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The comparison of optimization algorithms on unit root testing with smooth transition

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Abstract

The aim of this study is to search for a better optimization algorithm in applying unit root tests that inherit nonlinear models in the testing process. The algorithms analyzed include Broyden, Fletcher, Goldfarb and Shanno (BFGS), Gauss-Jordan, Simplex, Genetic, and Extensive Grid-Search. The simulation results indicate that the derivative free methods, such as Genetic and Simplex, have advantages over hill climbing methods, such as BFGS and Gauss-Jordan, in obtaining accurate critical values for the Leybourne, Newbold and Vougos (1996, 1998) (LNV) and Sollis (2004) unit root tests. Moreover, when parameters are estimated under the alternative hypothesis of the LNV type of unit root tests the derivative free methods lead to an unbiased and efficient estimator as opposed to those obtained from other algorithms. Finally, the empirical analyses show that the derivative free methods, hill climbing and simple grid search can be used interchangeably when testing for a unit root since all three optimization methods lead to the same empirical test results.

Keywords: Nonlinear trend; Deterministic smooth transition; Structural change; Estimation methods

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1. Introduction

Testing stationarity properties of economic variables has attracted a great deal of attention among economists in the last three decades; and as a result, following the seminal work of Dickey and Fuller (1979) many unit root tests have been proposed. These unit root tests can be generally classified under three classes – standard linear unit root tests, unit root tests using a nonlinear framework², and unit root tests that allow for a break in mean and/or trend. This study will concentrate on the third class, namely the unit root tests that allow for break in mean and/or trend.

Several researchers including Perron (1989, 1990), Rappoport and Rechlin (1989), Zivot and Andrews (1992), Lumsdaine and Papell, and Bai and Perron (1998) have recognized alternative trend specifications in testing for the unit root hypothesis. This strand of literature has focused on models with segmented line trends; and single or multiple breaks (Vougas, 2006). Yet, another strand of literature has developed unit root tests where the alternative hypothesis is that of stationarity around a smoothly changing trend. Leybourne, Newbold and Vougos (1996, 1998) (LNV, hereafter) and Sollis (2004) used logistic trend functions³ that allow for a smooth break in the deterministic trend of the data. Bierens (1997) modeled nonlinear trend using Chebyshev polynomials, while Becker et al. (2006) used trigonometric functions (via means of Fourier transformations) to model possible gradual breaks in the data generating process. The use of either Chebyshev polynomials or trigonometric functions might be problematic, because there is no unique way of choosing the order of polynomials or the frequency components for the trigonometric functions. However, in the case of logistic trend functions the parameters of interest in the gradually changing trend function may be estimated using a convenient nonlinear estimation algorithm. By the same token, smooth transition regression (STR) models have also been proved to capture gradual structural breaks quite well (e.g., Granger and Teräsvirta, 1994; Lin and Teräsvirta, 1994; Greenaway et al. 1997). Moreover, the STR type trend modeling can incorporate broken or unbroken trend lines, thereby allowing for gradual as well as abrupt break (Vougas, 2006). Along these lines, the STR type of trend modeling can also be seen as a generalization of the first strand of trend modeling. Due to all these reasons, researchers should focus on STR type of trend modeling more seriously. Fortunately, Vougos (2006) has investigated the neglected numerical issues that necessitate the re-calculation of critical values for the LNV tests. The comparison of alternative estimation algorithms is yet another important issue within the context of LNV type unit root tests. Chan and Mc Aleer (2002) and Maugeri (2012) have compared the nonlinear optimization algorithms in the STAR-GARCH models and in non-linear co-integration frameworks, respectively. According to these authors, concentrating the sum of squares method and some other popular nonlinear optimization algorithms were not found as efficient as they were expected to be. Therefore, the comparison of alternative nonlinear optimization algorithms for unit root estimation serves as an important research question that has only been partially answered so far in the literature.

Nonlinear estimation inherits various problems such as convergence and good starting values. These problems may represent an obstacle for the estimation process like the inability to find global optima. Consequently, these kinds of problems lead to biased and inefficient estimates of the true data generating process. In this study our main focus is on the LNV type unit root tests which naturally encounter these kinds of problems due to the STR type nonlinearity inherent in the deterministic components of the testing process. For this purpose, we organize a simulation study by generating data under the alternative hypothesis of the LNV unit root tests and compare the estimation results of different optimization algorithms by employing statistical tools such as mean square error (MSE) and root mean square error (RMSE). Comparing the estimation results of the nonlinear data generation processes by using different optimization algorithms is crucial to measure the losses and gains (by means of MSE and RMSE) of the specific type of optimization algorithm employed. Such an analysis is therefore needed to obtain better critical values and to carry out power and size analysis at a

² Such as; Kapetanios et al., G. (2003) in time series, and the Ucar and Omay (2009) in panel analysis.

³ Vougos (2006) pointed out that the trend models employed by LNV are deterministic and must be distinguished from stochastic STR models.

minimum cost where the minimum cost principle forms the basis of virtually every statistical analysis of data⁴.

The purpose of this paper is to investigate the performance of the various optimization algorithms that can be applied to the LNV type of unit root testing. The five methods analyzed in this study are BFGS, Gauss-Jordan, Simplex, Genetic, and Extensive Grid-Search. We have especially included in this study the algorithms that are commonly used within the context of the LNV type of nonlinear unit root tests, and found out that derivative free methods have advantage over hill climbing methods while obtaining the accurate critical values. On the other hand, increasing the complexity of data generating process simple algorithms has advantages over more complex algorithms in computing the parameter estimates. Finally, we have found out that depending empirical study no matter which the optimization algorithms are employed the empirical tests results are not changing.

The rest of the paper is structured as follows. Section 2 introduces and discusses the various optimization algorithms employed in the study. Section 3 investigates the performance of the alternative optimization algorithms through Monte Carlo simulation studies. It reports and compares the critical values of the LNV and Sollis (2004) unit root tests obtained by employing each optimization algorithm along with the biases of the estimated parameters for each alternative optimization method under the alternative hypotheses of these tests. Section 4 provides an empirical application of the aforementioned optimization methods to the purchasing power parity (PPP) hypothesis for 9 countries. Section 5 is reserved for concluding remarks.

2. The estimation of STAR models and the optimization algorithms

The model that is employed in this paper is a logistic trend model that allows for a smooth break in the deterministic trend of the data. Following the model of LNV, we consider the following representation for the logistic trend function;

$$y_t = \alpha_1 + \alpha_2 F_t(\gamma, \tau) + \varepsilon_t, \mu_{i0} = 0, \varepsilon_t \sim NID(0,1) \quad (1)$$

$$F_t(\gamma, \tau) = \frac{1}{1 + e^{-\gamma(s_t - \tau)}}$$

Estimation of the parameters in the STR model is a relatively straightforward application of the nonlinear least squares (NLS) technique. The parameters $\psi = (\alpha_1, \alpha_2, \gamma, \tau)'$ of the STR model can be estimated as;

$$\hat{\psi} = \arg \min_{\psi} \mathcal{Q}_T(\psi) = \arg \min_{\psi} \sum_{t=1}^T [y_t - S(\psi)]^2$$

where $S(\psi) = \alpha_1 + \alpha_2 F_t(\gamma, \tau) + \varepsilon_t$ is the skeleton of the model, that is equation (1).

