

DEVELOPING ACADEMIC SOFTWARE FOR TEACHING TIME SERIES ANALYSIS: A CASE STUDY

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Abstract

The academic training on time series analysis requires not only a sound theoretical background on the methods but also the use of specific academic software to appreciate the methods' capabilities, limitations and proper applicability. It is desirable for students to program the routines and algorithms by themselves but this is not always feasible, particularly during short courses and workshops in which the interest is to understand the information supplied by several analytical methods. Considering the time constraints and the need to stress the interpretative rather than the computational skills, the authors have developed the software package UATSA (University of Arizona Time Series Analysis) that incorporates many analytical tools commonly used in time series analysis in an organized and sequential manner: exploratory statistics, markovian processes, univariate and multivariate analyses (ARMA models), frequency decomposition algorithms, principal components, canonical correlations and cluster analyses are included within the current version of the package. UATSA is a stand-alone executable file compiled in MATLAB[®] that has been used in courses of time series analysis in hydrology at the University of Arizona and in

several workshops offered by the authors between 2004 and 2007. The software aims to easily illustrate the use of algorithms in the synthesis and decomposition of time series, providing a background to the methods and a visual platform that is user friendly and data extensive. The software has evolved through the years, incorporating suggestions made by students to improve its appearance and widen its scope. The software also has contributed to a shift in teaching dynamics by allowing students and instructors to focus on interpreting and analyzing outcomes rather than just learning the set of mathematical tools.

Introduction

Time series play a fundamental role in virtually all sciences and technical fields of knowledge. Each discipline, according to its own needs and interests, has contributed to the development of a wide range of tools to analyze time series. Time Series Analysis (TSA) is an active field of research that specializes in the development and application of methods to tackle a variety of scientific issues related to time series datasets.

Universities regularly offer introductory and advanced graduate courses on TSA with

contents that vary according to the requirements of specific groups. In introductory courses it is a common practice to include standard methods on the time and frequency domains and the spatial analysis of distributed univariate and multivariate time series.

The desirable goal of letting the students write their codes to gain a full understanding of the algorithms (particularly in advanced courses) is usually challenged by the following aspects: the course's time constraints; the fact that not all the students in a course group, which usually consists of people with diverse backgrounds and interests, are familiarized with mathematical methods or have the required programming skills to either manage existing libraries or write their own scripts; the large datasets that must be handled and the complexity of managing several methods to analyze and synthesize the information in short time. TSA courses, therefore, involve the use and development of software to speed up the learning process and increase the number of methods that can be covered during a regular semester. There are several software options, both commercial (i.e., MATLAB[®], MATHEMATICA[®], S and SAS[®]) and freeware (i.e., R, Octave), that include TSA libraries and allow users to run their own programs.

People who are interested in applying the methods to analyze their datasets but lack the skills or are simply short of time to program their own codes may look for alternative software toolkits that are rigorous in their algorithms and have an interface that is simple to use and sufficiently descriptive of the methods used (these aspects of software development are discussed by [1] in detail). Many toolkits that perform statistics and time series analysis with different scopes and varying degrees of complexity are already available online as public domain software. Examples of these kind of software are: TISEAN[2] for nonlinear analyses, SSA-MTM Toolkit for spectral analysis[3], extRemes[4] for the analysis of extreme events, ASTSA[5] for introductory methods on time series analysis,

KSpectra toolkit[6] for spectral analysis and the free statistics and forecasting software[7] based on R libraries.

It is within this context that the authors have developed the public domain software UATSA (University of Arizona Time Series Analysis) intended mainly for instruction on the fundamentals of TSA in hydrology. This paper describes the structure of UATSA, briefly introduces the main technical aspects of its modules and discusses the authors' experience in using it as an aid in introductory TSA graduate courses and short workshops.

Package Structure

UATSA is an executable, stand-alone application compiled in MATLAB[®][8]. The package requires only the installation of an additional interpreter file (MCRInstaller.exe) to read the compiled libraries in the end-user's computer (this interpreter works also for any other executable file compiled in MATLAB[®]). The decision to use MATLAB[®] was based on the author's own experience working with the computational and graphical capabilities of the software (that already includes many libraries on statistics and TSA), including the possibility to design and compile Graphical User Interfaces (GUIs) as stand-alone applications.

