Particularities and commonalities of singular spectrum analysis as a method of time series analysis and signal processing

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Abstract

Singular spectrum analysis (SSA), starting from the second half of XX century, has been a rapidly developing method of time series analysis. Since it can be called principal component analysis for time series, SSA will definitely be a standard method in time series analysis and signal processing in the future. Moreover, the problems solved by SSA are considerably wider than that for PCA. In particular, the problems of frequency estimation, forecasting and missing values imputation can be solved within the framework of SSA. The idea of SSA came from different scientific communities such as time series analysis (Karhunen-Loeve decomposition), signal processing (low-rank approximation and frequency estimation) and multivariate data analysis (principal component analysis). Also, depending on the area of applications, different viewpoints on the same algorithms, choice of parameters, and methodology as a whole are considered. Thus, the aim of the paper is to describe and compare different viewpoints on SSA and its modifications and extensions to give people from different scientific communities the possibility to be aware with potentially new aspects of the method.

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1 Introduction

References The origin of singular spectrum analysis (SSA) is usually referred to the papers (Broomhead & King, 1986a) and (Fraedrich, 1986). SSA became widely known in climatology after publication of (Vautard & Ghil, 1989; Vautard, Yiou, & Ghil, 1992). After several years, the book (Elsner & Tsonis, 1996) summarized the basic information about SSA existing to that moment. In parallel, SSA (named “Caterpillar”) was created in Russia; the results were published in (Danilov & Zhigljavsky, 1997) (in Russian). A theoretical breakthrough was performed in the fundamental book (Golyandina, NeKRutkin, & Zhigljavsky, 2001), where the theory is put together with examples. The next book is (Golyandina & Zhigljavsky, 2013) in the series Briefs in Statistics; it contains a brief description and some updates from 2001, including description of SSA as a set of filters.

From 2013, a large jump was performed in SSA, when it starts to be considered from the general point of view for analysis of objects of different dimensions and shapes. Also, the R-package Rssa (Korobeynikov, Shlemov, Usevich, & Golyandina, 2017) was developed with a very fast implementation of SSA for the whole range of objects. This structured approach to SSA, its multivariate extensions (MSSA and 2D-SSA) together with algorithms and description of the implementation in Rssa are contained in the recent book (Golyandina, Korobeynikov, & Zhigljavsky, 2018).

Three mentioned monographs of Golyandina and coauthors cover a very wide range of problems solved by SSA; however, they only briefly discuss practical applications of SSA to stationary processes. On the other hand, the applications of SSA to stationary time series were developed by the team from UCLA (starting from (Yiou, Sornette, & Ghil, 2000)), mostly for climatic data. Some practical applications, in particular, in economics and biomedicine, are considered in numerous works of H.Hassani, S.Sanei and their coauthors (see e.g. the book (Sanei & Hassani, 2015) and the review (Hassani & Thomakos, 2010)). A separate branch is related to real-life problems in geophysics, where traces of straight lines should be extracted; a preliminary processing is performed by the Fourier transform of the image rows and then Complex SSA is applied to the Fourier coefficients (S. R. Trickett, 2003; Oropeza, 2010). It seems that these branches are developed separately; however, it would be very helpful to enrich one another.

Sketch of algorithm The SSA algorithm consists of two stages. The first stage is called Decomposition, where the initial object (e.g. time series) is transformed to a trajectory matrix (a Hankel matrix) and then the singular value decomposition is applied to the trajectory matrix to obtain a decomposition into elementary rank-one matrix components. The second
stage, which is called Reconstruction, creates grouped matrix components in a clever way and transforms the grouped matrix decomposition back to a decomposition of the initial object.

The first stage was developed earlier than the second stage. For example, the first stage of the Multichannel (or Multivariate) version of SSA for analysis of several time series (multivariate time series) was suggested in (Weare & Nasstrom, 1982).

Another origin of SSA traces back to properties of Hankel matrices (Gantmacher, 1959). Sometimes, an origin of SSA is drawn from (de Prony, 1795), where the modelling a sum of exponential series was considered; this origin is related to the parameter (frequency) estimation problem.

We can call the method by SSA if both Decomposition and Reconstruction stages are involved. The methods based on Decomposition stage only are called subspace-based methods. Although many subspace-based methods were developed before SSA, these methods may be called SSA-related.

**Motivation** Depending on the area of applications, different points of view on the same algorithms, choice of parameters and methodology as a whole are considered. The aim of the present paper is to describe and compare different points of view on SSA and its modifications and extensions to give people from different scientific communities the possibility to be aware with potentially new aspects of the method.

**Structure** Section 2 contains the description of singular spectrum analysis starting from its algorithm and basic ideas. We briefly discuss SSA from different viewpoints to show that SSA has connections to a very wide area of problems related to time series analysis and signal processing. Section 3 contains specific problems of time series analysis and their solution by SSA in comparison with other methods. In Section 4, we briefly describe implementations of SSA, since in the era of big data the effective implementation of a method is a key point for its use in real-life problems. Section 5 concludes the paper.

This review paper is supported by the monograph (Golyandina et al., 2018), which describes and organizes the algorithms of SSA-related methods and their implementation in the R-package *Rssa* (Korobeynikov et al., 2017) with numerous examples. The monograph contains the description of different aspects of SSA itself. In this paper, we put an emphasis on different external viewpoints on SSA and their connection with other methods. To avoid the repetition of figures and to give the readers convenient possibility to look at the illustrative pictures, we put into footnotes the links to the examples from the companion website [https://ssa-with-r-book.github.io](https://ssa-with-r-book.github.io) to the book (Golyandina et al., 2018).
2 A general review of SSA

2.1 Time series and digital images: problems

2.1.1 Decomposition

Let us observe \( X = (x_1, \ldots, x_N) \), where \( X = T + P + N \), \( T \) is a trend, \( P \) contains regular oscillations and \( N \) is noise. The common problem is to construct a decomposition \( X = \tilde{T} + \tilde{P} + \tilde{N} \), see Fig. 1, which allows one to estimate the trend \( T \), the whole signal \( S = T + P \), or periodic components \( P \) (\( P \) can consist of periodic components with different fundamental periods). If the signal is estimated and its structure is detected, different signal-based methods such as forecasting can be applied.

If the time series does not contain a signal, then the problems of filtering can be reduced again to decomposition into low-frequency and high-frequency components.

![Reconstructed Series](image)

Figure 1: ‘MotorVehicle’, monthly sales: Decomposition.

Problems of analysis of digital images are similar to that. Let

\[
X = \begin{pmatrix}
  x_{11} & \ldots & x_{1N_1} \\
  \vdots & \ddots & \vdots \\
  x_{N_11} & \ldots & x_{N_1N_1}
\end{pmatrix}
\]

be a digital image, which again has a decomposition \( X = T + P + N \) to a pattern, regular oscillations (e.g. a texture) and noise.

See Fig. 2, which demonstrates the extraction of a pattern (which is obtained after removal of regular oscillations). Note that the frequency filtering is even more frequently used for digital images than the decomposition into identifiable components.

‘Digital images’ is a common name for 2D data, since one of the dimensions can be temporal. The decomposition problem for multidimensional data can be reasonable for higher dimensions. For example, we can consider both 3D spatial data and 2D data with the third temporal dimension as 3D data; and so on. We call data with \( n \) dimensions as \( n \)D data.
2.1.2 Another time series/image problems

The results of decomposition (in particular, of signal extraction) allow one to solve many problems for objects with different dimensions and shapes; among these problems are

- trend/tendency extraction;
- smoothing/filtration;
- noise reduction;
- periodicity extraction (including seasonal adjustment);
- frequency estimation;
- construction of a model and parameter estimation;
- forecasting/prediction (of the extracted signal);
- missing data imputation;
- change-point detection.

2.2 Singular Spectrum Analysis

We consider application of Singular Spectrum Analysis (SSA) for most of the problems mentioned above. We mean SSA in both a narrow sense and a broad sense. We say about SSA in a narrow sense meaning the algorithm of decomposition of an object into a sum of interpretable components. We say about SSA in a broad sense for methods that use results of the SSA decomposition.

2.2.1 An idea of SSA: to create samples of structure

In multivariate data, there are many observations, which are sampled from the same probability distribution. In data like time series or digital images, we have only one object and therefore need to create many samples of the object’s structure to detect it. This can be done by a moving procedure.

Let us start with time series \( \mathbf{X} = (x_1, \ldots, x_N) \). Choose a window length \( L, 1 < L < N \), and consider \( K = N - L + 1 \) moving subseries \( \mathbf{X}_1 = (x_1, \ldots, x_L)^T, \mathbf{X}_2 = (x_2, \ldots, x_{L+1})^T, \ldots \)
(the procedure looks like a caterpillar is moving; this step gave one of the method’s name “Caterpillar”).

For digital images

$$X = \begin{pmatrix} 
  x_{11} & \ldots & x_{1N_1} \\
  \ldots & \ldots & \ldots \\
  x_{N_21} & \ldots & x_{N_2N_1}
\end{pmatrix},$$

the size of the moving 2D window is $L_1 \times L_2$, the moving procedure is performed in two directions, from the left to the right and from the top to the bottom:

$$X_{l,k}^{(L_1,L_2)} = \begin{pmatrix} 
  x_{l,k} & \ldots & x_{l,k+L_1-1} \\
  \ldots & \ldots & \ldots \\
  x_{l+L_2-1,k} & \ldots & x_{l+L_2-1,k+L_1-1}
\end{pmatrix},$$

$l = 1, \ldots, K_1$ and $k = 1, \ldots, K_2$, where $K_1 = N_1 - L_1 + 1$, $K_2 = N_2 - L_2 + 1$

2.2.2 An idea of SSA: to find a common structure using the SVD

Using a set of sub-objects of the given object, we should find a common structure. There is a standard statistical method for this, Principal Component Analysis (PCA), which is usually applied to data in matrix form.

Therefore, the moving sub-objects are transformed to vectors and are stacked to the matrix called trajectory matrix.

Note that PCA is applied to matrices, whose rows and columns have different nature, cases and variables. In the case of SSA, the rows and columns of the trajectory matrix as a rule have the same structure. Whereas PCA consists of centering or standardization by variables of the data matrix and then of application of the SVD to the transformed matrix, in SSA it is natural to change PCA to the singular value decomposition (SVD), without transformations. This version of SSA is called Basic SSA.

Due to the approximation properties, the SVD allows one to extract the signal (i.e., to remove noise). Due to bi-orthogonality of the SVD, the separation of the signal components (trend, periodic components) one from another is possible.

For the separation of the signal components, the approximation properties are not necessary. Therefore, other techniques (not the SVD) can be applied after the signal extraction. One can see an analogy with the factor analysis, where after detection the number of factors, rotations are performed to extract interpreted factors. After rotation, the extracted factors do not have approximation properties.

2.2.3 Basic SSA algorithm

Here we introduce the algorithm for time series decomposition. The general form of the algorithms is given in (Golyandina et al., 2018) and Section 2.7.

Let $X = (x_1, \ldots, x_N)$ be a time series of length $N$.

**Decomposition stage** (Parameter: window length $L; \ 1 < L < N$)
1. Embedding

Construction of the trajectory matrix by means of the embedding operator $T$, which maps a time series to the following $L \times K$ Hankel matrix:

$$T(X) = X = \begin{pmatrix} x_1 & x_2 & \cdots & x_K \\ x_2 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ x_L & x_{L+1} & \cdots & x_N \end{pmatrix}. \quad (2)$$

2. Singular Value Decomposition (SVD)

The SVD is given by $X = \sum_{m=1}^{d} \sqrt{\lambda_m} U_m V_m^T$, where $\{U_m\}_{m=1}^{d}$ and $\{V_m\}_{m=1}^{d}$ are orthonormal systems of left and right singular vectors of $X$, respectively, $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_d > 0$ are squared singular values.