If the assumption that ε_t is normally distributed prevails, NLS is equivalent to maximum likelihood; otherwise, the NLS estimates can be interpreted as quasi maximum likelihood estimates. The STR models can be estimated using any conventional nonlinear optimization procedure. (Potscher and

⁴ A cost arises because Monte Carlo simulations conducted to obtain critical values are time consuming. For an accurate critical value, 50000 replications are needed. Under these circumstances, a researcher would want to optimize this process with the best possible solution available and that involves improving the simulation time and obtaining exact critical values.

Prucha (1997) have demonstrated that NLS is consistent and asymptotically normal under appropriate regularity conditions. However, some issues deserve particular attention; such as the choice of starting values for the optimization algorithms, concentrating the sum of squares function (CSQ) and the estimate of the smoothness parameter γ in the transition function.

We have mentioned above that the STR models can be estimated using any conventional nonlinear optimization procedure and the burden on the optimization algorithm can be alleviated by using good starting values. For fixed values of the parameters γ and τ in the transition function, the STR model is linear in the parameters α_1 and α_2 ; and therefore, can be estimated by OLS. Hence, a convenient way to obtain sensible starting values for the nonlinear optimization algorithm is to perform a two-dimensional grid search over γ and τ ; and then to select those parameter estimates that minimize the variance of the residual term or the residual sum of squares.

In this study, we suggest an extensive grid search (EGS) method to initiate the parameter estimates of the STR model. This EGS methodology displays characteristics similar to the procedure used to estimate the Threshold Autoregressive Regression models (TAR). Hence, to explain this methodology it is better to first give a brief explanation of the way TAR estimation is conducted when the threshold parameter τ is unknown. The popularity of the TAR models stems from the fact that it allows for different degrees of autoregressive decay. Consider the following two-regime version of the threshold autoregressive (TAR) model developed by Tong (1983):

$$y_t = I_t \left[\alpha_0 + \sum_{i=1}^p \alpha_i y_{t-i} \right] + (1 - I_t) \left[\beta_0 + \sum_{i=1}^p \beta_i y_{t-i} \right] + \varepsilon_t \quad (2)$$

where y_t is the series of interest, the α_i , and β_i are coefficients to be estimated, τ is the value of the threshold, p is the order of the TAR model and I_t is the Heaviside indicator function such that;

$$I_t \begin{cases} 1 & \text{if } y_{t-1} \geq \tau \\ 0 & \text{if } y_{t-1} < \tau \end{cases} \quad (3)$$

The nature of the system is that there are two states of the world. In one state of the world, y_{t-1} exceeds the value of the threshold τ so that, $I_t = 1$ and $((1 - I_t) = 0$. As such, y_t follows the autoregressive process $\alpha_0 + \sum \alpha_i y_{t-i}$. Similarly, in the low state y_{t-1} falls short of the threshold τ , so that $I_t = 0$ and $((1 - I_t) = 1$ and y_t follows the autoregressive process $\beta_0 + \sum \beta_i y_{t-i}$. In a sense, there are two attractors or potential “equilibrium” values. In the ‘high’ state, the system is drawn towards $\alpha_0 / (1 - \sum \alpha_i y_{t-i})$; whereas in the ‘low’ state the system is drawn towards $\beta_0 / (1 - \sum \beta_i y_{t-i})$. Moreover, the degree of autoregressive decay will differ across the two states if for any value of i $\alpha_i \neq \beta_i$. The key feature of the TAR model is that a sufficiently large ε_t shock can cause the system to switch between states. Chan (1993) shows how to obtain a super-consistent estimate of the threshold parameter. To estimate a TAR model, the procedure is to order the observations from smallest to largest such that:

$$y^1 < y^2 < y^3 \dots < y^T$$

For each value of y^j let $\tau = y^j$ set the Heaviside indicator according to this potential threshold and estimate a TAR model. The regression equation with the smallest residual sum of squares contains the consistent estimate of the threshold. In practice, the highest and lowest 15% of the $\{y^j\}$ values are excluded from the grid search so as to ensure an adequate number of observations on each side of the threshold.

Likewise the methodology outlined above, in our EGS method the first stage starts with the consistent estimation of the parameters τ and γ , where γ is the slope parameter of the STR model. Simultaneous estimation of the parameters τ and γ carried out using Tong's (1983) methodology can be categorized as two dimensional grid searches for STR type models. Tong (1983) has introduced limitations on the highest and lowest 15% of the state variable, however in our case the state variable is time and we are searching for the break instead of the threshold values. Thus, we have changed this restriction for our purposes and discarded different highest and lowest percents for the parameter τ and ranged it in these intervals by 0.01 increments in order to obtain the most efficient estimate. For the slope parameter (γ) we have followed the same computation method and ranged it (after scaling) from 1 to 10 or 1 to any arbitrary positive integer number by 0.1 increments.

As recommended by Leybourne et al. (1998), concentrating the sum of squares function is another method used to simplify the estimation problem like grid search. Since the STR model is linear in the autoregressive parameters for given values of γ and τ , the nonlinear least square sum of squares function can be concentrated with respect to α_1 and α_2 as

$$SS = \sum_{t=1}^T (y_t - \hat{\pi}' x_t)^2 \quad (4)$$

where

$$\hat{\pi} = (\hat{\alpha}_1, \hat{\alpha}_2)' = \left(\sum_{t=1}^T x_t x_t' \right)^{-1} \sum_{t=1}^T x_t y_t \quad (5)$$

and

$$x_t = x_t(\hat{\gamma}, \hat{\tau}) = \{1, F_t(\hat{\gamma}, \hat{\tau})\}' \quad (6)$$

Therefore, the NLS estimation reduces to minimizing the sum of squares function with respect to just the two parameters γ and τ .

These two computational approaches (grid search and concentrated sum of squares) greatly simplified the estimation process for STR models; hence, different optimization algorithms which use the hill climbing methodology, such as BFGS and Gauss-Jordan, were employed to obtain parameter estimates of STR models. Nonetheless, we have used two derivative free methods in this study. These derivative free methods, namely "Simplex" and "Genetic" are provided in RATS (Regression Analysis for Time Series) software package. These two methods are explained as follow⁵:

Although the Simplex method requires the underlying function to be continuous, it is essentially a derivative free method that does not necessitate the function to be also differentiable. In the first step, the algorithm chooses K+1 points in K-space, where K refers the number of parameters. Simplex is the name of the geometrical object that is created when these points are connected. Initial values correspond to one of these vertices⁶. The RATS program equalizes each other point to the initial value plus a perturbation to only one of the parameters. As opposed to a general grid search method, the initial values obtained need not encompass the optimum. At each step the worst K+1 vertices are selected and replaced with their reflection through face opposite. While the hill climbing optimization algorithms search for a direction where the function increases, the Simplex method progresses uphill by omitting the directions where the function decreases. Although this makes the Simplex method more immune to the way the function behaves and the choice of initial conditions, it is found to

⁵ See RATS 8 user manual.

⁶ The only relationship between this and the Simplex method of linear programming is that each method utilizes a Simplex.

converge more slowly than hill-climbing methods where the latter is deemed to be more suitable⁷. On the other hand, Genetic algorithms, by administering great computational power and an elegant model of “evolution” with random “mutations, are created to tackle troublesome optimization problems. The RATS software utilizes the so called differential evolution. In this model, at each iteration every parameter vector is compared with a feasible successor from a given “population” of parameter vectors. The parameter vector that gives the better function value is maintained and the other is eliminated. For developing successors a number of ways exist and in all at least one parameter must be mutated, in other words some random number should be added to it. In differential evolution, the discrepancy between the parameter in two randomly chosen elements of the population determines the magnitude of mutation in a parameter. These mutations will be large in size when the values that a specific parameter takes are widely scattered throughout the population. However, the mutations will be fairly small if the parameter in question can be well determined, so that it takes values that can be tightly gathered in a group⁸.