UATSA's modular, user-friendly interface provides quick numerical and visual results of several methods of time series analysis (in time, frequency and space domains) that are commonly taught in graduate introductory courses in hydrology. Each module consists of (figure 1): an interactive panel that displays the data and the plots generated during the analysis; a menu bar that includes options to manage files and graphs, run the methods and open the users' guide document (a hypertext that briefly introduces the methods employed and has a step-by-step description on how to work with data and save output files and figures); a tool bar (with features from the MATLAB[®] GUIDE editor) that includes tools to dynamically interact with the panel plots (i.e., data matching,

dragging and zooming); additional windows that display specific figures which may be edited and saved directly by the user with a default editor bar provided by the MATLAB[®] compiler.

The modules, which are designed to work independently, follow a logical progression from exploratory data statistics to the formulation of stochastic models based on the analysis, decomposition and reconstruction of data's deterministic and stochastic components. The modular structure facilitates also the package upgrading and the inclusion of new tools and methods as they are considered in the course work. Currently the toolbox includes:

1. Exploratory data analysis: sample statistics, detrending, data augmentation and gap filling.
2. Analysis and synthesis in the time domain: univariate models (annual and seasonal) and multivariate models (annual and seasonal).
3. Analysis and synthesis in the frequency domain: spectral analysis, multichannel singular spectrum analysis and wavelets.
4. Analysis and synthesis in space/time domains: principal components, canonical correlation and clusters.
5. State-space models: Kalman filter.

A brief explanation of these modules follows (this paper does not focus on the theory behind the methods but includes references to sources that discuss each in detail).

Exploratory data analysis

The module on exploratory data analysis provides analytical tools and graphical outputs to examine the statistical structure of time series (Figure 1). Its aim is to familiarize users with powerful, yet simple tools to visualize and quantitatively characterize time series. As with all the modules, data can be either imported from ASCII files written in specified formats or directly pasted in a table created in the interactive panel. The module allows the analysis of both single and multiple data series which may have missing values. Users can

choose among several plot options (histograms, autocorrelograms, periodograms, box whisker and phase state diagrams) to represent the data series.

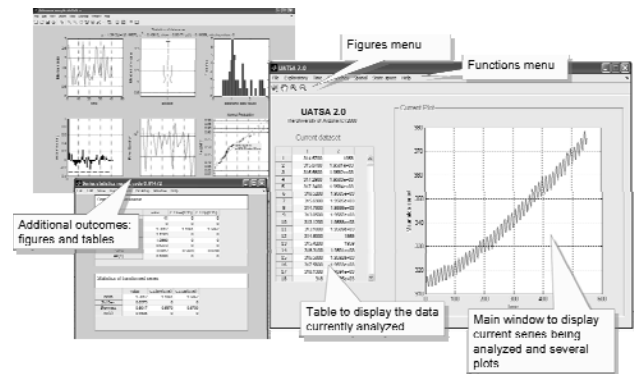


Figure 1. Home menu, interactive panel and some of the plots generated with the module of exploratory data analysis.

After a visual inspection, users may choose among several probability distribution functions to fit the data using the Kolmogorov-Smirnov confidence test as a criterion of acceptance or rejection[9]. A probability plot with the results of the test is generated in the main panel. Users can also detrend the data series using linear regression, differentiation and smoothing techniques (an option is provided to detrend the series with the module of analysis and synthesis in the frequency domain). The module provides also tools for data augmentation and gap filling using smoothing and cross correlation techniques for multiple time series.

Analysis in the time domain

Once the data's main features have been identified, users can proceed with the module on time domain analysis and synthesis (see Figure 2) which provides tools to visualize the autocorrelation functions (ACF) and partial ACF (PACF) for univariate and multivariate analysis to identify ARMA models and to generate annual and seasonal series[10]. Each analysis is divided in three main steps: 1) verification of normality and stationarity conditions, 2) determination of the ARMA model that best fit the observed data and

3) generation of synthetic series.