Reconstruction stage (Parameter: way of grouping $\{1, \ldots, d\} = \bigcup I_j$)

1. Grouping

The SVD components are grouped: $X = X_{I_1} + \ldots + X_{I_c}$, where $X_I = \sum_{m \in I} \sqrt{\lambda_m} U_m V_m^T$.

2. Diagonal averaging

Each matrix $X_I$ is transferred to the nearest Hankel matrix $\tilde{X}_I$ by hankelization and then $\tilde{X}_I$ is transformed to a series as $\tilde{X}^{(l)} = T^{-1}(\tilde{X}_I)$.

Thus, the output of the SSA algorithm is the decomposition $X = \tilde{X}^{(I_1)} + \ldots + \tilde{X}^{(I_c)}$.

2.2.4 Comments to Basic SSA

Singular Value Decomposition (SVD) The SVD expansion $X = \sum_{m=1}^{d} \sqrt{\lambda_m} U_m V_m^T$ is the bi-orthogonal decomposition into a sum of rank-one matrices, $d = \text{rank} X$. By the Eckart-Young theorem (Eckart & Young, 1936), it provides the best low-rank approximation in the Frobenius norm.

Construction of the SVD can be reduced to finding eigenvectors $\{U_m\}$ and eigenvalues $\{\lambda_m\}$ of the matrix $XX^T$, which can be called lag-covariance matrix; $V_m = X^T U_m / \sqrt{\lambda_m}$. The collection $(\sqrt{\lambda_m}, U_m, V_m)$ is called the $m$th eigentriple (ET).

If the trajectory matrix $X$ is considered as a transposed data matrix with $K$ cases and $L$ variables, the SVD of $X$ is closely related to principal component analysis. If rows of $X$ are centered, the SVD exactly corresponds to PCA. Therefore, according to statistical terminology, $V_m$ and $\sqrt{\lambda_m} V_m$ are called factor scores and principal components, respectively.

Grouping Let $X = X^{(1)} + X^{(2)}$ and therefore the following equality be valid for the trajectory matrices: $X = X_{I_1}^{(1)} + X_{I_2}^{(2)}$. In the case, when there exists a grouping $\{1, \ldots, d\} = I_1 \cup I_2$ such that $X_{I_1}^{(1)} = X_{I_1}$ and $X_{I_2}^{(2)} = X_{I_2}$ (this is called separability, see Section 2.3.1), the eigenvectors $\{U_m\}_{m \in I_j}$ form a basis of $\text{colspace}(X^{(j)})$; therefore, $U_m$ for $m \in I_j$ repeats the
behavior of $X(j)$ (recall that the columns of $X(j)$ are subseries of $X(j)$). Thus, we can say that an eigenvector repeats the behaviour of a component that produces this eigenvector. Thereby, we can identify slowly-varying $U_m$ and gather them into the trend group, then identify regular oscillations and gather them into the periodicity group, and so on.

An elementary grouping, when each group consists of one component, produces the so-called elementary reconstructed time series. Since Grouping and Diagonal averaging are linear operations, it does not matter if to group and then perform diagonal averaging or vice versa. Therefore, elementary reconstructed components are helpful for Grouping.

There is a particular case, when we observe a noisy time series and want to extract the signal. Formally, this is the case of two groups, signal and noise. Since we need only the signal group, the grouping is reduced to the choice of a signal group $I$. Due to approximation properties of the SVD, the group $I$ corresponds to signal usually consisting of $r$ leading components $I = \{1, \ldots, r\}$. Thus, the way of grouping is reduced to the choice of $r$.

### 2.2.5 A view from the Karhunen-Loeve transform

For a stochastic process $\xi_t$, $t \in [0, T]$, the structure is contained in the autocovariance function $K(s, t) = E(\xi_s - E\xi_s)(\xi_t - E\xi_t)$; and the Karhunen-Loeve transform (KLT) based on the eigendecomposition of $K(t, s)$ is considered to express this structure in the form of a decomposition. Originally, the Karhunen-Loeve decomposition of $\xi_t$ is the decomposition into an infinite sum of white noises $\varepsilon_k$, $k = 1, 2, \ldots$, with coefficients obtained from the eigenfunctions $u_k(t)$ of the autocovariance function.

However, for discrete time and a finite time series length, the KLT of $(\xi_1, \ldots, \xi_N)$ in fact coincides with PCA of the multivariate random variable $(\xi_1, \ldots, \xi_N)^T$. Then, the Karhunen-Loeve transform is the decomposition into a finite sum of white noises $\varepsilon_k$, $k = 1, \ldots, N$, with coefficients obtained from the eigenvectors $U_k$ of the covariance matrix. For a time series $(x_1, \ldots, x_N)$ of length $N$, which can be considered as a realization of $(\xi_1, \ldots, \xi_N)$, the empirical KLT is constructed on the base of eigenvectors of the estimated covariance matrix. If the time series is centered or, alternatively, centering is applied to the rows of the trajectory matrix $X$, then $XX^T$ can be considered as an estimate of the (auto)covariance matrix.

The question is how to construct the sample version of $\varepsilon_k$, $k = 1, \ldots, N$. In PCA, we have many samples of $(\xi_1, \ldots, \xi_N)^T$. Then the sample version of $\varepsilon_k$ is the $k$th principal component of the multivariate data. For time series, we have only one realization of length $N$. The trajectory matrix $X$ is the way to create $L$ samples of length $K = N - L + 1$. Then $\sqrt{\lambda_m}V_m$ can be considered as the sample version of $\varepsilon_m$, $m = 1, \ldots, \min(L, K)$.

Thus, up to the above assumptions, the empirical KLT formally corresponds to Decomposition stage of the SSA algorithm. People, who studied the theory of random processes and then looked at the SSA algorithm, sometimes say that it is nothing new, just the KLT. Note that Reconstruction stage is not included to the KLT decomposition. Also, the point of view on SSA from stochastic processes theory leaves a mark on the methodology of applications of SSA (see e.g. (Khan & Poskitt, 2013)).

Authors in different countries (independently) came to Decomposition stage of the SSA algorithm. See e.g. (Basilevsky & Hum, 1979), (Efimov & Galaktionov, 1983). Since the idea to put together subseries from one time series and then apply PCA/KLT is straightforward,
the decomposition stage of SSA can be found in many papers; it is hard to detect, which paper was first.

2.2.6 A view from stationary processes

People who deal with stationary processes look at SSA in a different way. For (weakly) stationary random processes, the autocovariance function \( K(s, t) \) depends on \(|t - s|\). Therefore, one of main characteristics of a stationary random process \( \xi_t, t \geq 0 \), with mean \( \mu \) is its autocovariance function \( C(|s - t|) = K(s, t) = \text{E}(\xi_s - \mu)(\xi_t - \mu) \) of one variable. For discrete time and a sequence \( \xi_1, \ldots, \xi_N \), this means that the autocovariance matrix \( \{\text{E}(\xi_i - \mu)(\xi_j - \mu)\}_{i,j=1}^N \) is Toeplitz and has size is \( N \times N \). However, in practice, we cannot accurately estimate covariances with large lags, since there are only one pair of observations with lag \( N - 1 \), two pairs of observations with lag \( N - 2 \), and so on. In SSA, autocovariances are estimated up to the lag \( L \); then not smaller than \( K \) pairs of observations can be used for estimating the autocovariances with lags not larger than \( L \). Since autocovariances are proportional to autocorrelations, it is not important, to consider either covariances or correlations.

In Basic SSA, the lag-covariance matrix \( L \times L \) has the form \( C = XX^T/K \), which is close to a Toeplitz matrix if the time series is stationary (we assume that the time series is centered); however, this is not exactly a Toeplitz matrix. In Toeplitz SSA, the lag-covariance matrix is estimated in a way to obtain exactly Toeplitz matrix. The conventional estimation \( \tilde{C} = \{\tilde{c}_{ij}\}_{i,j=1}^L \) of the autocovariance matrix is \( \tilde{c}_{ij} = \frac{1}{N-|j-i|} \sum_{k=1}^{N-|j-i|} x_k x_{k+j-i} \). In both Basic and Toeplitz SSA, Decomposition step can be expressed as \( X = \sum_m P_m(X^T P_m)^T \). In Basic SSA, \( P_m = U_m \) are eigenvectors of \( C \), whereas in Toeplitz SSA, \( P_m \) are the eigenvectors of \( \tilde{C} \).

Since the intention of Toeplitz SSA is in a better estimation of the autocovariances, not large window lengths are usually chosen to obtain stable estimates of the autocorrelations, which should be estimated for lags, which are not larger than the chosen window length.

Note that in (Vautard & Ghil, 1989), the Toeplitz version is called VG according to the author’s names, while the basic version with the SVD decomposition is called BK, since it was suggested in (Broomhead & King, 1986a).

It is important to note that the only form of the decomposition step which is invariant with respect to transposition of the trajectory matrix (that corresponds to the change \( L' = K \) and \( K' = L \)) is the SVD. In particular, for Toeplitz SSA the decompositions for \( L, K \) and \( L' = K, K' = L \) are different.

It seems that this view from stationary processes limits the application of SSA, since Toeplitz estimates of autocorrelation matrices have sense for analyzing stationary processes only, while the range of problems solved by SSA is much wider. Since the VG (Toeplitz) version was suggested for analysis of data in climatology, this version is still considered as main one in many applications; probably, sometimes this is used just through habit. However, it should be noted that the VG (Toeplitz) version of SSA is linked to spectral estimation; in such case, this version is appropriate.
2.2.7 A view from dynamical systems

It is interesting that the origin of SSA is referred to the papers devoted to dynamical systems (Broomhead & King, 1986a) and (Fraedrich, 1986), where the problem is based on the Takens embedding theorem. It seems that the connection between SSA and the Takens theorem is mostly historical. However, the terminology in SSA is partly taken from dynamical systems.

The dynamical system approach introduced the name “trajectory matrix” due to interpretation of columns of the trajectory matrix as a sequence of vectors (a trajectory) in a multidimensional space.

2.2.8 A view from structured low-rank approximation

It is well-known that rank-deficient Hankel matrices corresponds to time series of a certain structure, see e.g. (Gantmacher, 1959). Developed independently of the main stream of SSA, the algorithm of SSA (as an algorithm of signal extraction) practically coincides with one step of the iteration algorithm suggested in (Cadzow, 1988) and later named as Cadzow iterations.

The matrix called ‘trajectory’ in SSA, was called enhanced matrix in the Cadzow’s paper and subsequent papers (e.g. (Hua, 1992) constructs the enhanced matrix in the 2D case for 2D frequency estimation).

2.3 Decomposition

Here we consider the problem of decomposition of time series into a sum of identifiable components such as a trend, periodic components and noise. The first question is if SSA allows finding such decomposition; then, if the answer is “yes”, how to identify the time series components with the help of information on the SVD components. Also, the question about the choice of window length $L$, which leads to a better decomposition, arises. We start with the first question.

2.3.1 Separability

The (approximate) separability of the time series components is required to perform a grouping of the SVD components to (approximately) extract these components.

Let us observe a sum $X = X^{(1)} + X^{(2)}$, $X = X^{(1)} + X^{(2)}$. The SVD step of Basic SSA provides an expansion $X = X_1 + \ldots + X_d = \sum_{m=1}^{d} \sqrt{\lambda_m} U_m V_m^T$. Separability means that the set of eigentriples in the decomposition of the sum $X^{(1)} + X^{(2)}$ is equal to the union of eigentriples $(\sqrt{\lambda_{m,j}}, U_{m,j}, V_{m,j}^T)$ produced by each time series $X^{(j)}$, $j = 1, 2$. If this is true, the grouping that separates the series $X^{(1)}$ and $X^{(2)}$ exists and it is sufficient to identify the corresponding eigentriples. When the grouping is fixed, Diagonal averaging step provides the decomposition of the original time series.