3. Monte Carlo Design and Simulation results

In this section the performances of different optimization algorithms are compared using Monte Carlo simulations. The algorithms considered in the study include BFGS, Gauss-Jordan, Genetic, Simplex and EGS. To this end, first, the effects of using different algorithms on the critical values of the LNV statistics are assessed. Vougos (2006) has argued that he has obtained the *accurate* critical values for the LNV statistics based on constrained optimization via sequential quadratic programming (SQP) method. In the light of Vougos’s conclusion, the critical values obtained under each algorithm can be evaluated according to whether they closely match the accurate critical values or not. However, a critical question emerges here: “Is it sufficient to compare the results of other algorithms to the critical values obtained using SQP?” In order to find an answer to this question and to analyze the efficiency of different optimization algorithms, we have organized a Monte Carlo design⁹. In this design, alternative hypothesis of the LNV unit root test is used in which the STR type trend function is directly parameterized. Hence, the use of different optimization algorithms will allow us to see whether the true parameter values can be obtained. In order to calculate the biases of the estimated parameters, the mean square error (MSE) and root mean square error (RMSE) criteria are used.

In the table given below five different sets of critical values are reported for the LNV statistics using the methods explained in section 2, where the sample range is $T=100$. The original critical values of Leybourne et al. (1998) obtained by concentrating the sum of squares (CSQ) function via the BFGS algorithm are tabulated in column 4 of this table. In column 1, the more accurate critical values of Vougos (2006) are presented. In columns 2, 3, 5, and 6, the critical values obtained from the Genetic, Simplex, Gauss-Jordan algorithms and the extensive grid search (EGS)¹⁰ methods are given, respectively. The ordering of the columns is important because the optimization algorithms that are placed in the columns are sorted by their proximity to the accurate critical values given by Vougos

⁷ For further information see RATS (8) user’s guide page-116.

⁸ For further information see RATS (8) user’s guide page-117.

⁹ In implementing the Genetic, Simplex and EGS algorithms; while the parameter values can be obtained, the standard errors cannot be computed as they could be with normal estimation. Estimation or obtaining the trend function is the first and the most crucial step of LNV type of unit root testing. Therefore, obtaining the true trend function is very important to acquire the accurate critical values. Hence, any method which gives the true trend function can be used in this stage of the LNV type of unit root testing.

¹⁰ We have obtained the critical values from EGS method, directly using the computed initial values of slope and threshold values by using the ordinary least square (OLS) estimation. May be this type of evaluating critical values named as two stage optimization procedure.

(2006) in column 1. In other words, starting with the second column the consequent columns are arranged in a descending order with respect to the closeness of the critical values to the accurate critical values reported in column 1.

Table 1. The critical values obtained from different optimization algorithms for LNV (1998)

	1	2	3	4	5	6
%1	-4.87	-4.887	-4.865	-4.882	-4.788	-4.757
%5	-4.25	-4.257	-4.240	-4.232	-4.142	-4.108
%10	-3.93	-3.937	-3.911	-3.909	-3.818	-3.788

- 1) Constrained optimization via sequential quadratic programming (Vougos, 2006),
- 2) Concentrating the sum of squares using the Genetic method,
- 3) Concentrating the sum of squares using the Simplex method,
- 4) Concentrating the sum of squares using the BFGS method (used by LNV, 1998),
- 5) Concentrating the sum of squares using the Gauss Jordan method,
- 6) Direct implementation of extensive grid search (EGS) by using OLS.

Note: The results are reported for T=100.

The comparison of critical values obtained in using different algorithms clearly reveals that the accuracies of the critical values' can be increased. From Table 1 we can recognize that the use of the Genetic method to concentrate the sum of squares function yields critical values that are very close to those obtained via SQP, which is the method claimed to produce the most accurate critical values. Hence, it is possible to use Genetic algorithm instead of SQP to obtain the accurate critical values for the LNV type of unit root testing. On the other hand, Gauss-Jordan and the EGS methods seem to be the most inefficient methods to obtain the said critical values. Nevertheless, the differences among the critical values obtained using the four methods (the ones given in columns 1, 2, 3, and 4) are trivial. Hence, using different optimization algorithms in empirical studies would barely alter the test results. In order to robustify this conclusion, we have organized a Monte Carlo design as follows (which we mentioned above).

The data generation process for the first simulations is:

$$y_t = \alpha_1 + \alpha_2 S_t(\gamma, \tau) + \varepsilon_t, \quad \mu_{i0} = 0, \quad \varepsilon_t \sim NID(0,1)$$

$$S_t(\gamma, \tau) = \frac{1}{1 + e^{-\gamma(s_t - \tau t)}}$$

where $\alpha_{i,1} = 1.0$, $\alpha_2 = 10.0$, $\gamma = 0.5$, and $\tau = 0.5$ ⁸.

Table 2 Simulation results of parameter estimates of LNV (1998)

		Ex. Grid Search	G and J	BFGS	Simplex	Genetic
α_1	MSE	0.02540	0.02475	0.02478	0.02480	0.02731
	RMSE	0.15938	0.15733	0.15743	0.15747	0.16526
α_2	MSE	0.05040	0.05008	0.05015	0.04979	0.05222
	RMSE	0.22449	0.22378	0.22394	0.22314	0.22851
γ	MSE	0.01054	0.02725	0.00872	0.01011	0.00825
	RMSE	0.10268	0.16508	0.09340	0.10055	0.09082
τ	MSE	$2.269 e^{-5}$	$1.871 e^{-5}$	$1.877 e^{-5}$	$1.852 e^{-5}$	$1.881 e^{-5}$
	RMSE	0.00476	0.00433	0.00433	0.00430	0.00434

Note: The other relevant statistics and density functions obtained from these simulations are given in Appendix A.

Table 2 reports the MSE and RMSE criteria for the parameters α_1 , α_2 , γ and τ obtained using the five different algorithms considered in this study. When Table 2 is analyzed, the first thing to note is that among the five methods employed none of them is superior to the other in terms of estimating the parameters. For obtaining α_1 Gauss-Jordan seems to be the best algorithm. Gauss-Jordan algorithm is followed by BFGS, Simplex, and EGS methods; and the Genetic algorithm appears to be the last in this ranking. For α_2 the ordering of the estimation algorithms from best to worst changes to Simplex, Gauss-Jordan, BFGS, EGS, and the Genetic algorithm. The algorithm ordering totally changes when we compute the MSE and RMSE for the slope parameter γ . An inspection of Table 2 clearly reveals that; while the best algorithm for the estimation of γ is the Genetic algorithm, the worst one is Gauss Jordan. For the parameter τ we observe a similar pattern, with Simplex yielding the best algorithm and EGS the worst. From all of these results we can deduce that the accuracy of the estimates of the parameters γ and τ are crucial for unit root testing. From the accuracy comparison made in Table 1, we have seen that the Genetic algorithm produces the most accurate LNV statistics. The Genetic algorithm is followed by the Simplex, BFGS and Gauss-Jordan algorithms in terms of obtaining the accurate LNV critical values. Table 2 reveals that the EGS algorithm estimates the parameters α_1 and α_2 as accurate as any other optimization algorithm. However, we cannot arrive at the same conclusion for the parameters γ and τ . Similar arguments can be made with respect to the Gauss-Jordan optimization algorithm except for the estimation of τ . The Gauss-Jordan algorithm estimates τ as better as any other optimization algorithm. Regarding the BFGS, Simplex and Genetic algorithms; all of the parameter estimates are similar in accuracy except for the estimation of parameter α_1 via the Genetic algorithm. On the other hand, the Genetic algorithm is found to be the best algorithm for estimating the parameter γ with respect to MSE and RMSE criteria. Specifically, the precise estimation of γ directly affects the accuracy of the critical values of the LNV type of unit root testing.

