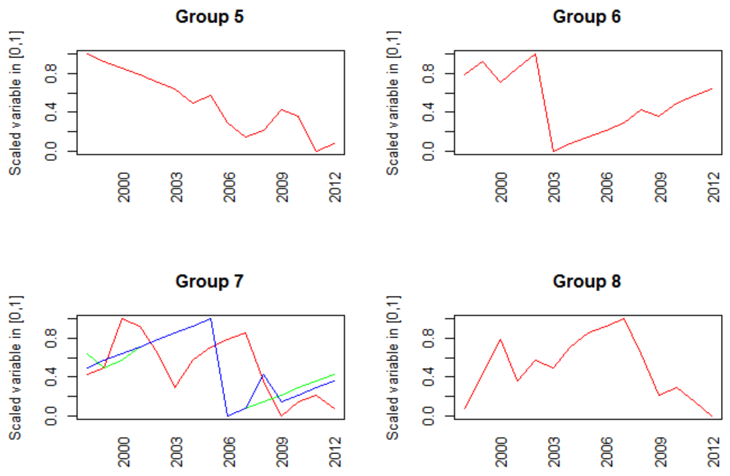


Figure 29: Cluster plots for the function `tseriesca`.

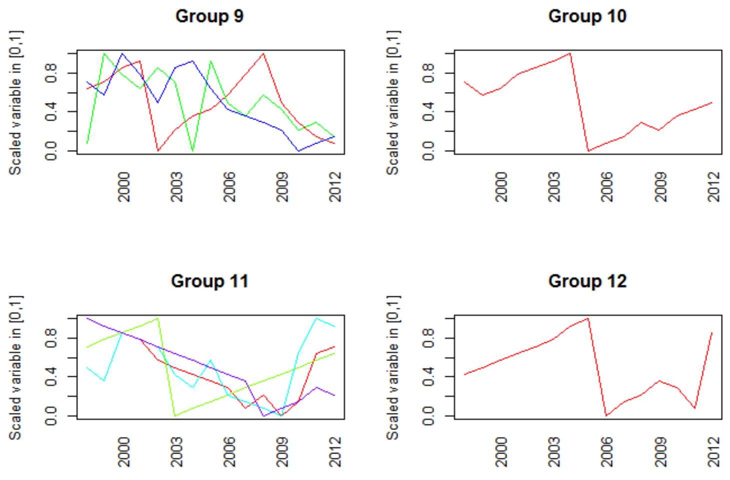


Figure 30: Cluster plots for the function `tseriesca`.

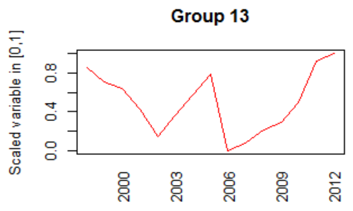


Figure 31: Cluster plots for the function `tseriesca`.

References

[1] Nieto-Barajas, L.E. & Contreras-Cristán A. (2014): *A Bayesian Nonparametric Approach for Time Series Clustering.* Bayesian Analysis, Vol. 9, No. 1 pp. 147-170.