There are two versions of separability related to non-uniqueness of the SVD which is caused by multiple eigenvalues. *Weak separability* means that there is an SVD decomposition, which allows the grouping of its components to fit the time series components. *Strong separability* means the any SVD allows the proper grouping. Strong separability is necessary in practice.
**Proposition 1** Let \( L \) be fixed. Two series \( X^{(1)}_N \) and \( X^{(2)}_N \) are weakly separable, if their column trajectory spaces are orthogonal and the same is valid for their row trajectory spaces, that is, \((X^{(1)})^T X^{(2)} = 0_{K,L}\) and \((X^{(1)}(X^{(2)})^T) = 0_{L,L}\).

Two series \( X^{(1)}_N \) and \( X^{(2)}_N \) are strongly separable, if they are weakly separable and the sets of singular values of their \( L \)-trajectory matrices are disjoint, that is, \( \lambda_{k,1} \neq \lambda_{j,2} \) for any \( k \) and \( j \).

Thus, the assumption for (approximate) weak separability is the (approximate) orthogonality of subseries of lengths \( L \) and the same for subseries of length \( K \). For example (Golyandina et al., 2001, Section 6.1), \( x_n^{(j)} = A_j \cos(2\pi \omega_j n + \phi_j), j = 1, 2, n = 1, \ldots, N \), are asymptotically weakly separable for any \( 0 < \omega_1 \neq \omega_2 < 0.5 \). For exact weak separability, the condition that \( L\omega_j \) and \( K\omega_j \) are integers should be fulfilled. For strong separability we additionally need \( A_1 \neq A_2 \), since it is easily to find that \( \|X^{(j)}\|^2 = A_{j}^2 LK/2 \) and therefore \( \lambda_{m,j} = A_{j}^2 LK/4, m = 1, 2 \) and \( j = 1, 2 \).

Examples of approximately separable series are: trend and oscillations; slowly-varying components and noise; sinusoids with different periods, seasonality and noise.

Theoretically, the approximate separability is a consequence of the asymptotic separability as \( N \to \infty \). Therefore, the accuracy of decomposition depends on the convergence rate as \( N \to \infty \). For example, for separability of sine waves, the convergence rate is \( C/\min(L,K) \), where \( C \sim 1/|\omega_1 - \omega_2| \), see (Golyandina et al., 2001, Example 6.7). Therefore, for weak separability of sine waves, the choice \( L \approx N/2 \) is recommended. Also, a worse separability occurs for sine waves with close frequencies.

### 2.3.2 How to identify the SVD components

The most sophisticated step of SSA is the way of grouping of elementary components. Here we well demonstrate how it can be done in an interactive way.

Let us enumerate the basic approaches (Golyandina et al., 2001, Section 1.6):

1. To construct the trend group, choose the eigentriples with slowly varying eigenvectors. The same can be done on the basis of factor vectors or elementary reconstructed components.

2. To extract the periodicity with period \( T \), find pairs of components similar to sine/cosine with periods \( T/k, k = 1, \ldots, [(T - 1)/2] \) and one saw-tooth component, which corresponds to the period 2 if \( T \) is even. The mentioned pairs of sine/cosine can be detected in 2D scatterplots of sequential eigenvectors.

3. Possible approach to the choice of the components is their separability, which can be checked by means of \( w \)-correlation matrix. Elementary components with strong \( w \)-correlation should be put into the same group. In particular, noise produces correlated components; this can be seen in the \( w \)-correlation matrix. Note that the name ‘correlation’ can be a bit ambiguous here, since the vectors are not centered; that is, the measure called \( w \)-correlation is related to the cosine of the angle between vectors.

The enumerated properties can be formalized to obtain methods of automatic identification.
A special task is the choice of components related to the signal. To extract the signal, we should choose a number \( r \) of the leading components. If the signal is used for e.g. forecasting, \( r \) can be chosen by minimization of the forecasting errors for historical data.

### 2.3.3 Example

Let us demonstrate how to perform the SSA decomposition by a simple example. In the 1D scatterplots (Fig. 3), one can find a slowly varying component (ET 1), whereas in 2D scatterplots (Fig. 4) regular polygons say about pairs of sine-wave components. In these figures, \( U_i(k) \) denotes the \( k \)th coordinate of the \( i \)th eigenvector obtained in the SVD step of SSA. The eigenvector numbers are indicated at the captions of the graph.

![Eigenvectors](image1)

**Figure 3:** Fortified wines, \( L = 84 \): 1D graphs of eigenvectors \( (k, U_i(k)) \), \( k = 1, \ldots, L \).

![Pairs of eigenvectors](image2)

**Figure 4:** Fortified wines, \( L = 84 \): 2D scatterplots of eigenvectors \( (U_i(k), U_{i+1}(k)) \), \( k = 1, \ldots, L \).

The resultant decomposition into the trend, the seasonality and noise is depicted in Fig. 5. This example is performed by the code from Fragments 2.1.1–2.1.3\(^1\) of (Golyandina et al., 2018).

---

\(^1\)https://ssa-with-r-book.github.io/01-chapter2-part1.html#fragments-211-australian-wines-input-and-212-fort-reconstruction
Figure 5: Fortified wines, $L = 84$: decomposition for groups ET1, ET2–11 and ET12–84.

2.4 Filtering

It is known that the time series components reconstructed by SSA can be considered as a result of linear filters applied to the initial time series (Hansen & Jensen, 1998; Harris & Yan, 2010; Bozzo, Carniel, & Fasino, 2010) and (Golyandina & Zhigljavsky, 2013, Section 3.9). Certainly, the coefficients of these filters have nonlinear dependence on the time series. Therefore, these filters are called adaptive. This approach is more natural if $L$ is small, since then a larger part of the reconstructed time series is obtained by the same linear filter (see Section 3.6 for details).

2.4.1 Example

The following example shows that SSA can be considered from the viewpoint of decomposition on components from different frequency ranges, that is, not necessarily as a decomposition of trend, periodic components and noise. Fig. 6 shows the decomposition, which was obtained by grouping the components according their frequency range. Fig. 7 with components’ periodograms depicted together confirms this.

This example is performed by the code from Fragment 2.8.1 (Golyandina et al., 2018).

2.5 Modelling

We mentioned that SSA combines non-parametric (model-free) and parametric approaches; certainly, the latter is possible if a parametric model is stated. Consider the following model of signals that is used in SSA. Let $S = (s_1, \ldots, s_N)$ be a signal (or, more precisely, a time series component of interest). Set a window length $L$, $1 < L < N$; $K = N - L + 1$. Consider

\footnote{https://ssa-with-r-book.github.io/02-chapter2-part2.html#fragment-281-tree-rings-frequency-decomposition}
Figure 6: ‘Tree rings’: Frequency decomposition.

Figure 7: ‘Tree rings’: Periodograms of the series components.

the trajectory matrix:

\[ S = \begin{pmatrix}
    s_1 & s_2 & \cdots & s_K \\
    s_2 & \ddots & & s_{K+1} \\
    \vdots & & \ddots & \vdots \\
    s_L & s_{L+1} & \cdots & s_N
\end{pmatrix}. \]

Let \( r \) denote the rank of \( S \).

Different forms of the model are:

- \( S \) is a Hankel low-rank matrix of rank \( r < \min(L, K) \); the model can be parametrized by a basis of \( \text{colspace}(S) \) or of its orthogonal completion. Such time series are called time series of finite rank.
• The time series is governed by a linear recurrence relation (LRR)

$$s_n = \sum_{k=1}^{r} a_k s_{n-k}, a_r \neq 0, n = r + 1, \ldots \tag{3}$$

Such time series is called a *time series governed by an LRR*.

• The time series has an explicit parametric form of a finite sum:

$$s_n = \sum_{k} P_k(n) \exp(\alpha_k n) \sin(2\pi \omega_k n + \phi_k), \tag{4}$$

where $P_k(n)$ is a polynomial of $n$, $\exp(\alpha_k n) = \rho_j^n$ for $\rho_j = e^{\alpha_j}$.

The first model is more general; however, under some non-restrictive conditions (for example, for infinite time series), these three models are equivalent, see e.g. (Hall, 1998, Theorem 3.1.1) and (Golyandina et al., 2001, Section 5.2).

Let us describe how the minimal LRR (the irreducible LRR of order which is as low as possible), which governs the time series, determines its explicit parametric form. A more convenient form of (4) is as follows:

$$s_n = \sum_{m=1}^{p} \left( \sum_{j=0}^{k_m-1} c_{m,j} n^j \right) \mu_m^n, \tag{5}$$

where $\mu_m$ coincide with $\rho_j e^{\pm 2\pi \omega_j}$ for some $j$. Thus, the complex parameters $\mu_m$ determines frequencies $\omega_j$ and exponential bases $\rho_j$.

The polynomial $P_r(\mu) = \mu^r - \sum_{k=1}^{r} a_k \mu^{r-k}$ of order $r$ is called characteristic polynomial of the LRR (3). Roots of the characteristic polynomial are called characteristic roots of the corresponding LRR. The roots of the characteristic polynomial of the minimal LRR governing the series, determine the values of parameters $\mu_m$ and $k_m$ in (5) as follows. Let the time series $S_\infty = (s_1, \ldots, s_n, \ldots)$ satisfy the LRR (3). Consider the characteristic polynomial of the LRR (3) and denote its different (complex) roots by $\mu_1, \ldots, \mu_p$, where $p \leq r$. All these roots are non-zero as $a_r \neq 0$ with $k_m$ being the multiplicity of the root $\mu_m$ ($1 \leq m \leq p$, $k_1 + \ldots + k_p = r$). We refer for an extended summary to (Golyandina et al., 2018, Section 2.1.2.2).

### 2.5.1 Subspace-based approach

The question is how to find the structure (the basis of $\text{colspace}(S)$, the coefficients of the LRR, the parameters of $s_n$) of a signal $S$. Within SSA, the answer is as follows. Let us apply SSA and obtain the decomposition of the trajectory matrix $S = \sum_{m=1}^{r} \sqrt{\lambda_m} U_m V_m^T$.

Then

- $U_m$, $m = 1, \ldots, r$, form a basis of $\text{colspace}(S)$.
• The basis $U_m$, $m = 1, \ldots, r$, provides the coefficients $a_k$ in the LRR $s_n = \sum_{k=1}^r a_k s_{n-k}$, $n = r + 1, \ldots$. Denote $\pi_m$ the last coordinate of $U_m$, $U_m \in \mathbb{R}^{L-1}$ the vector $U_m$ with the last coordinate removed, and $\nu^2 = \sum_{m=1}^r \pi_m^2$. Then the elements of the vector

$$\mathcal{R} = (a_{L-1}, \ldots, a_1) = \frac{1}{1 - \nu^2} \sum_{m=1}^r \pi_m U_m$$

provide the coefficients of the min-norm governing LRR: $s_n = \sum_{k=1}^{L-1} a_k s_{n-k}$ (see a discussion of the min-norm LRR in (Golyandina & Zhigljavsky, 2013, Section 3.2.3)). If $L = r + 1$, (6) yields the minimal LRR, which is unique.

• The basis $U_m$, $m = 1, \ldots, r$, provides the estimates of $\alpha_k$ and $\omega_k$ in (4). Consider the signal in the complex-valued form $s_n = \sum_{j=1}^r c_j \mu_j^n$ (we simplify the form excluding polynomials). The relation between parameters is $\alpha = \ln(\text{Mod}(\mu))$, $\omega = \text{Arg}(\mu)/(2\pi)$. Apply the ESPRIT method (Roy & Kailath, 1989). Denote $U_r = [U_1 : \ldots : U_r]$ and let $U_r$ be the matrix with the last row removed and $\tilde{U}_r$ be the matrix with the first row removed. Then $\mu_i$ can be estimated by the eigenvalues of the matrix $\tilde{U}_r^\dagger \tilde{U}_r$, where $\dagger$ denotes pseudo-inversion.