In order to explain these stated points more pertinently, we organize another simulation study in which a variant of the LNV type of unit testing is applied. This LNV variant unit root test proposed by

Solis (2004) applies the threshold unit root testing methodology utilized by Enders and Granger (1998) instead of the ADF test regression in the last step of the LNV unit root test. Therefore, in the alternative hypothesis of the LNV test now we are dealing with a TAR type of data generation process for the residual term. As a first empirical investigation, we obtained the critical values of Solis (2004) unit root test by using the aforementioned methods¹¹. The acquired critical values are tabulated in Table 3 given below.

Table 3. The critical values obtained from different optimization algorithms for Solis (2004)

	1	2	3	4	5
	Solis t				
%1	-3.994	-3.971	-3.935	-3.882	-3.854
%5	-3.417	-3.424	-3.418	-3.366	-3.326
%10	-3.169	-3.177	-3.155	-3.105	-3.062
	Solis F				
%1	12.244	12.090	11.963	11.613	11.518
%5	9.191	9.212	9.115	8.758	8.602
%10	7.844	7.897	7.770	7.458	7.325

- 1) Concentrating the sum of squares with using the BFGS method (Solis, 2004),
- 2) Concentrating the sum of squares with using the Genetic method
- 3) Concentrating the sum of squares with using the Simplex method,
- 4) Concentrating the sum of squares with using the Gauss Jordan method.
- 5) Direct implementation of extensive grid search (EGS) by using OLS.

Note: The results are reported for T=100.

Table 3 reveals a similar pattern to that described previously in Table 1, namely the comparison of different optimization algorithms based on critical values obtained shows that the accuracies of the critical values' can be increased. The critical values obtained using the Genetic algorithm (in column 2) were found to be in close agreement with those obtained by Solis (2004) using the BFGS algorithm, ascertaining the use of Genetic algorithm instead of the BFGS method to obtain the accurate critical values for the Solis unit root tests. Following the argument of Vogous (2006), we can also claim that the critical values obtained using the Genetic algorithm are accurate critical values for the Solis (2004) unit root test. On the other hand, the most inefficient methods to obtain critical values for the Sollis (2004) unit root test seem to be the Gauss-Jordan and EGS algorithms. However, among the three methods (1, 2, and 3) the critical value differences are trivial.

¹¹ In this study the RATS program is used to analyze the performance of different algorithms. Hence, the study is constrained with the programs available in the RATS 8.1 software package. Therefore, in order to use the same simulated data for all algorithms and thereby to be internally consistent, the SQP algorithm was not employed in the rest of the study.

The evidence based on careful examination of these results leads us once more to conclude that using different optimization algorithms in empirical studies would not cause much difference in the interpretation of the empirical test results. In order to robustify this conclusion, we again re-organize a Monte Carlo study that is the same with the first one. If the Genetic algorithm is again found to generate the most accurate critical values using the MSE and RMSE criteria, then this will clearly demonstrate the value of using the Genetic algorithm in conducting the LNV type of unit root tests in many of its extensions like the Sollis (2004) test.

As discussed above, in the next simulation exercise we have used an alternative data generation specification especially for the noise term:

$$y_t = \alpha_1 + \alpha_2 S_t(\gamma, \tau) + \varepsilon_t, \quad \mu_{i_0} = 0,$$

$$\Delta \varepsilon_t = \alpha + \rho_1 I_t \varepsilon_{t-1} + \rho_2 (1 - I_t) \varepsilon_{t-1} + \eta_t, \quad \eta_{it} \sim NID(0,1)$$

where $\alpha_{i,1} = 1.0$, $\alpha_2 = 10.0$, $\gamma = 0.5$, and $\tau = 0.5$ is defined as before, and the following parameter values are used; $\rho_1 = -0.3$ and $\rho_2 = -0,1$.

Table 4. Simulation results of parameter estimates of Solis (2004)

		Ex. Grid Search	G and J	BFGS	Simplex	Genetic
α_1	MSE	1.43143	7.31656	1.62272	1.61982	1.44381
	RMSE	1.19643	2.70491	1.27386	1.27272	1.20159
α_2	MSE	1.38531	9.78787	1.83266	1.82542	1.54451
	RMSE	1.17699	3.12856	1.35376	1.35108	1.24278
γ	MSE	0.07407	0.08382	0.08356	0.08107	0.07521
	RMSE	0.27215	0.28951	0.28907	0.28472	0.27425
τ	MSE	$4.168 e^{-4}$	0.00146	$5.103 e^{-4}$	$5.072 e^{-4}$	$4.592 e^{-4}$
	RMSE	0.02042	0.03819	0.02259	0.02252	0.02143

The results from these power experiments for a sample size of 100 and employing 50000 replications are given in Table 4. The simulation results obtained from this data generation process do not deviate much from those of the first simulation reported in Table 2, except for the performance of the EGS method, which was not unanticipated given the evidence presented in Table 3. From Table 4 we notice that among the five methods; now EGS is superior in estimating the four parameters with respect to the MSE and RMSE criteria. This is the only crucial difference between this and the first simulation results that we have presented in Table 2. For estimating α_1 , EGS seems to be the best algorithm. The EGS algorithm is followed by the Genetic, Simplex, and BFGS algorithms with Gauss-Jordan being the worst algorithm for estimating this parameter. For all the other three parameters this ordering does not change using both the MSE and RMSE criteria. This ordering can be referred as the accuracy

ordering of the Solis (2004) critical values as well. Therefore, the EGS method which we have proposed in section 2 is the best way to conduct power analysis for the Solis (2004) unit root test than the Genetic, Simplex, BFGS and Gauss Jordan algorithms. Although the Genetic algorithm is still the best method to obtain critical values for the Solis (2004) type of unit root test, a careful investigation of Table 4 reveals that the MSE and RMSE of the Genetic algorithm are in close agreement with those obtained using the EGS algorithm. Hence, we can conclude that the difference is trivial. The superiority of Genetic algorithm in obtaining the LNV type trend function is authenticated by all simulation studies. In line with Vougas (2006) we can claim that the Genetic algorithm is superior as much as the SQP approaches in computing the desired critical values of the LNV type of unit root tests. Moreover, the Genetic algorithm is a derivative free method which is easier to use in the estimation process than the BFGS, Gauss-Jordan and the rest of the algorithms which can be classified as hill-climbing methods using derivatives (i.e, BHHH¹² and SQP). The same argument follows for the Simplex method. From this perspective, considering the results with respect to the EGS method from Table 4, we can conclude that using simpler optimization algorithms as the complexity of the data generating process increases leads to unbiased and efficient parameter estimates.