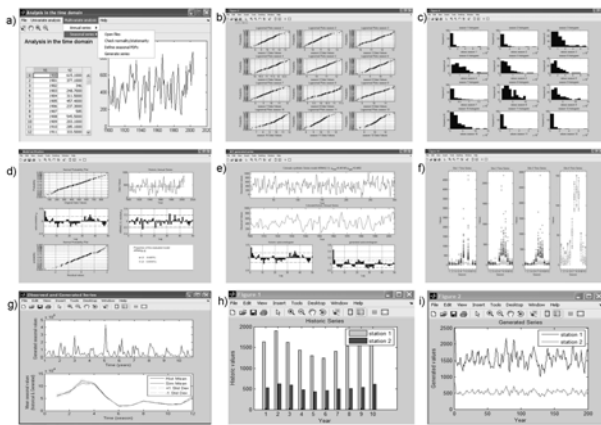


Figure 2. Univariate and multivariate analysis plots for generation of ARMA models: a) main module panel; b) normal plots; c) histograms; d) verification plots; e) generated series; f) multiple distributions; g) generated series and confidence intervals; h) multivariate series; i) generated correlated series.

Users must check first that series are normally distributed and stationary before choosing and running the appropriate ARMA model. For univariate annual analysis the module generates a window containing five plots (Figure 2d): the first two, representing the series and its distribution over a normal probability scale, serve to check the assumptions of normality and stationarity; the third and fourth plots, representing the autocorrelograms of both the series and its residual after subtracting the ARMA component, and the fifth plot, representing the residual in a normal probability scale, help to determine what kind of autoregressive model better fits the data (i.e., the closer the residual values are to a normal distribution the better the model fits the series). If data are neither stationary nor normally distributed, users may subtract any significant trends and periodic components using either the exploratory module or the frequency domain module to obtain the residual series to work with.

Once the ARMA model that best fit the series has been identified, users can generate time series of any given length. The result is an output file containing the generated series and its statistical properties and a figure showing the generated and historical series and their respective autocorrelograms (Figure 2e). The subtracted trends and periodic components are presented in separate tables and their values must be added back to the generated series to obtain the representation of the whole process. For the annual multivariate case the module additionally generates a comparative bar plot of the multiple time series chosen (Figure 2h).

In addition to verify normality and stationarity conditions, seasonal analyses require users to define the probability distribution that best fits the seasonal data for every season considered (currently the module only incorporates normal and lognormal distributions). The module displays the generated time series as well as the mean seasonal values of both the observed and generated series bounded by a confidence region representing one standard deviation above and below the historical mean seasonal values (Figure 2g). Once the different distribution functions for all the seasons and series have been determined, users can generate correlated ARMA series. Users must review the results by comparing the generated and observed series and checking that first and second order statistical properties are preserved.

Analysis in the frequency domain

The module of analysis in the frequency domain aims at helping users identify, decompose and extract meaningful information from time series, such as trends and periodical components. It includes three mathematical tools: Fast Fourier Transform (FFT), Multichannel Singular Spectrum Analysis (MSSA) and wavelets.

Fast Fourier Transform (FFT)

The procedure is divided in four main steps: 1) frequency identification, 2) frequency decomposition, 3) extraction of significant components and 4) analysis of the residual. In the first step the module generates the FFT periodogram to identify significant frequencies in the series. In the second step, users choose the window length or embedding dimension to decompose the series in its main frequencies. The relative weights of these components (i.e., trends and periodicities) are represented by their eigenvalues plotted in descendent order (Figure 3a). W-correlations of the full decomposition eigenvalues are also depicted in a grayscale matrix from full correlation (black) to zero correlation (white) (Figure 3b). These graphs allow users to identify and choose significant components in terms of their correlation values.

In the third step users may extract and plot the significant components (i.e., trends and periodicities) that were previously decomposed. The module generates phase state plots of paired harmonics to refine the identification of those components of the spectrum that are in phase-quadrature (Figure 3c). A diagram shows the power spectrum of each selected component. In the fourth step, users subtract those previously identified significant components to obtain a residual series which is supposed to represent a random process. The module generates a plot that superimposes the sum of significant components to the original series and plots also the residual series and its spectrum (Figure 3d). Users may repeat the process over the residual series until it exhibits no significant frequencies in its power spectrum.