This is called \textit{subspace-based approach}. It can be extended to 2D, 3D, ... cases; certainly, the $n$D theory for $n > 1$ is much more complicated than the one-dimensional case.

\textbf{Subspace-based approach in real-life problems} In real-life problems we observe $X = S + R$, where $S$ is the structured component of interest (e.g. a signal), $R$ is a residual (e.g. noise).

Suppose we have an approximate separability ($\approx$ approximate orthogonality) of $S$ and $R$. Then

1. Apply SSA and obtain the set of $U_m$, $m = 1 \ldots, L$.
2. Identify the SVD components with numbers $G = \{i_1, \ldots, i_r\}$, which are related to the series component of interest.
3. Take the set $U_i$, $i \in G$, as an estimate of the basis of the component trajectory subspace. The same formulas from the subspace-based approach, which are used in the noiseless case, are applied to this basis to get estimates of the LRR coefficients and the time series parameter.

\textbf{2.5.2 Signal extraction}

Consider a particular case of $X = S + N$, $X = (x_1, \ldots, x_N)$, where $S$ is a signal of rank $r$, $N$ is noise. Set parameters: the window length $L$ and the signal rank $r$.

Introduce two projections in Frobenius norm: $\Pi_r : \mathbb{R}^{L \times K} \mapsto \mathcal{M}_r$, where $\mathcal{M}_r$ is the set of matrices of rank not larger $r$, and $\Pi_{\mathcal{H}} : \mathbb{R}^{L \times K} \mapsto \mathcal{H}$, where $\mathcal{H}$ is the space of Hankel matrices. Let $\mathcal{T}$ be defined in (2).
Scheme of SSA for signal extraction:

\[
X \xrightarrow{R} X = \begin{pmatrix} x_1 & x_2 & \ldots & x_K \\ x_2 & x_3 & \ldots & x_{K+1} \\ \vdots & \vdots & \ddots & \vdots \\ x_L & x_{L+1} & \ldots & x_N \end{pmatrix} \xrightarrow{\text{SVD:} (\sqrt{\lambda_m, U_m, V_m}), \Pi_r} \Gamma \xrightarrow{\Pi_H} \tilde{S} = \begin{pmatrix} \tilde{s}_1 & \ldots & \tilde{s}_K \\ \tilde{s}_2 & \ldots & \tilde{s}_{K+1} \\ \vdots & \vdots & \vdots \\ \tilde{s}_L & \ldots & \tilde{s}_N \end{pmatrix} \xrightarrow{T^{-1}} \tilde{S}.
\]

A concise form of the SSA algorithm for signal extraction is

\[
\tilde{S} = T^{-1}\Pi_H\Pi_r TX.
\]

2.5.3 Example

Consider the decomposition depicted in Figure 5. This decomposition was created without the use of a model. However, we can detect the model and estimate its parameters. The model is a sum of products of polynomials, exponentials and sine waves. The subspace-based method allows one to construct the parametric model of the signal of rank \( r \).

The subspace-based approach gives us the following form:

\[
\tilde{s}_n = C_1 0.99679^n + C_2 0.99409^n \sin(2\pi n/12 + \phi_2) + \\
+ C_3 1.00036^n \sin(2\pi n/4 + \phi_3) + C_4 1.00435^n \sin(2\pi n/5.97 + \phi_4) + \\
+ C_5 1.00175^n \sin(2\pi n/2.39 + \phi_5) + C_6 0.98878^n \sin(2\pi n/3.02 + \phi_6).
\]

The coefficients \( C_i \) and the phases \( \phi_i \) can be estimated by the linear least-squares method. An example of the R-code can be found in Fragment 3.5.9\(^3\) and 3.5.11\(^4\) of (Golyandina et al., 2018).

2.6 Choice of parameters in SSA

The two parameters of SSA are the window length \( L \) and the way of grouping. There are no strict recommendations for their choice. Moreover, these recommendations are different for different problems and different assumptions about the time series nature.

For example, if the signal is of finite rank, then \( L \approx N/2 \) is recommended (simulations provide the recommendation \( L \approx 0.4N \) (Golyandina, 2010)).

If the signal is not of finite rank or has a complex structure (a large rank and its trajectory has a large condition number), then a smaller window length is recommended.

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\(^3\)https://ssa-with-r-book.github.io/03-chapter3.html#fragment-359-fort-estimation-of-parameters-by-basic-ssa

\(^4\)https://ssa-with-r-book.github.io/03-chapter3.html#fragment-3511-fort-estimation-of-parametric-real-valued-form
If the period of a periodic time series component is known, then it is recommended to take the window length divisible by the fundamental period.

For analysis of stationary processes, the recommendation can be special. In particular, the window length should allow a good estimation of the autocovariance matrix. This means that $L$ should be small enough.

Formalization of the grouping way is difficult. One approach is based on the separability notion (e.g. on $w$-correlations as a measure of separability) and on visual inspection of eigentriples. Another approach can be used in the case of finite-rank signals. Then methods of rank detection can be applied (see a brief discussion in paragraph ‘Signal identification’ of Section 3.14).

### 2.7 General scheme of SSA decompositions

We refer to (Golyandina et al., 2018) for discussion of the general scheme of SSA modifications and variations in detail. A general form of SSA-family algorithms for object decomposition can be presented in the following form. A wide range from time series to $n$D shapes can be considered as the input.

**Input:** An object (for example, a time series).

1. **Embedding.** Object is transformed to a structured trajectory matrix from a set $\mathcal{H}$ by an embedding operator $\mathcal{T}$ (e.g., $\mathcal{H}$ is a set of Hankel matrices).

2. **Decomposition.** Trajectory matrix is decomposed into a sum of one-rank elementary matrices (e.g., by the SVD).

3. **Grouping.** Elementary matrices are grouped in an appropriate way.

4. **Return to the object decomposition.** Grouped (summed) matrices are transformed to the form of initial objects by projection to $\mathcal{H}$ (e.g. by hankelization) and performing $\mathcal{T}^{-1}$.

**Output:** Decomposition of the initial object into the sum of identifiable objects (e.g., of a trend, oscillations and noise).

The algorithm in the general form is easily scaled to different dimensions by the change of the embedding operator $\mathcal{T}$. Also, modifications of Decomposition step do not depend on the shape/dimension of the decomposed object, since they are localized in Decomposition step, whereas the specific of the shape/dimension is localized by means of the embedding operator $\mathcal{T}$ in the first and last steps.

### 2.8 SSA and multivariate/multidimensional extensions

Multivariate/multidimensional extensions differs by the embedding step; that is, by definition of the embedding operator $\mathcal{T}$. Let us list different versions of Embedding step:

- SSA for time series (1D-SSA): $\mathcal{T}(X)$ is a Hankel matrix;
- MSSA for systems of time series: $\mathcal{T}(X)$ is a stacked Hankel matrix;
• 2D-SSA for digital images: $\mathcal{T}(X)$ is a Hankel-block-Hankel matrix;

• Shaped SSA for any shaped objects: $\mathcal{T}(X)$ is a quasi-Hankel matrix;

• M Shaped 3D-SSA for several 3D images of some shapes provides a stacked quasi-Hankel trajectory matrix;

• Shaped nD-SSA $(n > 1)$ can be considered as a general $n$-dimensional extension of SSA for shaped objects.

2.8.1 MSSA

Decomposition, forecasting, missing data imputation, and other subspace-based methods are performed in the same manner as for 1D-SSA, see examples from (Golyandina et al., 2018, Chapter 4)\(^5\).

By applying SSA, we cannot say about causality, since the MSSA method is invariant with respect to shifts of time series. However, we can say about supportiveness of one series with respect to another series. Supportiveness means that the second time series improves the accuracy of signal estimation or forecasting in comparison with the use of the first series only. If the series have a large portion of common structure, their simultaneous processing is better than the separate processing of each time series. The common structure within the SSA framework means similar signal trajectory spaces. The success of signal extraction depends on relation between signal and noise matrices. Even if the two time series have signals of the same structure, a large noise level in the second time series can cause this series to be not supportive.

It is important to stress that in MSSA there are a lot of different notations, which are sometimes controversial. In 1D-SSA, it is not important, what we call left or right singular vectors, eigenvectors or factor vectors/principal components, since the transposed $L$-trajectory matrix coincides with $K$-trajectory matrix, $K = N - L + 1$. Usually, longer vectors are called factor vectors (principal components). Another approach is to fix the embedding dimension $L$ (which is equal to the window length $L$) and to call the right singular vectors factor vectors/principal components. Then increasing the time series length $N$ will increase the length $K$ of factor vectors. Since usually $L \leq K$, both approaches provide the same terminology.

However, for MSSA, this is not the case. In MSSA, the trajectory matrix is constructed from stacked trajectory matrices of time series from the considered collection. The stacking can be either vertical or horizontal. In the case of horizontal stacking,

$$\mathcal{T}_{\text{MSSA}} = [X_1 : \ldots : X_s],$$

where $X_i$ is the trajectory (and therefore Hankel) matrix of the $i$th time series. Then left singular vectors correspond to time subseries of length $L$, while right singular vectors consist of stacked subseries of different time series from the collection. Thus, in contrast to 1D-SSA, left and right singular vectors have different structure.

\(^5\)https://ssa-with-r-book.github.io/04-chapter4.html
Vertical stacking is not something different; left and right singular vectors interchange (if to interchange $L$ and $K = N - L + 1$); therefore, the way of stacking influences no more than terminology, choice of parameters and possibly computational cost.

Originally, a small window length $L$ was applied to each of $s$ time series with vertical stacking of trajectory matrices (Weare & Nasstrom, 1982), where $L = 3$ (after reordering of rows of the matrix $X$); then $K$ is large, left singular vectors have the length $Ls$; the left singular vectors of length $Ls$ are called EEOFs (extended empirical orthogonal functions). Right singular vectors provides factor vectors (or principal components if to multiply by singular values). They have almost the same length as the series themselves and therefore can be used instead of time series in further investigations.

In (Golyandina, Korobeynikov, Shlemov, & Usevich, 2015) and (Golyandina et al., 2018), horizontal stacking is considered to fix the number of rows (that is, the dimension of the column space of the trajectory matrix). This choice is explained by the possibility of different series lengths and keeping the dimension as the time series lengths increase.

The above consideration that the horizontal and vertical stackings are just different forms of the same methods are valid for Basic (M)SSA, where the SVD of the trajectory matrix is considered. That is, the form of stacking in MSSA, which was suggested in (Broomhead & King, 1986b), is not important. For Toeplitz (M)SSA, this is not the case. Let $C_i$ be the autocovariance (Toeplitz) matrix of the $i$th time series, $C_{ij}$ be the cross-covariance matrix of the $i$th and $j$th time series. Then for horizontal stacking, the decomposition is constructed on the basis of eigenvectors of $\sum_{i=1}^{s} C_i$.

For vertical stacking, which is considered in the algorithm of Multichannel SSA, the decomposition is constructed on the basis of eigenvectors of

\[
\begin{pmatrix}
C_{11} & \cdots & C_{1s} \\
\vdots & \ddots & \vdots \\
C_{s1} & \cdots & C_{ss}
\end{pmatrix}.
\]

In climate investigation, the Toeplitz version of MSSA with vertical stacking is conventional (Plaut & Vautard, 1994).