4. Empirical example

In this section we empirically apply all the methods explained in section 2 to examine the validity of the purchasing power parity (PPP) hypothesis for 9 countries over the period 2003:6-2011:10. Monthly data on bilateral exchange rates of the national currency against the U.S. dollar and on consumer price indices (CPI) were taken from International Monetary Fund's *International Financial Statistics* (IFS) database. The base year for the CPI is 1997. The analysis includes 9 countries, namely Argentina, China, Canada, Germany, France, Italy, Japan, Saudi Arabia, Turkey and the United Kingdom. All variables were put into natural logarithms before the analysis. In addition to the LNV tests, we have also applied the Solis t and F tests to the real exchange rate series (RERs). The results are tabulated below in Table 5.

As can be readily seen from Table 5, the application of the LNV unit root tests suggests a random walk behavior of the RERs for 3 countries (or in other words PPP holds only in 3 countries out of 9). However, the crucial issue here is that the test results obtained using all the optimization algorithms are the same for all countries. This phenomenon clearly demonstrates that all the optimization algorithms can be used for obtaining valid tests statistics for the LNV unit root test¹³. The test results in given in italic; such as the test results obtained using the Simplex algorithm for Germany, test results obtained using the Genetic algorithm for Japan and tests results obtained using the EGS method for all countries except Argentina and China, deviate from those obtained via other methods. For the EGS method, the deviations seem to be very minor due to the increments which are taken for the search algorithm. For this study we have chosen 0.1 and 0.01 increments for γ and τ , respectively; and used these increments for the simulation studies as well. From the tests results one can note that even this level of grid search accuracy is sufficient for obtaining the true LNV statistics. In order to have a deeper understanding of the process by which critical values are obtained, we have tabulated the estimated values of γ and τ in Table 6.

¹² We have obtained the critical values and simulation studies of BHHH method. The obtained results are similar with BFGS. The results are shown that BHHH algorithm is not better than BFGS, but the discrepancies are trivial. The results are available upon request.

¹³ We have obtained similar results for the Solis t and F tests. The tests results are available upon request.

Table 5. LNV unit root test results using different optimization algorithms

C Name	<i>BFGS</i>		<i>Genetic</i>		<i>Simplex</i>		<i>Gauss Jordan</i>		<i>EGS</i>	
	Lag	LNV	Lag	LNV	Lag	LNV	Lag	LNV	Lag	LNV
Argentina	1	-2,156	1	-2,156	1	-2,156	1	-2,156	1	-2,156
China	9	-0,338	9	-0,338	9	-0,336	9	-0,338	9	-0,338
Germany	5	-4,095	5	-4,095	5	-4,095	5	-4,095	5	-4,077
France	5	-4,097	5	-4,097	5	-4,097	5	-4,097	5	-4,118
Italy	5	-4,270	5	-4,270	5	-4,270	5	-4,270	5	-4,283
Japan	0	-1,945	1	-2,150	0	-1,945	0	-1,945	0	-1,941
Saudi Arabia	0	-2,277	0	-2,277	0	-2,277	0	-2,277	0	-2,262
Turkey	0	-3,118	0	-3,118	0	-3,118	0	-3,118	0	-3,125
UK	0	-2,765	0	-2,765	0	-2,765	0	-2,765	0	-2,796

Notes: The maximum critical value obtained for the LNV statistics among the algorithms used equals -3.937 and corresponds to that obtained using the Genetic algorithm. The minimum critical value is obtained using the EGS method and is equal to -3.788 at the 10% significance level. The values written in bold represent significance at 10% level and lower levels.

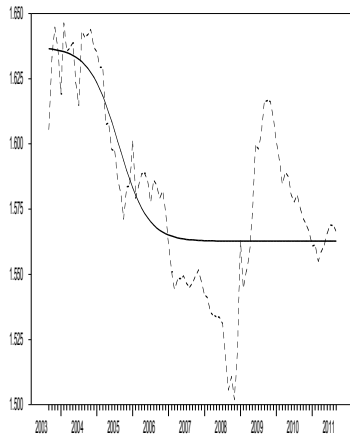
Table 6. Estimated gamma and threshold parameters

C Name	<i>BFGS</i>		<i>EGS</i>	
	$\hat{\gamma}$	$\hat{\tau}$	γ	τ
Argentina	0.204 (4.712)	0.250 (15.301)	0.2	0.24
China	0.192 (5.077)	0.147 (7.064)	0.2	0.15
Germany	0.431 (2.840)	0.454 (23.985)	0.4	0.44
France	0.458 (2.795)	0.454 (25.433)	0.5	0.44
Italy	0.387 (3.558)	0.456 (27.872)	0.4	0.45
Japan	0.204 (3.905)	0.743 (24.685)	2.8	0.65
Saudi Arabia	0.187 (9.335)	0.682 (78.974)	0.2	0.66
Turkey	0.086 (6.038)	0.291 (8.503)	0.1	0.30
UK	3.257 (0.915)	0.662 (196.201)	2.4	0.64

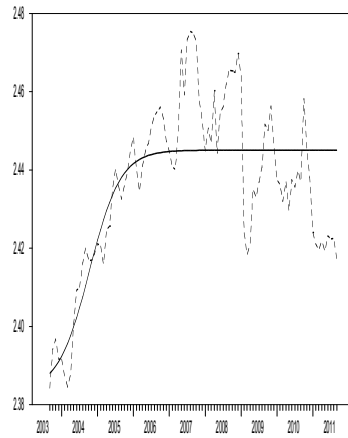
Inspection of Table 6 reveals that the slope of transitions and locations of the threshold for breaks are different for all countries. In spite of this fact, however, we can still classify all countries into three groups with respect to the gamma parameter as follows: *slow* change, *moderate* change and *abrupt* change. This type of grouping can be made with respect to threshold value as well, depending on whether the location of the threshold is at the *beginning* of the sample, at the *middle* or at the *end* of the sample. According to these groupings, Germany, France and Italy can be classified under the *Moderate and Middle* group where the transition is moderate and the threshold location is in the middle; Argentina and China in the *Moderate and Beginning* group; and Japan and Saudi Arabia under the *Moderate and End* group. Turkey and the UK have different slope parameters than the rest of the sample, with Turkey categorized as *Slow and Beginning* and UK can be classified under *Abrupt and End*. The biggest deviation in the test results presented in Table 6 occurs for the Genetic Algorithm in the Japanese case, where the deviation equals 0.205. This result can be attributed to the fact that only a different lag structure is chosen for the Genetic algorithm in Japan using the Akaike Information Criteria (AIC). Although for the EGS algorithm, the AIC criteria produces results that are same with those obtained under other algorithms; still there are deviations in the test results except for Argentina and China due to the fact mentioned above. Therefore, these groupings do not seem to be that much effective on the test results.