Multichannel Singular Spectrum Analysis (MSSA)

MSSA is a data-adaptive, nonparametric technique that allows the analysis of multiple signals (channels) simultaneously and the extraction of their common significant trends and oscillations[3, 11-13] (the analysis of single series is known simply as SSA). The procedure

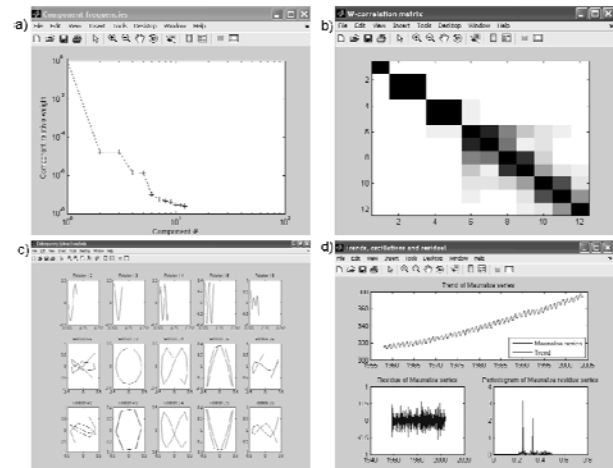
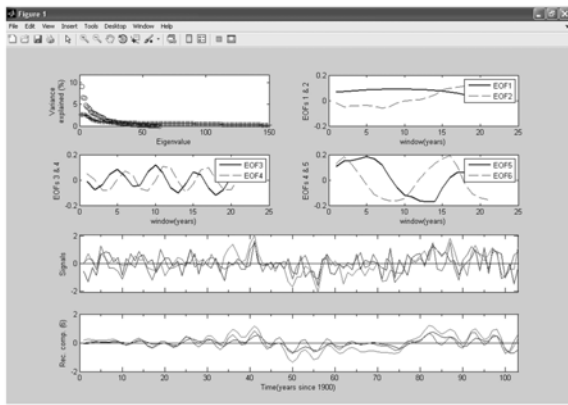


Figure 3. Example of plots displayed in the spectral analysis using FFT: a) eigenvalue decomposition, b) w-correlation matrix, c) phase-state diagrams of selected frequencies and d) reconstruction of trends and oscillations and residual periodogram.

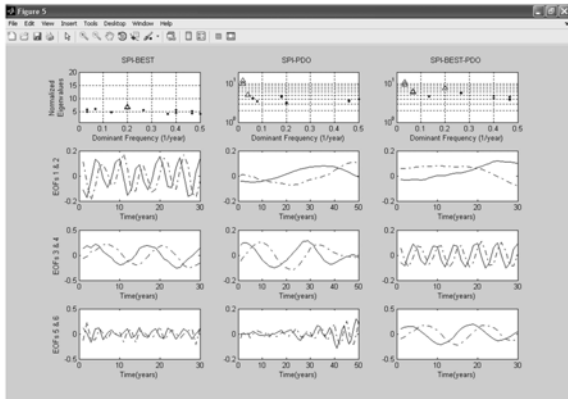
in the module—adapted from a code written by[14]—is divided in four steps: 1) identification of signal structure, 2) signal decomposition, 3) extraction of significant components and 4) reconstruction of significant components and analysis of the residual. Users must choose the window size or embedded dimension to do the analysis and decide which components are significantly different from red noise, which is calculated automatically by generating Monte Carlo simulations of AR(1) processes with the same first and second order statistics of the series. Series must have the same length and be concurrent. The module displays the eigenvalues against the variance explained and their dominant frequencies, pairs of eigenvectors in decreasing order and the observed and reconstructed series using significant components selected by the user (Figures 4a and b)

Wavelets

Wavelets are useful tools in the time-frequency domain for the analysis of non-stationary variances at different time scales. Wavelets decomposition helps identify



a)



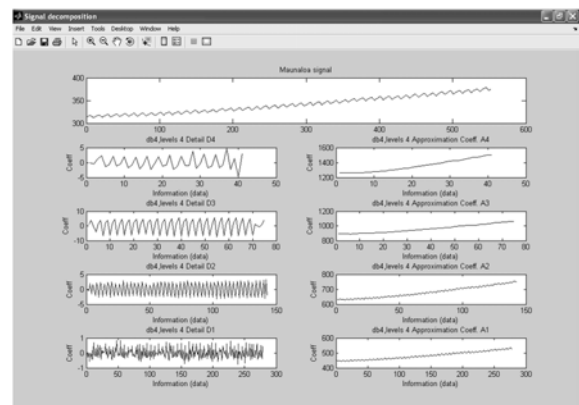
b)

Figure 4. MSSA analysis plots for signal decomposition and reconstruction (three signals analyzed): a) variance explained by eigenvalues, EOF structures and observed and reconstructed series; b) eigenvectors' dominant frequencies and EOF pairs.