### 2.8.2 2D-SSA

For digital images $X = X_{N_1,N_2} = (x_{ij})_{i,j=1}^{N_1,N_2}$, a 2D window size $L_1 \times L_2$ should be chosen. The trajectory matrix consists of vectorized moving 2D windows. This trajectory matrix can be written in the form of a Hankel-block-Hankel matrix:

\[
X = \mathcal{T}_{2D-SSA}(X) = \begin{pmatrix}
H_1 & H_2 & H_3 & \cdots & H_{K_2} \\
H_2 & H_3 & H_4 & \cdots & H_{K_2+1} \\
H_3 & H_4 & \ddots & \cdots & \vdots \\
\vdots & \vdots & \ddots & \cdots & \vdots \\
H_{L_1} & H_{L_1+1} & \cdots & \cdots & H_{N_1}
\end{pmatrix},
\]

where each $H_j$ is the $L_1 \times K_1$ trajectory (Hankel) matrix constructed from $X_{:,j}$ (the $j$th column of the 2D array $X$).
The estimation of frequencies by 2D-ESPRIT is the most frequent use of such trajectory matrix (Sahnoun, Usevich, & Comon, 2017), see Fragments 5.3.1\(^6\) and 5.3.2\(^7\) from (Golyandina et al., 2018). Also, 2D-SSA is used for the problems of smoothing and noise reduction, see Fragments 5.4.2–5.4.6\(^8\).

### 2.8.3 Shaped SSA

In (Golyandina et al., 2015), a general approach to singular spectrum analysis is suggested. Shaped SSA is the universal version of SSA, applicable to arbitrary shapes and dimensions of the objects. The moving window can be of arbitrary shape. For example, both the digital image and the moving window can be circular-shaped, not rectangular. Shaped SSA allows one to present all possible versions of SSA, including SSA for objects with missing data, 1D-SSA, MSSA, 2D-SSA and their circular versions in a unified manner. See Fragment 2.6.\(^9\) for the 1D case, Fragments 5.2.2–5.2.3\(^10\) for the example with a shaped image, a circle window and Fragment 5.4.6\(^11\) for decomposition of data given on a cylinder (Golyandina et al., 2018).

There is a limitation for this approach. The points within the window and the window locations should be linearly ordered. Then, the columns of the trajectory matrix consist of the points of windows taken in the given order and these columns are stacked to the matrix according to ordered locations of shaped windows. Many objects can be considered as linearly ordered. The standard technique is to consider the object as a subset of a multidimensional box of the same dimension, with natural ordering. For example, a piece of the sphere (after its projection to the plane) can be circumscribed by a rectangle; however, there is no continuous planar projection of the whole sphere. Therefore, at the present moment, SSA for data given on the whole sphere is not elaborated.

### 2.8.4 Complex SSA

Complex SSA (C. Keppenne & Lall, 1996) is Basic SSA applied to complex-valued time series. The only difference in the algorithm is the change of transpose to conjugate transpose. Generally speaking, Complex SSA is not a method for multivariate time series; although, it can be considered as a special method for analysis of two time series.

Most applications of Complex SSA are related to the so-called F-xy eigenimage filtering (S. R. Trickett, 2003). This name is related to analysis of digital images in geophysics, when

\(^{6}\)https://ssa-with-r-book.github.io/05-chapter5.html#fragment-531-mars-parameter-estimation-with-2d-esprit

\(^{7}\)https://ssa-with-r-book.github.io/05-chapter5.html#fragment-532-mars-parameter-estimation-with-shaped-2d-esprit

\(^{8}\)https://ssa-with-r-book.github.io/05-chapter5.html#fragment-542-brecon-beacons-decomposition

\(^{9}\)https://ssa-with-r-book.github.io/01-chapter2-part1.html#fragment-262-incomplete-decomposition-for-a-series-with-a-gap

\(^{10}\)https://ssa-with-r-book.github.io/05-chapter5.html#fragments-521-auxiliary-plot-of-2d-image-and-522-mars-mask-specification-and-decomposition

\(^{11}\)https://ssa-with-r-book.github.io/05-chapter5.html#fragments-546-kruppel-analysis-of-data-given-on-a-cylinder
Discrete Fourier Transform is applied to each row of the image matrix and then the complex-valued series from values, which were obtained for each frequency in the Fourier transform, are analysed by Complex SSA. Note that the authors of papers devoted to F-xy analysis usually omit the word ‘Complex’ in Complex SSA. The specific of the studied images is that they contain lines on the geophysical images; these lines are transformed by the algorithm to complex exponentials, which have rank 1 in Complex SSA. Therefore, lines can be separated from noise very well.

2.9 SSA: Modifications of the SVD step

Almost independently from extensions of the embedding step, different modifications of the decomposition step can be considered in the form \( X = X_1 + \ldots + X_r \), where the matrices \( X_i \) are of rank one.

In Basic SSA, the SVD is considered. It is the best approximating bi-orthogonal decomposition. If there is no information about the time series, the SVD is optimal. Thus, modifications of Decomposition step are related to different assumptions about the time series.

2.9.1 The use of apriori information

Decompositions adjusted to the series structure are:

- **SSA with projection** if the model of the signal is partly known; for example, if it is assumed that the signal has a linear trend, see Section 3.5. We refer to (Golyandina & Shlemov, 2017) for details, where the general approach with preliminary projections is described. SSA with centering (Golyandina et al., 2001, Section 1.7.1) is a particular case of SSA with projection, since the centering of a vector can be considered as the projection to the subspace spanned by the vector of ones. SSA, where rows of the trajectory matrix are centered, came from PCA; however, this is not natural for time series, since the rows and columns of the trajectory matrix have the same structure. Double (row and column) centering is much more natural for trajectory matrices. It is shown in (Golyandina & Shlemov, 2017) that SSA with double centering helps to extract linear trends in the presence of periodic components (see Fragment 2.8.7\(^{12}\)).

- **Toeplitz SSA** if the series is stationary (see Section 2.2.6). In application related to stationary time series, Toeplitz SSA is considered as a main version. Details are described in Section 3.13.

2.9.2 Refined decompositions of the signal

Another reason to modify the SVD step is related to improving the separability. In Basic SSA, the SVD is used for decomposition of trajectory matrices. Two main properties of the SVD (bi-orthogonality and optimality) allow one to decompose a time series into interpretable components. Optimality (we mean the approximation properties of the SVD)

\(^{12}\text{https://ssa-with-r-book.github.io/02-chapter2-part2.html#fragment-287-hotel-ssa-with-projection-linear-trend-detection}\)
provides the possibility to separate signals from noise. Bi-orthogonality helps to separate time series components if they (approximately) orthogonal. It appears that many time series components such as trends and sine waves with different frequencies are asymptotically orthogonal (separable); although, we need separability for finite-size time series. Moreover, the problem of lack of strong separability (the problem of equal eigenvalues in the SVD) can not be solved even asymptotically.

There are methods of matrix decomposition, which weaken the orthogonality condition. However, most of methods, which remove the bi-orthogonality, simultaneously drop the approximation properties. Therefore, the improvement of separability is performed in two steps. First, the trajectory space of the signal is estimated by means of grouping the signal elementary matrix components in the SVD step of Basic SSA. Then, the signal grouped matrix is decomposed by a refined expansion (we call such kind of refined expansions nested decompositions).

Examples of SSA modifications with nested decompositions are:

- SSA with derivatives. This modification can help if the components of the signal were mixed due to equal contributions of components (no strong separability) (Golyandina & Shlemov, 2015). Application of SSA with derivatives is demonstrated in Fragment 2.8.6\textsuperscript{13} for the 1D case. Fragment 5.2.5\textsuperscript{14} shows that the same approach works in the 2D case.

- Iterated Oblique SSA. This helps to solve the problem of no orthogonality (no weak separability) (Golyandina & Shlemov, 2015), see e.g. Fragment 2.8.2\textsuperscript{15}.

An approach, which uses additional rotations of mixed components, is also considered in (Groth & Ghil, 2011), where Multichannel SSA with factor rotations is suggested to solve the problem of lack of strong separability in MSSA. Recall that this problem is caused by equal eigenvalues in the SVD decomposition of the trajectory matrix. In the paper (Groth & Ghil, 2011), the problem of equal eigenvalues is called degeneracy of eigenvalues (this is the notion, which is sometimes used in PCA for explanation of unstable eigenvectors for close eigenvalues). At the same time, this problem was discussed ten years before in (Golyandina et al., 2001, Sections 1.5 and 6.1), where it was connected with the very important notion of separability in SSA (more precisely, the strong separability).

### 2.9.3 Tensor SSA

The general scheme of SSA can be even more extended in the embedding step if to consider the embedding operator $\mathcal{T}$ mapping to a set of tensors of some order instead of the matrix set. Then the scheme of the SSA algorithm is the same, a decomposition into elementary components, grouping and return back to decomposition of the initial object.

\textsuperscript{13}https://ssa-with-r-book.github.io/02-chapter2-part2.html#fragment-286-us-unemployment-improvement-by-derivssa
\textsuperscript{14}https://ssa-with-r-book.github.io/05-chapter5.html#fragments-524-mars-identification-and-525-mars-improvement-by-derivssa
\textsuperscript{15}https://ssa-with-r-book.github.io/02-chapter2-part2.html#fragment-282-fort-basic-ssa-and-iterative-o-ssa-trends
The shortcoming is that tensor decompositions are not unique and time-consuming. Sometimes, tensor decompositions can be reduced to matrix decomposition. For example, the trajectory matrix in 2D-SSA can be represented in the form of a tensor of fourth order (Golyandina & Usevich, 2010).

New algorithms can be obtained by tensor decompositions, which are not reduced to matrix ones. For example, there is a version of SSA, where the embedding operator transfers the initial object to a 3D array instead of a matrix (a 2D array)) and then a tensor decomposition (PARAFAC) is applied, see e.g. (Kouchaki, Sanei, Arbon, & Dijk, 2015), (Yang et al., 2017).

Note that the idea of the use of tensor decompositions arose much earlier in the subspace-based and low-rank approximations framework (Papy, De Lathauwer, & Van Huffel, 2005).

3 SSA and different problems

3.1 SSA and nonlinearity. Is SSA a linear method?

In the literature, a critic of SSA sounds as “SSA is a linear method”.

Let us explain what this means. First, note that the algorithm is nonlinear. Components, which can be extracted by SSA, are generally nonlinear. However, the class of time series, which produce rank-deficient trajectory matrices, consists of time series governed by homogeneous linear recurrent relations (LRRs) in the form \( x_n = \sum_{i=1}^{r} a_i x_{n-i} \). LRRs are closely related to linear differential equations (LDEs) \( \sum_k b_k s^{(k)}(t) = 0 \), since LRRs are generated by the finite-difference method applied for solving linear differential equations. In the area of dynamical systems, the methods, which are related to linear differential equations, are called linear. For example, let \( s(t) + bs'(t) = 0 \) be a LDE of order 1; consider 1, 2, 3, ... as discretization of \( t \) and the finite-difference approximation \( s'(i) \approx s_{i+1} - s_i \); then we obtain \( s_{i+1} + b(s_{i+1} - s_i) = 0 \) or, the same \( s_{i+1} = (1 - 1/b)s_i \), that is, an LRR of order 1.

The answer to the criticism of SSA linearity is as follows.

First, the class of solutions of LDE is wide enough, since it contains any finite sums of products of polynomials, exponentials and sine waves. Then, to deal with signals governed by LRRs (e.g., to extract signals from noisy time series), a large window length (optimally, around \( N/3-N/2 \), where \( N \) is the time series length) is recommended. However, smaller windows allow taking into consideration only local finite-rank approximations. For example, a modulated sinusoid with a slowly-varying amplitude is well approximated by an exponentially-simulated sinusoid in the time frame of several periods. Therefore, SSA with a small window length equal to several periods produces reasonable results. It can be stated that the coefficients of the approximating LRR should be the same for each time series segment to obtain an appropriate signal estimation. Thus, a small window length allows one to deal with nonlinearity of the model in some common cases such as modulated harmonics and trends.

A very important feature of SSA is that it does not use the explicit parametric form of the time series. For example, to predict the value of an exponential series \( s_n = Ae^{\alpha n} \), one approach is to estimate \( A \) and \( \alpha \) and to forecast by the explicit formula. However, a more flexible approach is to estimate coefficients of a governed LRR and to perform forecasting
by the estimated LRR. Thus, SSA methods try to avoid estimation of explicit time series parameters to make the method more robust with respect to deviations from the model.