If the data had been well behaved with respect to the STR type of trend function (or if the data generating process of series were consistent with STR type trend), the slope and threshold parameters for the break would not be detrimental in obtaining the LNV type of unit root test. In the case that the data generating process of series are not consistent with STR type trend function, different trend specifications can be tried. For example in the linear trend function case, ADF type of unit root testing can be employed in line with Leybourne et al. (1998). If there is more than one break in trend, multiple break type STR function can be employed using the double transition function. These are the alternative solutions for the LNV type of unit root testing. However, although sometimes the STR type of trend function can be consistent with the data, there can still be convergence problems due to the gamma parameter and the threshold parameters. These kinds of problems can be solved using good initial values, by imposing constraints in nonlinear optimization problems and by other suitable methods. But, the general solution to these problems is to use identification tests that specify the features of the series in hand. The first appropriate identification test for this purpose may be the linearity test used in Teräsvirta (1992) and Lin and Teräsvirta (1994). By using this linearity test under the alternative of STR type nonlinearity, we can investigate whether the series are linear or nonlinear. The second appropriate identification test may be a break test such as the one developed in Bai-Perron (1998). And the last one may be the remaining structural shift test as done in the STAR literature in order to identify the second transition function. Thus, we can determine the features of the series in hand and employ the most appropriate unit root test at the beginning without facing any difficulties. These kinds of identification tests are not used in this study, because these issues are beyond the scope of this study. However, the EGS method can be used as a diagnostic test depending on the simulation study and empirical analysis. In the EGS method, we are not confronted with any problem such as good starting values or convergence problem. Hence, it is better to start with the EGS method to obtain the LNV test results. If there is a big deviation in the obtained gamma and threshold values; and tests results using the EGS method from those obtained using the other optimization algorithms (i.e., BFGS, Gauss-Jordan), then employ the other identification tests (i.e., break tests) that we have suggested to obtain better LNV type unit root test results. The visual inspection of STR type trends can be seen below in Figure 1.

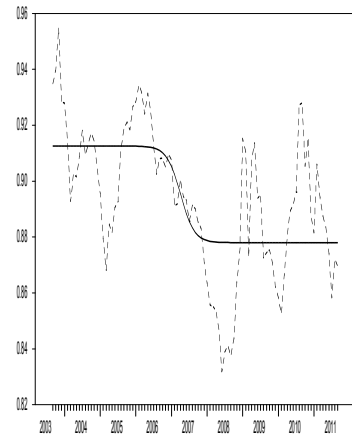
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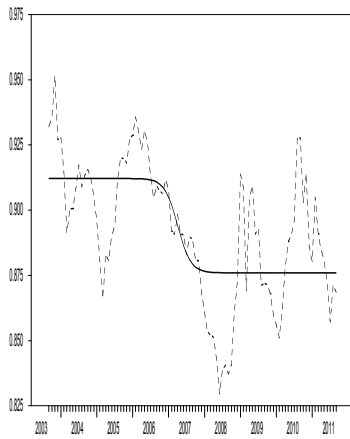
China



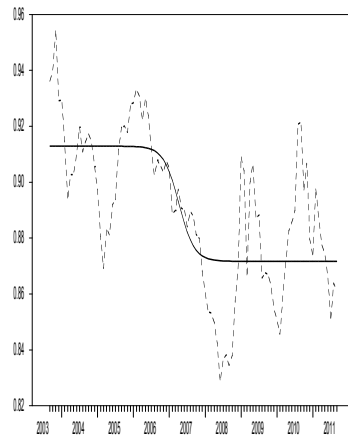
Germany



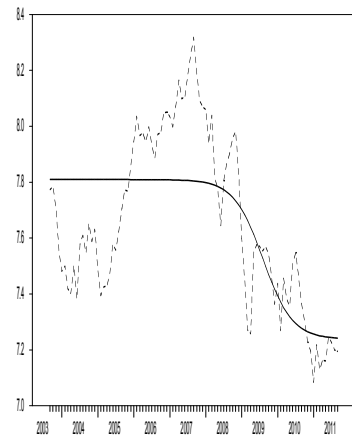
France



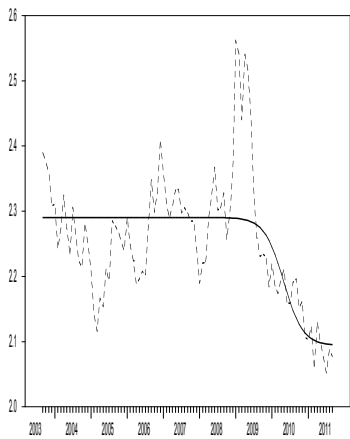
Italy



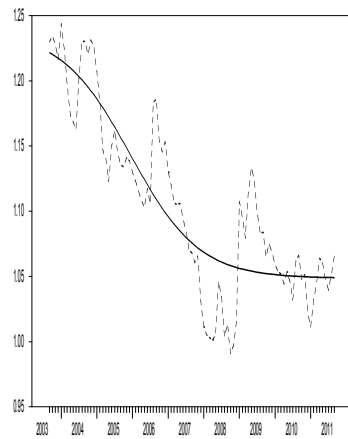
Japan



South Africa



Turkey



UK

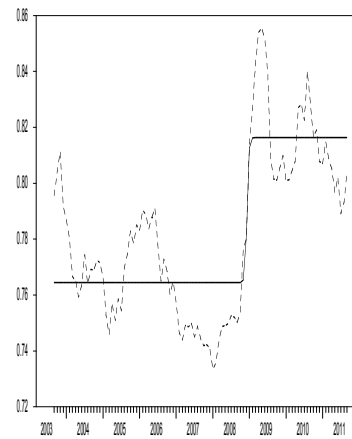


Figure 1. Estimated STR type trend functions for all countries

5. Concluding Remarks

In this study we have compared different optimization algorithms in conducting LNV type of unit root tests in order to obtain more accurate critical values, to conduct better power analysis and to arrive at consistent empirical results. From all of the simulation exercises undertaken in this study, we arrive at the general conclusion that the Genetic algorithm has more advantages than the other methodologies. This can be attributed to the fact that we have obtained the most accurate critical values for the LNV and Solis (2004) unit root tests by using the Genetic algorithm. The second best method seems to be the Simplex method, which is the second derivative free method used in our study. In general, we can claim that the derivative free methods have advantages over hill climbing algorithms in obtaining more accurate critical values. On the other hand, the BFGS algorithm is the best hill climbing method that has a similar performance with the Simplex method in obtaining the accurate critical values for the LNV and Solis (2004) unit root tests. However, the Gauss-Jordan optimization algorithm as a hill climbing method was expected to display a better performance than that observed in this study. From the simulation studies we have seen that its performance is not better than a simple grid search methodology.

From the simulation studies, depending on whether the alternative hypothesis is of LNV or Solis type of unit root test, as expected, we have obtained similar results with the critical value accuracy results. In the first simulation exercise tabulated in Table 2, the Genetic algorithm has outperformed the other algorithms with respect to the gamma parameter. For the rest of the other three parameters, the performance of the Genetic algorithm is similar with that of other methods. From the second simulation study, which is tabulated in Table 4, again the Genetic algorithm is found to outperform all the other algorithms except the EGS method with respect to all parameters considered. In the empirical part, we have estimated the gamma and threshold parameters using the EGS method. These estimation results reveal that the algorithm that we have used works well for estimating the STR trend function. However, these results seem to be good approximations of the estimated parameters $\hat{\gamma}$ and $\hat{\tau}$ due to the increments selected (0.1 and 0.01 for gamma and threshold, respectively) for the grid search analysis. In the power analysis, the selected parameter values for the slope and the threshold parameters are: $\gamma = 0.5$ and $\tau = 0.5$. Therefore, the selected increments for γ and τ give advantages to the EGS method over other methods in the simulation study. Fortunately, when the table values of second simulation study are investigated we realize that the differences between the MSE and RMSE values of the Genetic and EGS methods are trivial. This fact is another piece of evidence that corroborates the conclusion that the Genetic algorithm outperforms the other methods used in the study. Even though we have obtained similar results for the EGS algorithm with respect to other algorithms in the first simulation study, we have observed that the performance of this algorithm is better in the second simulation study. This fact gives us a general conclusion about the structure of optimization algorithms in the sense that as the complexity of the data generation process increases, it is better to use simpler optimization algorithms to obtain unbiased and efficient parameter estimates.