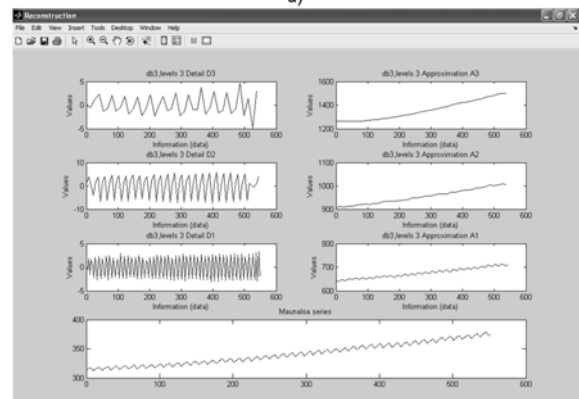
dominant modes of variability and changes of variability with time[15]. The procedure in the module allows users to: decompose, reconstruct and de-noise a signal in several levels or scales using different wavelet families as filters (i.e., Deubechies, Symlets) (Figure 5). Users define the wavelet filter and the levels to scale or de-noise the signals.

Spatial and temporal analysis

Time series in hydrology are generally associated with processes and variables that are distributed in space. Therefore, the analysis of time series is not restricted to the time and frequency domains but includes the spatial analysis of patterns and features evolving through time. This module aims at introducing



a)



b)

Figure 5. Wavelets analysis plots: a) signal decomposition and b) signal reconstruction at different levels.

techniques that are useful for analyzing spatially-related attributes associated with distributed time series. The module includes principal components, canonical correlation and clustering analyses.

Principal components analysis (PCA)

PCA is a non-parametric technique that transforms a multidimensional set of correlated variables into a set of components that are uncorrelated (orthogonal), with each component explaining a specific amount of variance from the original variables (usually the components are organized in decreasing order of variance explained, being the first components those that explain the most of the variance). The technique is commonly employed to reduce the dimensionality of problems that involve huge datasets (i.e., spatial analysis of distributed

variables) by focusing only on those components that explain a significant part of the variance (for a detailed description of PCA see[16]).

The PCA procedure incorporated in the module (Figure 6) allows users to obtain the eigenvalues and their explained variances (in a Pareto diagram, Figure 6a) and the eigenvectors and principal components of a set of observations on several variables (the module centers automatically the variables on their mean values). The module may be employed either to determine principal components of several variables in the same time sequence or to determine principal components of a single variable uniformly distributed in space (each case requires a specific format to introduce the data). If the spatial option is enabled, users can also plot the distribution of mean values and the coefficients of the eigenvectors in the space by specifying the properties of the grid to be plotted (i.e., number of grids in latitude and longitude, grid size or resolution and the coordinates of the bottom left corner). Border lines representing basin limits can also be mapped. Figure 6d shows the spatial plots

generated by the module for the mean values and the first three EOFs of the analyzed variable (precipitation in the Colorado Basin).

Canonical correlation analysis (CCA)

CCA is a multivariate statistical technique that correlates multiple dependent variables with multiple independent variables by creating canonical functions from linear composites of the dependent and independent variables (canonical variables) and maximizing the correlation among them (for a detailed description of the method see[17]). The CCA procedure incorporated in the module calculates the eigenvalues and eigenvectors of the cross correlation of two matrices $X(n \times m)$ and $Y(n \times k)$ which may have different number of sites or variables but the same number of observations. The module normalizes the two sets of variables X and Y introduced by the user and calculates the matrices of canonical correlation coefficients (linear combinations of variables in X and Y) and the matrices of transformed canonical variables (U and V in Figure 7). The module produces a plot of the transformed variables as shown Figure 7.