Whereas a slowly changing amplitude is admissible, a changing frequency is not appropriate for SSA applied to the whole time series (except the case of varying the frequency around one main value, which is called “phase noise”). In the case of changing frequency, methods like EMD + HHT (Huang & Wu, 2008) can be working for extraction of oscillations with changing frequency; however, they only work well if noise is small enough.

**Local SSA**  The standard approach to time series with a slowly-changing structure is to analyse moving subseries of the original time series. In the framework of SSA, this is the so-called subspace tracking (see e.g. (Badeau, Richard, & David, 2003)). In papers devoted to subspace tracking, the primary focus is on construction of fast algorithms. The other use of subspace tracking is the change-point detection (Moskvina & Zhigljavsky, 2003), (Golyandina et al., 2001, Chapter 3), see example in Fragment 3.5.1216.

For estimation of time series components such as trends and signals, SSA applied to moving subseries is used (see e.g. (Leles, Sansao, Mozelli, & Guimaraes, 2018)). The main problem is how to combine different decompositions to one decomposition. In (Leles et al., 2018), for moving time series the central parts of the signal reconstructions are used and then stacked. The idea to use the central part is promising, since the reconstruction of end points is less accurate. However, the question is why not to use only central points (by analogy with the LOESS method (Cleveland, 1979)); certainly, this can be done if the computational cost is acceptable.

As a result of local SSA, we obtain a signal estimation or just a smoothing. The problem is how to forecast the extracted signal, since its estimates may have different structures at different time intervals. In local version of SSA, we do not obtain a nonlinear model; we have stacked linear models. However, many nonparametric local methods including e.g. LOESS have the same drawback.

**SSA as linear filter**  Another reason to call SSA a linear method is its connection with linear filters (see Section 2.4 for the references). Certainly, the coefficients of the SSA linear filter are produced by the time series in a nonlinear way.

### 3.2 SSA and autoregressive processes

It is important to remark that the basic model of signals in SSA and the model of autoregressive processes (AR) are similar only at a superficial glance. The models are totally different.

For SSA, the signal model is \( s_n = \sum_i a_i s_{n-i} \) and the observed series has the form \( x_n = s_n + \epsilon_n \), where \( \epsilon_n \) is typically noise (a non-regular oscillation; for example, a realization of a stochastic process).

For autoregressive processes, we have noise innovations at each step: \( x_n = \sum_i a_i x_{n-i} + \epsilon_n \).

Under some conditions on the coefficients, such innovations yield a stationary stochastic process.

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16[https://ssa-with-r-book.github.io/03-chapter3.html#fragment-3512-sunspots-subspace-tracking]
process, while \( s_n = \sum_i a_i s_{n-i} \) is a deterministic and not necessarily stationary signal. The coefficients \( \{a_i\} \) in the SSA model can be arbitrary.

In both AR and SSA analysis, characteristic polynomials are constructed on the basis of coefficients \( a_i, \ i = 1, \ldots, r \). In terms of SSA, we are concerned about characteristic roots of the governing LRR, that is, about roots of the polynomial \( t^r + a_1 t^{r-1} + \ldots + a_r \). The roots, which have moduli larger/smaller than 1, correspond to a growing/damped time series components, whereas roots with unit moduli correspond to a stationary deterministic component like undamped sine waves (see e.g. (Golyandina et al., 2001)).

For AR, this polynomial is reversed (therefore, its roots are inverse). The stationarity corresponds to roots with moduli larger than 1. The case of roots with unit moduli corresponds to non-stationarity (an example is Brownian motion \( x_n = x_{n-1} + \varepsilon \) and characteristic polynomial \( t - 1 \); the same characteristic polynomial corresponds to a constant signal in SSA).

In the context of SSA used for signal extraction, AR is mostly considered as a noise model (see e.g. a discussion of Monte Carlo SSA in Section 3.11).

There is a common form of forecasting for signals governed by an LRR and of constructing of mean forecast of AR processes. They both are performed by the LRR with estimated coefficients. The difference is in the approach for estimating these coefficients. Also, the forecasting values in the AR model are always converging to zero (or the mean value).

Note that there is an application area, where AR forecasting is performed for leading reconstructed components obtained by SSA (Toeplitz version) (Penland, Ghil, & Weickmann, 1991; C. L. Keppenne & Ghil, 1992). The authors consider the AR model for climate data; however, the example with a noisy finite-rank signal (a sum of two sinusoids) is considered as an example for numerical investigation of the method quality. Therefore, it is not clear, whether the AR prediction of SSA components is justified for time series forecasting.

Additionally, SSA can be applied to an estimate of autocovariance function \( C(l) \) to find the autoregressive coefficients, since the series \( C(l) \) is governed by the LRR with the same coefficients: \( C(l) = \sum_i a_i C(l-i) \) (the Yule-Walker equations).

### 3.3 SSA and parameter estimation

Let the signal have the explicit parametric form of a finite sum

\[
s_n = \sum_k A_k \exp(\alpha_k n) \sin(2\pi \omega_k n + \phi_k)
\]

and the observed time series be \( x_n = s_n + r_n \). Here we simplified the general model, where a polynomial multiplier can be presented in each summand, see Section 2.5. The complex-valued form of (8) is

\[
s_n = \sum_{j=1}^r c_j \mu_j^n,
\]

\[\mu_j = \rho_j e^{i2\pi \omega_j}.\] Here \( \omega_j = \text{Arg}(\mu_j)/(2\pi) \), \( \rho_j = |\mu_j| \). Note that \( \mu_j \) are the roots of the characteristic polynomial of the minimal LRR governing the signal. If \( s_n \) are real, each
complex $\mu_j$ should have its complex conjugate $\mu_k = \mu_j^*$. Then $c_j \mu_j^n + c_k \mu_k^n$ can be made real by a suitable choice of complex-valued $c_j$ and $c_k$.

A more general signal model is given by the signal rank: $\text{rank } S = r$, where $r$ is known in advance or is estimated. In the latter case, we consider $s_n = A_1 e^{\alpha_1 n} + A_2 e^{\alpha_2 n}$ and $s_n = A e^{\alpha n} \cos(2\pi \omega n + \phi)$ belonging to the same model for $r = 2$, whereas for the explicit representation (8), these are two different parametric models.

The Cramér-Rao lower bounds (CRLB) for the variance of parameter estimates are known (see e.g. (Stoica & Moses, 2005; Badeau, David, & Richard, 2008)). Let us consider a simple case of undamped sinusoids. Then it is interesting that the CRLB for the frequency has order $1/N^3$, while the CRLB for the amplitude has order $1/N$.

The common approach for parameter estimation is the nonlinear least-squares method, which implies the explicit form:

$$\sum_{n=1}^{N} (x_n - s_n(\{\alpha_j, \omega_j, A_j, \phi_j\}))^2 \rightarrow \min \{\alpha_j, \omega_j, A_j, \phi_j\}.$$  

It is a very complicated time-consuming optimization problem, since the objective function has many local minima and the problem is nonlinear and therefore needs iterative methods for solution.

The second approach is called *subspace-based* (Section 2.5.1). Let us consider the complex-valued form (5). The nonlinear parameters $\mu_j$ are estimated by one of the subspace-based methods (e.g. ESPRIT), which are based on $U_1, \ldots, U_r$ obtained in Decomposition stage of SSA (Section 2.2.3). The linear parameters can be found by the conventional linear least squares. Consider the Vandermonde matrix generated by $\mu_j$:

$$M = \begin{bmatrix} \mu_1 & \mu_1^2 & \cdots & \mu_1^N \\ \mu_2 & \mu_2^2 & \cdots & \mu_2^N \\ \vdots & \vdots & \ddots & \vdots \\ \mu_r & \mu_r^2 & \cdots & \mu_r^N \end{bmatrix}.$$  

Then (9) has the form $S = (s_1, \ldots, s_N) = C^T M$, where $C = (c_1, \ldots, c_r)^T$. If $s_n$ and $\mu_j$ are estimated (the signal $S$ is estimated as the reconstructed time series $\tilde{S}$ obtained by SSA; $\mu_j$ are estimated as $\tilde{\mu}_j$ obtained by ESPRIT), we come to the approximate equality $\tilde{S} \approx C^T \tilde{M}$; then $\hat{C}$ can be found by the LS method.

One can see that the described approach is very simple and all we should know about the signal is its rank. As methods for the frequency estimation, the subspace-based algorithms are called high-resolution, since they provide the estimates with the variance of the same order $1/N^3$ as the CRLB has (see (Badeau, Richard, & David, 2008) for the undamped case: for $s_n = C e^{i2\pi \omega n}$, the ESPRIT estimation of $\omega$ has variance $D \tilde{\omega} \sim 1/N^3$).

### 3.4 SSA and structured low-rank approximation (SLRA)

Let us apply SSA to extract a finite-rank signal from a noisy time series. The algorithm of SSA can be written down in a compact form by means of projections (see Section 2.5.2):
\[ \tilde{S} = T^{-1} \Pi_H \Pi_r T X. \]

However, in practice, the estimate \( \tilde{S} \) is generally not of finite rank. The problem of finding the estimate \( \tilde{S}_N \) of rank \( r \) can be solved by different methods. There is a subset of methods, called SLRA, which state the problem of approximation of the time series trajectory matrix by a low-rank Hankel matrix: \( \min_{S \in M_r \cap H} \| X - S \|_F \). The most famous method is called Cadzow iterations and was introduced in (Cadzow, 1988). This method consists of alternating projections and can be expressed as \( S^{(n)} = T^{-1}(\Pi_H \Pi_r)^m T X \). Thus, SSA as a method for signal extraction can be considered as one iteration of the Cadzow iterations. The Cadzow iterations were suggested in parallel with SSA.

Another approach is to use a parameterization of the set \( D_r \) of time series of rank not larger than \( r \). Then the problem of low-rank approximation \( \min_{S \in D_r} \| X - S \|_w \) is considered as a least squares problem and can be solved by ordinary weighted LS methods. If the noise is Gaussian, then by the choice of corresponding weights, the weighted LS estimates coincide with maximum likelihood estimates (MLE) and therefore they are asymptotically the best.

However, if \( S \) is parameterized by means of parametrization of series of rank not larger than \( r \), it is still called structured low-rank approximation method (see (Markovsky, 2019)), where the Hankel structure of the trajectory matrix is considered. However, the problem in (Markovsky, 2019) is formulated as the problem of weighted least squares for time series themselves and the result does not depend on window length. Therefore, in fact, this is not the problem of low-rank matrix approximation.

Both SSA and Hankel SLRA can be used for signal extraction, forecasting and frequency estimation. Comparing the approaches, we can say that

- SSA is fast, SLRA is time-consuming;
- SLRA can provide more accurate parameters estimates than SSA;
- for a signal which only approximately (or locally) satisfies the model, SLRA does not work; SSA does work;
- the outcome of SLRA allows simpler procedures for parameter estimation and forecasting.

Thus SLRA is applied mostly in signal processing for engineering problems, where the signals are exactly of finite rank.

For the general case of real-life time series, time series components, which are exactly of finite rank, is a rare case and therefore SSA is suitable in a much greater extent. For example, lowly-varying trends can be approximated by time series of finite rank but generally they are not exactly of finite rank. Also, amplitude modulations of periodic components are not exactly of finite rank for real-life data. However, this does not create a barrier for SSA to extract them. Nevertheless, a reasonable example of Cadzow iterations for extraction of an exponential trend can be found in Fragment 3.5.8\(^{17}\).