In the empirical part of the study we have found same test results for the LNV and Solis (2004) unit root tests for all countries by using all the optimization algorithms employed. Hence, while conducting empirical studies the researchers may use any optimization algorithm without loss of generality. If the data generating process of the series are consistent with a STR type of trend, then the slope and threshold parameters for the break are not detrimental in obtaining LNV type unit root tests, otherwise, different trend specifications can be experimented with. This approach is the alternative solution for the LNV type of unit root testing. However, sometimes the STR type of trend function can be consistent with the data, but still convergence problems may arise due to the gamma and threshold parameters. These kinds of problems can be solved using good initial values, by imposing constraints to the nonlinear optimization algorithms and by other suitable methods. The general solution to these problems aforementioned in section 4 is to use identification tests to specify the features of the series in hand. However, dealing with these problems is beyond the scope of this study; and further elaborations on these areas can be considered as recommendations for further research.

Appendix A

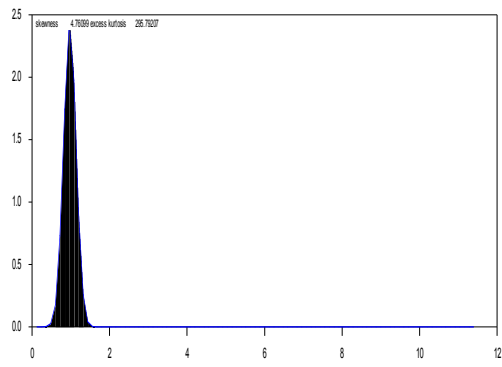
Table 1A. The simulation results for parameters α_1 and α_2 under normally distributed error terms

	$\alpha_1 = 1.0$					$\alpha_2 = 10.0$				
	Ex. Grid Search	Gauss Jordan	BFGS	Simplex	Genetic	Ex. Grid Search	Gauss Jordan	BFGS	Simplex	Genetic
Mean	0.973	0.972	0.972	0.972	0.973	10.028	10.030	10.031	10.030	10.030
Median	0.974	0.973	0.972	0.973	0.973	10.026	10.029	10.029	10.029	10.028
Variance	0.026	0.024	0.024	0.024	0.027	0.051	0.049	0.049	0.049	0.052
St. Error	0.163	0.154	0.155	0.155	0.164	0.227	0.221	0.221	0.221	0.228
Skewness	4.760	-0.019	-0.028	-0.121	-8.700	-1.695	0.020	0.023	0.059	3.340
Kurtosis	295.792	0.148	0.258	2.057	656.679	76.046	0.076	0.110	0.608	182.739
Minumum	0.209	-0.323	-0.600	-1.802	-11.483	-0.020	9.017	9.017	9.017	9.164
Maximum	11.113	1.659	1.660	1.659	1.558	11.031	11.446	11.724	12.928	22.613
01-%	0.607	0.609	0.610	0.610	0.611	9.513	9.518	9.518	9.518	9.164
99-%	1.339	1.331	1.331	1.331	1.332	10.550	10.549	10.550	10.549	10.548

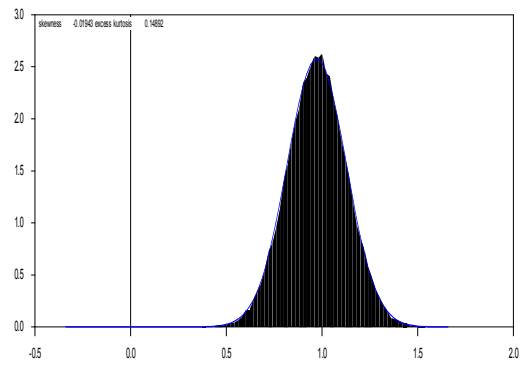
Table 2A. The simulation results for parameters γ and τ under normally distributed error terms

	$\gamma = 0.5$					$\tau = 0.5$				
	Ex. Grid Search	Gauss Jordan	BFGS	Simplex	Genetic	Ex. Grid Search	Gauss Jordan	BFGS	Simplex	Genetic
Mean	0.513	0.512	0.511	0.511	0.511	0.499	0.499	0.499	0.499	0.499
Median	0.500	0.500	0.500	0.500	0.500	0.500	0.499	0.499	0.499	0.499
Variance	0.010	0.027	0.008	0.008	0.008	0.000	0.000	0.000	0.000	0.000
St. Error	0.101	0.164	0.092	0.091	0.090	0.004	0.004	0.004	0.004	0.004
Skewness	16.716	131.730	4.118	1.883	1.684	2.496	-27.443	-27.797	-27.996	-28.889
Kurtosis	1500.535	24654.31	179.76	37.804	26.097	132.178	3048.61	3100.54	3130.73	3264.86
Minumum	0.300	0.262	0.262	0.262	0.274	0.480	0.019	0.016	0.015	0.009
Maximum	10.000	31.356	5.573	3.846	3.471	0.720	0.514	0.514	0.514	0.516
01-%	0.400	0.350	0.350	0.350	0.351	0.490	0.491	0.491	0.491	0.491
99-%	0.800	0.781	0.781	0.781	0.776	0.510	0.508	0.508	0.508	0.508

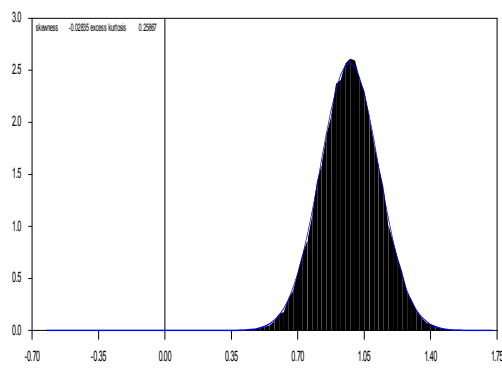
EGS



Gauss Jordan



BFGS



Simplex

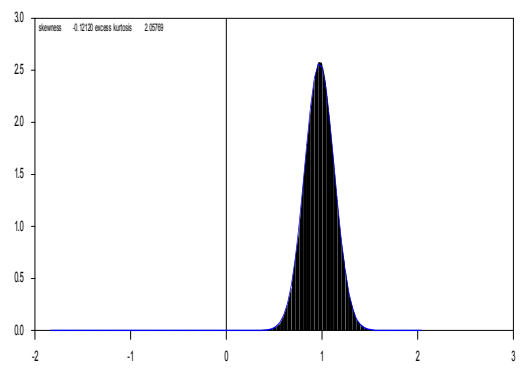
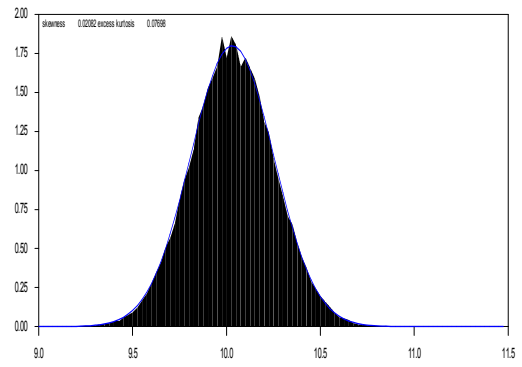
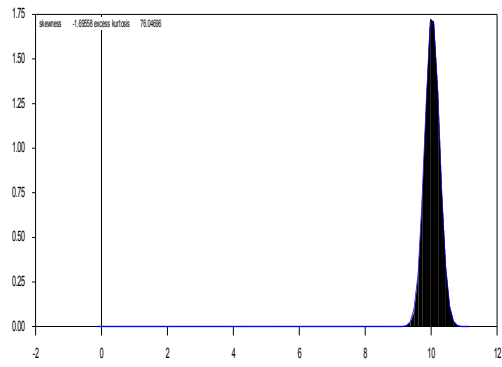