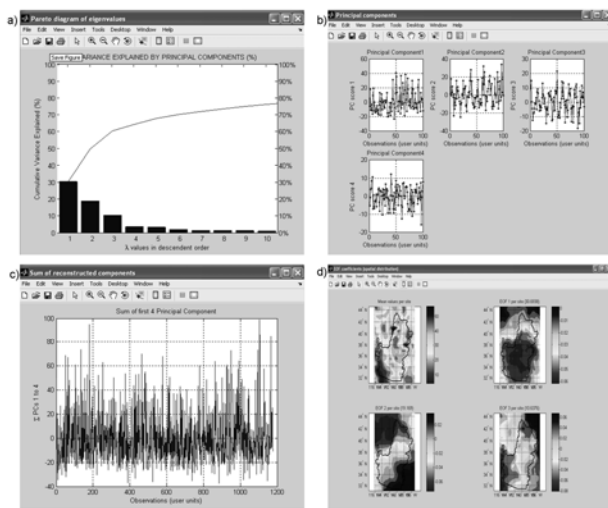


Figure 6. PCA plots: a) eigenvalues (explained variance), b) principal components, c) reconstructed signal and d) spatial distribution of EOF coefficients.

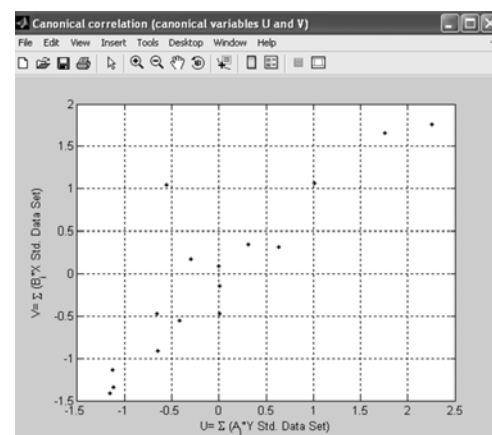


Figure 7. Canonical correlation plot for multiple dependent and independent variables (U and V are the canonical functions derived from the original variables).

Cluster analysis

Cluster analysis encompasses several statistical techniques employed to classify or group data into different sets according to similarity measures (i.e., correlation coefficients).

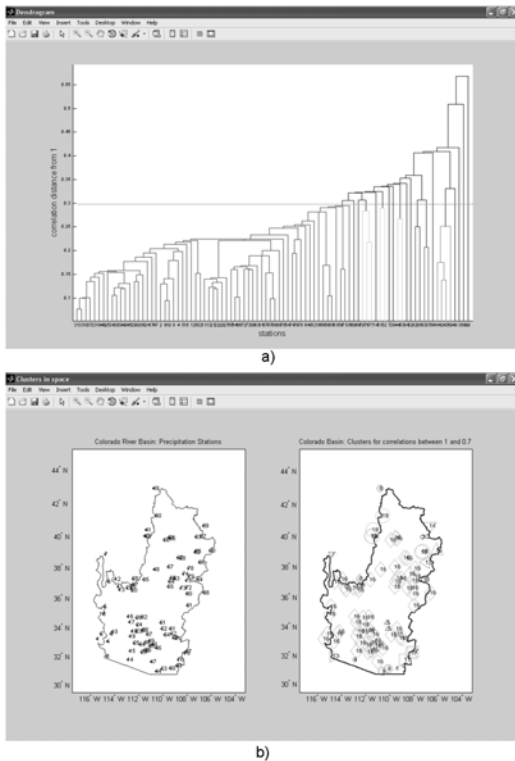


Figure 8. Cluster analysis plots: a) dendrogram and b) spatial distribution of clusters.

Clustering may be particularly useful to visualize spatial features associated with distributed variables[18]. The analysis currently available in the module (Figure 8) uses correlation coefficients as measure of similarity for hierarchical and k-means clustering. It performs the following steps: 1) standardize variables, 2) compute similarity measure (Euclidean distances for correlation coefficients), 3) group data with similar minimum distances (correlations) and 4) plot the clusters in a dendrogram (Figure 8a). The module also allows the mapping of clusters if coordinates are provided by the user (Figure 8b). The user chooses the threshold distance to define the clusters.

State-space models

A state-space model is a mathematical representation of a system defined by inputs, outputs and state variables related by first-order differential equations. Stochastic systems, as those commonly found in hydrology, are characterized by the presence of statistical noise in the system's dynamics and measures. It is, therefore, necessary to filter these noises to estimate the behavior underlying these stochastic systems. The Kalman filter[19] is a popular algorithm to efficiently estimate the most likely state of a stochastic system by recursively filtering the noise from observed signals (usually assumed as Gaussian). The module on state-space models currently implemented includes (Figure 9): a procedure for verifying the stability and convergence of Kalman filter parameter estimates given that