\(^{17}\)https://ssa-with-r-book.github.io/03-chapter3.html#fragment-358-fort-cadzow-iterations
3.5 SSA and linear regression (LS-estimator of linear trend)

As we discussed before, SSA can extract trends which are slowly-varying time series components and are approximated by finite-rank series. Ideally (but not necessarily) trend should be series of small rank \( r \). Linear series \( s_n = an + b, a \neq 0 \), belong to the class of series, which are governed by LRRs and have rank 2. However, linear functions are not natural for SSA (while exponential series are very natural). The reason is that the characteristic root for a linear series is 1 of multiplicity 2 and the minimal recurrence formula is \( s_{n+2} = 2s_{n+1} - s_n \). Presence of roots of multiplicity larger than 1 is very unstable. Any distortion of the coefficients of this LRR transforms the multiple unit root to two different roots, that is, a linear series to a sum of two exponentials with small exponential rates or a cosine series with large period.

There is a modification of SSA, which was called in (Golyandina et al., 2001, Section 1.7.1) SSA with double centering. In that book, the correspondence between SSA with double centering and extraction of linear trends is demonstrated. As it is shown in (Golyandina & Shlemov, 2017), SSA with double centering is a particular case of SSA with projection, where projections of its rows and columns to the given subspaces are produced, subtracted from the trajectory matrix, and then the SVD expansion of the residual matrix is performed. SSA with projection is positioned as SSA with the use of some information given in advance. At the present moment, only the use of SSA with projection for extraction of polynomial trends is considered (Golyandina & Shlemov, 2017).

Since the most standard method for estimation of linear trends is linear regression, where the least-squares method is used, let us summarize the comparison results. Certainly, if the time series consists of a linear trend and white noise, the least squares provides the best estimate. However, if the residual includes e.g. a periodic component, this is not true. It is numerically shown in (Golyandina & Shlemov, 2017) that for the case \( x_n = an + b + \sin(2\pi \omega n + \phi) + \epsilon_n \), where \( \epsilon_n \) is white noise, the LS method applied to the trend, which was extracted by SSA with double centering, generally overcomes the conventional LS estimate applied to the original time series (i.e., overcomes the ordinary linear regression).

3.6 SSA and filtering

Recall that linear finite-impulse response (FIR) filters are defined as \( f_n(X) = \sum_{i=-m}^{m} b_i x_{n-i} \). The main characteristic of FIR filters is the frequency-amplitude response \( A(\omega) \), which has a simple explanation: if \( x_n = \cos(2\pi \omega n) \), then \( f_n(X) = A(\omega) \cos(2\pi \omega n + \phi(\omega)) \).

SSA can be considered as a set of adaptive filters (see Section 2.4 for references). Each elementary reconstructed component for indices from \( L \) to \( N - L + 1 \) is obtained by a linear FIR filter applied to the original time series. If the window length is small, then the output of SSA can be considered mostly as a result of filtering by an adaptive FIR filter. However, if \( L \) is large, this view is not suitable. Generally, each point of the reconstructed series is a linear combination of values of the original series. However, for each point from \([1, L]\) and \([N - L + 1, N]\) we have different linear combinations.

The following result is valid: let SSA be applied with \( L \leq (N + 1)/2 \) and \( U = U_i \) be an eigenvector in the SVD of \( X \). Then the \( i \)th elementary reconstructed time series on the
interval \([L, N - L + 1]\) has the form

\[
\tilde{x}_s^{(i)} = \sum_{j=-(L-1)}^{L-1} \left( \sum_{k=1}^{L-\lvert j \rvert} u_k u_{k+\lvert j \rvert}/L \right) x_{s-j}, \quad L \leq s \leq K. \tag{10}
\]

This filter is called middle-point filter (MPF). It is shown in (Golyandina & Zhigljavsky, 2013, Section 3.9) that the frequency response \(A(\omega)\) of MPF is determined by the periodogram of \(U\). This explains why we can perform the grouping step based on frequency properties of eigenvectors \(U_i\).

Note that if \(U\) consists of equal numbers, we obtain the Bartlett (triangle) filter. A similar leading eigenvector is obtained if the time series is positive and \(L\) is small.

The other helpful properties are as follow. The filter bandwidth tends to be narrower as \(L\) (together with \(N\)) tends to infinity. That is, increasing \(L\) we can obtain a more refined decomposition. Recall that we discuss the behavior at \([L, N - L + 1]\).

The last-point filter (LPF) plays an important role, since it is used for reconstruction of the last point and therefore is connected with forecasting. It is not really a filter as it is used only for the reconstruction of the last point:

\[
\tilde{x}_N^{(i)} = u_L \sum_{i=0}^{L-1} u_{i+1} x_{N-i}.
\]

However, it is the only reconstruction filter that is causal (see (Golyandina & Zhigljavsky, 2013, Section 3.9.5) for discussions).

As a rule, causal filters have a delay. For example, the causal moving average with window width \(W\) has delay \(W/2\). The delay in SSA depends on the separability quality for the reconstructed component. If the separability is exact, then the delay is zero. This is the important advantage of SSA over moving averaging. This advantage is a consequence of adaptive properties of SSA.

### 3.7 SSA and ICA

Independent component analysis (ICA) is introduced for random processes and the word “independent” is related to the stochastic independence instead of the uncorrelatedness (orthogonality) in PCA based on the SVD. In SSA, mostly non-random signals are extracted and separated. Since signals extracted by SSA are generally not stochastic, the stochastic independence can be just formally applied to deterministic components. Therefore, the direct use of ICA in SSA is formal and leads to an improvement of separability not in stochastic sense. By the reasons explained in Section 2.9.2, ICA is used in SSA for a nested decomposition.

The SSA with SOBI-AMUSE version of ICA is described in (Golyandina & Lomtev, 2016). Note that this version is very similar to DerivSSA (Golyandina & Shlemov, 2015), which was created by a completely different approach. SSA with maximization of entropy is described in (Golyandina & Zhigljavsky, 2013, Section 2.5.4). In both versions, the modification of the decomposition step of the SSA algorithm can be called ICA, since the maximization problems stated in ICA are formally reformulated for non-random time series components.
Another connection between SSA and ICA is related to applications to blind signal separation and is considered in (Pietilä, El-Segaier, Vigário, & Pesonen, 2006). In that application, Basic SSA served for pre-processing, i.e. for removal of noise and dimension reduction; then ICA was applied for the extraction of independent components from their mixture in a conventional way. This is similar to the use of PCA before ICA for analysis of multidimensional data (Kato, Yen-Wei Chen, & Gang Xu, 2006).

3.8 SSA and EMD, FT, WT

**EMD** Empirical Mode Decomposition (EMD) (Huang & Wu, 2008) is frequently compared with SSA, since both are model-free techniques. It seems that EMD is an method without explicit approximation properties, whereas SSA has both separability and approximation properties. (The first components extracted by EMD is highly oscillating and the last component is referred to a trend; for SSA, it is opposite, since the signal corresponds to the leading components.) The advantage of EMD is its ability to extract periodic components with complex modulation and changing amplitudes. Probably, the combination of SSA and EMD can extend the range of real-life problems being solved.

**FT** Fourier Transform (FT) differs from SSA by the use of a fixed basis consisting of sines-cosines with frequencies from an equidistant grid against the construction of an adaptive basis in SSA. In (Bozzo et al., 2010) the relation between SSA and FT is discussed. In fact, SSA coincides with FT in the circular version of SSA (see terminology in (Shlemov & Golyandina, 2014)), where the data are considered given on a circle or on a torus in the 2D case.

From the viewpoint of frequency estimation (see Section 3.3), SSA and the related subspace-based methods allow to estimate frequencies with a better resolution than $1/N$, where $N$ is the time series length (see e.g. (Santamaria, Pantaleón, & Ibanez, 2000) and (Stoica & Soderstrom, 1991) for comparisons of FT, ESPRIT and MUSIC). The MUSIC method allows one to construct pseudo-spectrums similar to periodograms but with no limitation on frequencies. Comparing time series models that suitable for the methods, one can say that a sum of pure sinusoids corresponds to FT, while a sum of products of polynomials, exponentials and sinusoids (that is, a sum of sinusoids with amplitude modulation) corresponds to SSA.

Another application of FT is estimation of the spectral density by means of smoothed periodograms. SSA can be used for estimation of the spectral density, see e.g. (Golyandina et al., 2001, Section 6.4.3), where the application of results from (Grenander & Szegö, 1984) to SSA is discussed. If the spectral density is monotonic, different frequencies generally correspond to different eigenvectors; otherwise, the eigenvectors are mixed, i.e. they contain different frequencies with equal contribution. This is an explanation, why eigenvectors produces by white noise (with constant spectral function) are mostly irregularly oscillating. And, vice versa, the eigenvectors of red noise can be referred to different frequencies. Since the contribution of the eigenvectors is determined by the corresponding eigenvalues, for red noise the graph of dependence of the eigenvalues on the main frequencies of corresponding eigenvectors can be considered as the spectral-density estimate (see e.g. (Golyandina, 2019, Figs. 1–4) for numerical confirmation).
In (Yiou, Baert, & Loutre, 1996), the questions of application of SSA to spectral estimation in climatology are discussed.

**WT** Wavelet transform is the decomposition based on a fixed space-time basis. This yields both advantages and disadvantages. See discussion in (Yiou et al., 2000).

### 3.9 SSA: model-free method and modelling

In Section 2.5 we discussed the model of time series that suits SSA. These are time series of finite rank or series governed by linear recurrence relations. The latter class is narrower; although it is much more understandable in practice.

SSA is a multi-purpose method, which can be as model-free as used for modelling. Briefly:

1. As an exploratory method, SSA is a model-free technique, which can perform the time series decomposition and the frequency filtration without assumptions given in advance.

2. If the signal is governed by an LRR, SSA allows constructing the explicit form of the signal and estimating the parameters; i.e. SSA can perform parametric modelling.

3. If the signal satisfies an LRR only approximately (or locally), forecasting and missing data imputation can be performed in the framework of SSA without construction of the model; that is, SSA is an adaptable method. This is one of key advantages of SSA, which considerably extends the range of applications.

### 3.10 SSA, forecasting, gap filling

We put forecasting and gap filling (missing data imputation) together, since forecasting can be considered as a particular case of gap filling with the gap at the place of the predicted data. On the other hand, gap filling can be considered as forecasting internal data.

**Parameters finding via cross-validation** Generally, if an algorithm has parameters, their choice can be performed with the help of the cross-validation procedure, which consists of constructing the prediction on training data and then calculation of errors on the test data; parameters are chosen to minimize the cross-validation error.

For forecasting, a moving prediction is performed for cross-validation, where test sets step after training sets. For gap filling, artificial gaps are considered as test data located at arbitrary positions. Generally, errors of imputations of test data can be considered for the choice of forecasting parameters; however, the forecasting accuracy can significantly differ from the imputation accuracy, since for the imputation we have data from both sides, while the forecasting uses data from one side only and thereby is less stable. It is an important difference as in both forecasting and gap filling, we seek for a compromise between accuracy and stability.
**SSA forecasting**  In (Golyandina et al., 2001; Golyandina & Zhigljavsky, 2013) the model of time series, which is a sum of a signal of finite rank and noise, is considered. Several subspace-based forecasting methods are suggested: recurrent, vector and simultaneous ones. The recurrent forecasting is performed by a special LRR (the min-norm LRR, whose coefficients have a minimal norm), which approximately governs the signal (or the chosen series component, the trend or the seasonality, to forecast), see Section 2.5.1. This algorithm is known as the linear prediction algorithm (Kumaresan & Tufts, 1982), where the min-norm LRR is used for forecasting.

Let us comment the SSA recurrent prediction. The model of the signal is given by the minimal LRR \( s_n = \sum_{i=1}^{r} a_i s_{n-i} \). There are a lot of LRRs, which govern the same time series, with different suppressing properties: \( \text{Var}(\hat{s}_n) = \text{Var} \sum_{i=1}^{m} b_i (s_{n-i} + \delta_{n-i}) = ||B||^2 \sigma^2 \), where \( \delta_n \) are some perturbations, \( \sigma^2 = \text{Var} \delta_n \). The SSA forecasting LRR (6) has minimum norm of coefficients and therefore has the best suppressing properties. Examples of forecasting are shown in Fragment 3.2.1\(^{18}\).