Figure 1A. Density function and normal distribution of the parameter α_1

EGS

Gauss Jordan



BFGS

Simplex

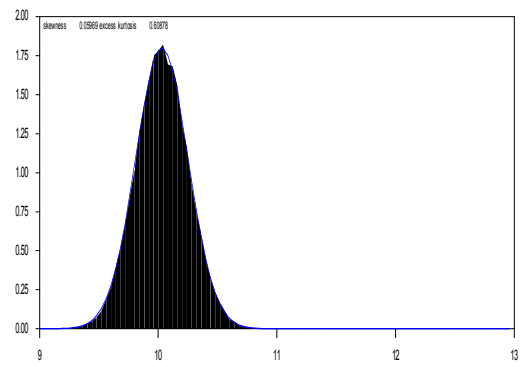
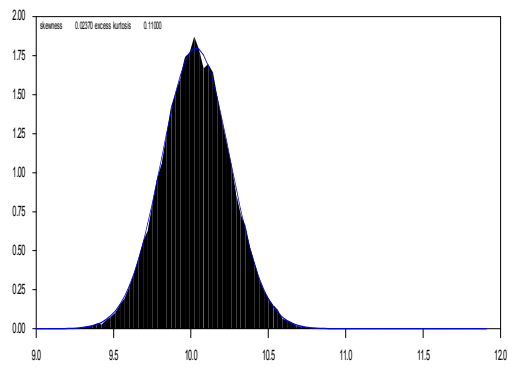
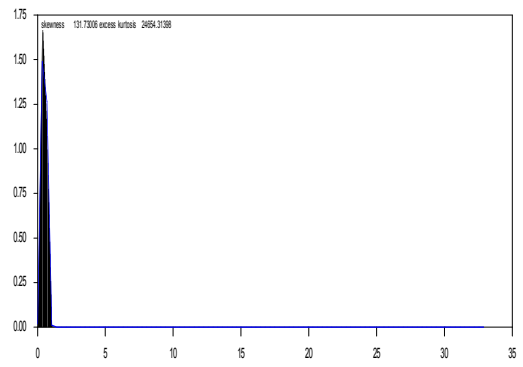
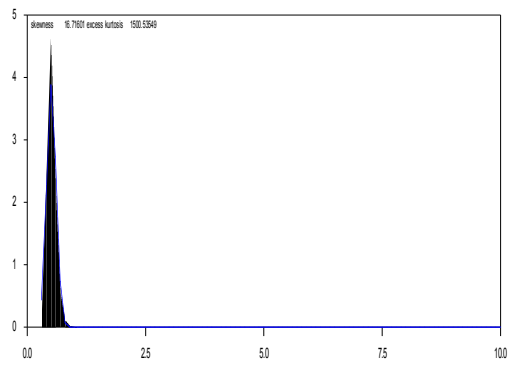


Figure 2A. Density function and normal distribution of the parameter α_2

EGS

Gauss Jordan



BFGS

Simplex

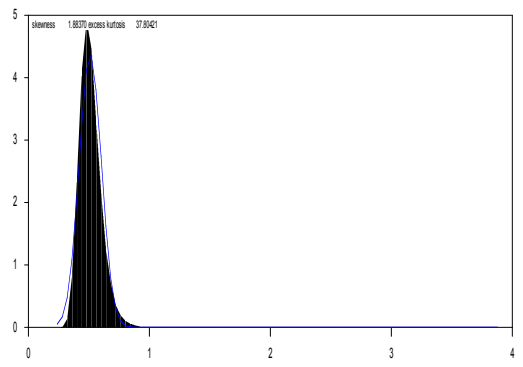
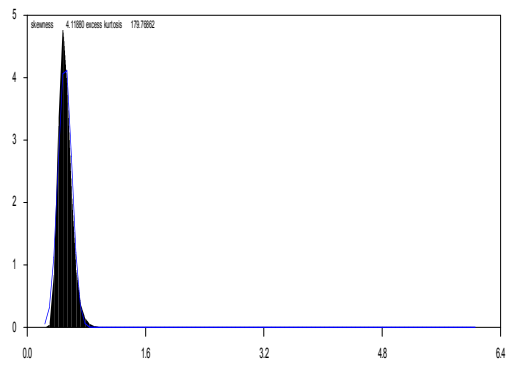
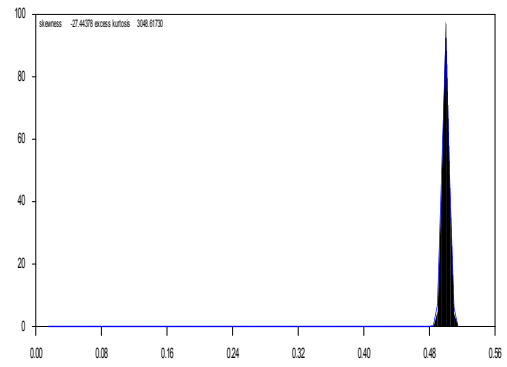
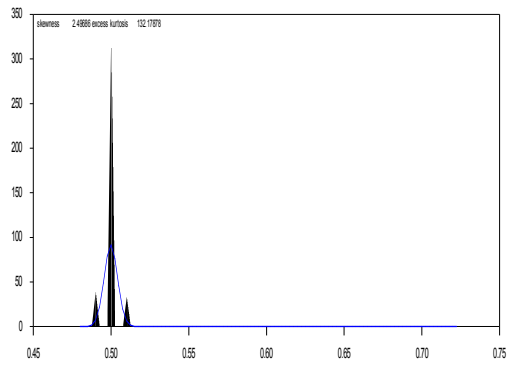


Figure 3A. Density function and normal distribution of the gamma parameter

EGS

Gauss Jordan



BFGS

Simplex

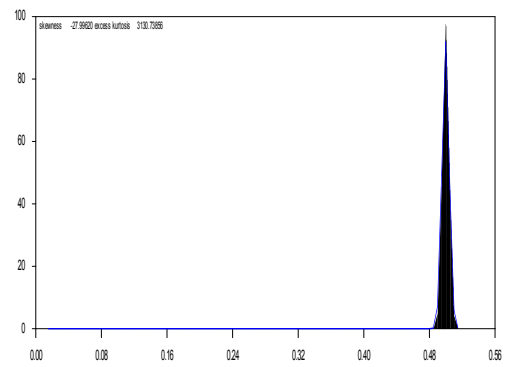
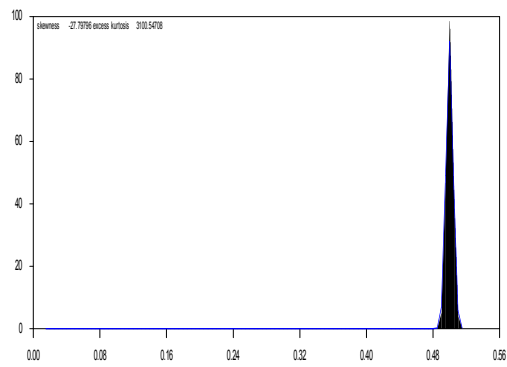


Figure 4A. Density function and normal distribution of the threshold parameter

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