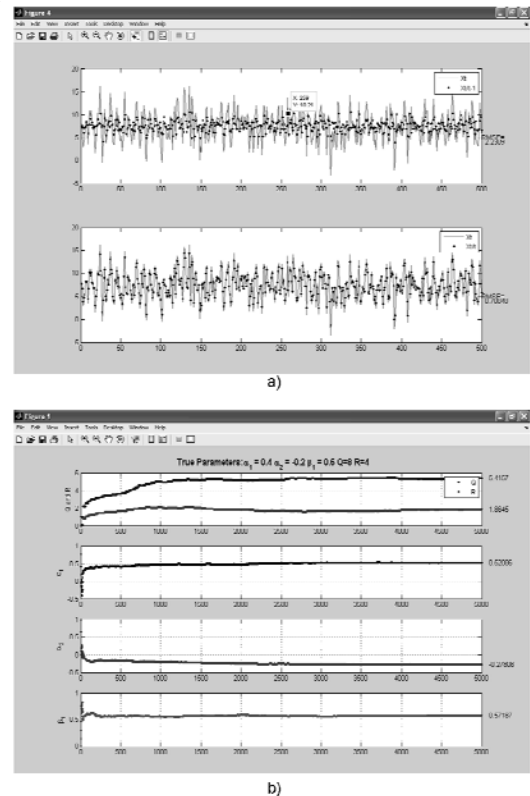


Figure 9. State-space analysis plots for parameter identification and model consistency using the Kalman filter.

both the observed and generated (system) series are known—an ideal situation used to illustrate the application and efficiency of the filter—and a Kalman filter to estimate the state of the system based on observed time series only.

Academic Training

The authors have used UATSA in several graduate courses and workshops on time series analysis at the University of Arizona and at the Universidad de Castilla-La Mancha (Spain) since 2004. The package and sample datasets are distributed among the attendants as an aid to solve homework assignments (participants who are willing to program their own algorithms or want to use other toolboxes are encouraged to do so).

Due to the complementary nature of the software as a teaching aid in structured courses on TSA, UATSA is currently distributed to course students and workshop attendants. In addition, the distribution to a limited group allows the identification of major design and operational issues before any intended release online. A major concern of the authors has been to make the package not only accurate but also user-friendly and appealing, since its main intended purpose is to serve as an academic toolbox (the package has been also employed as a visual aid to illustrate the methods' applications during class time).

Students and workshop attendants (in the order of 10 participants per course) have provided valuable criticism about the software design and have helped to debug the code. There were no evaluation forms for the software at the end of the courses, but rather a continuous feedback from the students as they were working with it along the semester. As a result of this feedback, the authors have incorporated changes in the interfaces and in the management of input and output files (figures and numeric results).

An issue detected by the users of the first version, for instance, was the relative uneasiness to prepare, store and save ASCII data files

because many of them were familiar with Excel tables (former versions of the package did not have the option to paste tabulated values directly in the modules). This difficulty was overcome in later versions, mainly with the inclusion of interactive tables. The formatting has also been simplified to define variables in columns and time series in rows for all the modules which facilitates the preparation of datasets by the user. Another issue has been to provide graphical outcomes that are useful for the analysis and require minimum additional editing from the users to be incorporated in their reports.

As mentioned by [1], some versatility is lost when developing and designing user interfaces. In the process of designing the interface, for instance, a critical aspect has been to keep a balance on the number of steps required to do the analysis: too many steps tend to discourage use, but too few reduces the procedure to a black box approach that is not adequate for educational purposes. The authors have opted for minimizing the number of steps that keep the meaning of the procedure clear, including steps for data acquisition, parameter definitions, routine selection and graphical and tabular outputs.

The use of UATSA to illustrate the methods as they are presented in the classroom has served the authors to modify some teaching dynamics by helping students to compare the outcomes from different methods as they dedicate time to understand the meaning of these outcomes and how to integrate them in the problem solving process. As the package evolves to include new methods and algorithms (i.e., Kalman Filtering and the treatment of missing data) it also facilitates the discussion of new topics during class time and workshops.

Developing the application (i.e., writing the software and designing a didactic, error-proof interface) is a time-consuming activity that requires empathy to the users' needs and expectations towards the software, which are neither unique nor convergent. In the authors'

experience, this process is most of the time rewarding since it improves the understanding of how to transfer state-of-the-art knowledge to groups using new technologies that goes beyond the conventional instructor-student class interaction.

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Biographical Information

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