**Subspace-based missing-data imputation**  In (Golyandina & Osipov, 2007), the same subspace-based approach is considered for missing data imputation. Moreover, if a prediction algorithm works, the same algorithm can be applied to fill in the gap by forward prediction from the left, by the backward prediction from the right and then by a combination of the results.

The subspace-based methods are fast and work well for forecasting. It is convenient, that we should not choose the number of components in advance. After decomposition, the time series components can be identified, grouped and each group can be forecasted by the corresponding forecasting LRR. However, as a method for gap filling, the subspace-based approach is suitable for a small number of gaps; generally, for several compactly located gaps to allow estimation of the subspace (Fragment 3.3.1\(^{19}\)).

**Iterative gap filling**  In (Kondrashov & Ghil, 2006) the approach from (Beckers & Rixen, 2003) is applied to time series. The approach suggested in (Beckers & Rixen, 2003) is very general and can be applied to data of arbitrary form. The algorithm is iterative and has two parameters (for SSA), the window length \( L \) and the rank \( r \). In the first step, missing data are filled in by some numbers; e.g., by the average. Then SSA(\( L, r \)) is applied to the time series with no missing data to obtain the reconstructed series. Next, the values at the positions without missing entries are restored to the original values and the iterations are repeated. Cross-validation is used to choose \( L \) and \( r \). This method is time consuming; however it is very universal for missing data imputation, since it is applicable for arbitrary gap location (see Fragments 3.3.2 and 3.3.3\(^{20}\)). For forecasting, this method is not stable, since it uses original data, which “hold” the imputation, only from the left.

\(^{18}\)https://ssa-with-r-book.github.io/03-chapter3.html#fragment-321-forecasting-of-co2

\(^{19}\)https://ssa-with-r-book.github.io/03-chapter3.html#fragment-331-subspace-based-gap-filling

\(^{20}\)https://ssa-with-r-book.github.io/03-chapter3.html#fragment-332-iterative-gap-filling-one-gap
AR and SSA forecasting  We refer to Section 3.2 for discussion of common and unique features of AR and SSA forecasting.

For the model of signals consisting of a trend and seasonality, Seasonal ARIMA can be concurrent with SSA. There are examples where ARIMA provides better accuracy; and vice versa; see e.g. (Hassani, Heravi, & Zhigljavsky, 2009; De Klerk, 2015a). One of the advantages of ARIMA is the choice of its model and orders by information criteria like Akaike information criterion (AIC) or Bayesian information criterion (BIC). The number \( r \) of signal components can be chosen in SSA on the basis of the AIC/BIC approach; however, at the present moment this approach is heuristic in application to SSA. Note that Seasonal ARIMA should know the period, whereas SSA does not need it. Moreover, observations of a few periods can be sufficient for SSA and definitely is insufficient for Seasonal ARIMA. Fragment 3.5.18\(^{21}\) contains an example of comparison of SSA, Seasonal ARIMA and ETS.

3.11 SSA and signal detection (Monte Carlo SSA)

The problem of signal detection is very actual in practice. If noise is strong, it is easy to find spurious signals, since noise (if to consider it as a stationary process) contains all frequencies. The mean contribution of each frequency is determined by the spectral density of the noise. In particular, this implies that if the spectral density is larger for low frequencies, the probability of spurious trends or spurious sine waves with low frequencies increases. This is exactly the case of the so-called red noise (AR(1) with a positive coefficient).

Since we observe one realization of time series, the contribution of each frequency from the grid \( \{ k/N \} \) (we consider the periodogram values, corresponding to these frequencies) is random with variance, which does not tend to zero as \( N \) tends to infinity. Moreover, asymptotically it has exponential distribution, that is, large values are likely.

The question of existence of a signal in noise can be reduced to construction of a criterion for testing the hypothesis that the time series is a pure noise; the criterion should be powerful again the alternative with presence of a signal. There are a lot of such criteria for different models of noise. The most of them are related to the white noise model.

In the framework of SSA, red noise is the other focus of attention. One of the reasons is that SSA was primarily popular in climatology, where the time series are conventionally modelled as red noise. In addition, the properties of red noise suit SSA, since red noise has a monotonic spectral function (see Section 3.8 for a short discussion).

The method of detection of a signal in red noise was called Monte Carlo SSA (M. Allen & Smith, 1996; R. M. Allen & Robertson, 1996; Palus & Novotná, 2004; Jemwa & Aldrich, 2006; Greco et al., 2011; Groth & Ghil, 2015; Garnot, Groth, & Ghil, 2018), since it uses simulations. Probably, the method’s name does not reflect the method specific as a method for hypothesis testing; however, this is the name the method is known.

The approach used in Monte Carlo SSA is straightforward: to choose a characteristic of data, create surrogate data according to null-hypothesis and construct the distribution of the chosen characteristics. If the chosen characteristic for the real-life data lies outside \((1 - \gamma)/2\) - and \((1 + \gamma)/2\)-quantiles of the constructed distribution, then the null hypothesis is

\(^{21}\)https://ssa-with-r-book.github.io/03-chapter3.html#fragment-3518-sweetwhite-comparison-of-ssa-arima-and-ets

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rejected at the significance level $1 - \gamma$. Certainly, there are different problems, which should be solved during application of the described scheme. For example, the parameters of the AR(1) process satisfying the null-hypothesis are unknown and should be estimated. Then, it is not enough to choose only one characteristic (one frequency in Monte Carlo SSA) to detect signals with different frequencies. That is, the problem of multiple tests arises.

We refer to (Golyandina, 2019) for description of a more strict statistical approach to construction of the Monte Carlo SSA criteria, where the problem of multiple tests is solved and an approach for controlling the type I error and estimating the criterion power is suggested.

### 3.12 SSA and outliers

The problem of robustness to outliers is actual for any method. Let us consider how this problem can be solved for SSA. Recall that for signal extraction, Basic SSA can be expressed through two projections: $\tilde{S} = \mathcal{T}^{-1}\Pi_{\Pi_{\mathcal{T}}}X$ (Section 2.5.2). In Basic SSA, both projections are performed in the Frobenius norm (which can be called the norm in $L_2$). The squared Frobenius norm is equal to the sum of squared matrix/vector entries.

There are two modifications of SSA, when the projection is performed in some other norm.

#### Weighted projections

The first approach is to use a weighted norm, produced by different weights of time series points, where points which are suspected to be outliers have smaller weights. In this approach, projections are performed in the weighted Frobenius norm. The weights are chosen by an iterative procedure like that used in LOWESS nonparametric smoothing (Cleveland, 1979) or in IRLS (Holland & Welsch, 1977), where the weights are chosen in dependence on the residual values in a specific way.

For this approach, SSA with weights should be implemented. SSA with special weights, where the ordinary SVD is changed to the oblique SSA, can be implemented with approximately the same computational cost as Basic SSA (Zvonarev & Golyandina, 2017). However, arbitrary weights of different time series points are not the case. The SVD with arbitrary weights has no closed form solution and needs an iterative approach to numerical computing. That is, the algorithm will contain inner and outer loops and will be very time-consuming. This approach is described in (S. Trickett, Burroughs, & Milton, 2012; Chen & Sacchi, 2014), where the authors consider the weighted projection to low-rank matrices; however, it seems they consider the unweighted projection to Hankel matrices (compare with (Zvonarev & Golyandina, 2017, Prop.2)).

#### $L_1$ projections

The second approach is also frequently used in approximation problems. To improve the robustness, the projections are performed in the $L_1$-norm. The idea to use the $L_1$-norm matrix approximation instead of the $L_2$-norm matrix approximation (that is, instead of the ordinary SVD if we talk about SSA) is very popular in data analysis. Again, $L_1$-SVD has no closed-form solution and therefore time-consuming iterative algorithms should be applied. There are many papers devoted to $L_1$ low-rank approximations. It is known that the optimal solution in the real-values case has computational cost of order $O(N^{dr})$, where $d$ is the rank of the data matrix and $r$ is the number of desirable components (Markopoulos,
Karystinos, & Pados, 2014). Therefore, suboptimal solutions are considered to decrease the cost (see e.g. (Kundu, Markopoulos, & Pados, 2014)).

Projection to Hankel matrices in $L_1$ is performed by the change of diagonal averaging to taking medians. The algorithm with the use of $L_1$-norm is considered in (Kalantari, Yarmohammadi, & Hassani, 2016). However, the question of its implementation with reasonable computational cost is still not solved.

The previous considerations were related to modifications, which robust to outliers. Another problem is to detect outliers. One common approach to outlier detection is to use a change-point detection method, then remove outliers and apply a method for data analysis. For example, the detection of outliers can be performed by subspace-based methods with the help of singular spectrum analysis, see (Golyandina et al., 2001, Chapter 3.6.1); or by standard statistical methods in the SVD step (or, similarly, PCA), see e.g. (De Klerk, 2015b).

3.13 SSA and apriori/aposteriori information

Let us consider what information about the time series can help to modify the SSA algorithm for more accurate estimates or to analyse the algorithm results. Note that the general rule is valid: if the used information is wrong, the modified algorithm can yield totally wrong results.

The most frequently used assumption is the stationarity of the time series; then Toeplitz SSA is used (Section 2.2.6). In Fragment 2.2.2 the comparison of Toeplitz SSA with Basic SSA in dependence on the exponential rate (the value 0 corresponds to stationarity) is demonstrated.

Another possible assumption is that the trend is polynomial. Especially for the linear trend, it is theoretically proved (Golyandina et al., 2001, Sections 1.7.1 and 6.3.2) and empirically confirmed that SSA with projection can considerably improve the trend extraction (Golyandina & Shlemov, 2017), see Section 3.5.

The second approach can be called posterior (Holmström & Launonen, 2013; Launonen & Holmström, 2017) or bootstrap. On the base of the bootstrap approach, bootstrap confidence intervals can be constructed for any characteristic, which is estimated by SSA; e.g., for the signal itself or for the signal’s parameters. The bootstrap approach includes estimation of the signal and noise parameters; then simulation of a sample consisting of the estimated signal plus simulated noise allows one to construct different confidence intervals. (The same approach is used in Monte Carlo SSA (which is actually Bootstrap SSA) for testing hypotheses and in forecasting for construction of bootstrap confidence intervals.) The approach used in (Holmström & Launonen, 2013; Launonen & Holmström, 2017) for the detection of trend/periodic components tests the stability of decomposition components to distinguish between noise and signal components.

[22]https://ssa-with-r-book.github.io/01-chapter2-part1.html#fragment-222-simulation-comparison-of-toeplitz-and-basic-ssa
3.14 SSA, automatic identification and batch processing

Let us describe approaches to automatic identification of eigentriples in SSA for their grouping for extraction of trend and periodic time series components.

**Trend identification** Probably, a more natural automatic detection is used for trend extraction, since the trend can be described in a nonparametric way as a low-frequency component of the time series.

In (Vautard et al., 1992) different methods for trend detection were suggested; in particular, the number of zeros or Kendall’s tau correlation coefficient were considered for detection of trend eigenvectors in the grouping step of the SSA algorithm. The number of zeros measures (in an indirect way) if the component is low-frequency. Kendall’s tau correlation reflects if the component is increasing or decreasing.

In (Alexandrov, 2009) and (Golyandina & Zhigljavsky, 2013, Section 2.4.5.2), low-frequency components are extracted in a direct way by analysis of component’s periodograms. More precisely, eigenvectors or factor vectors or elementary reconstructed components taken from the SSA decomposition are considered. Then a frequency range \([0, \omega_0]\) and a threshold are chosen. If the contribution of frequencies from the given frequency range is larger than the threshold, the component is referred as the trend one. This simple algorithm works very well if the trend components are separated from the residual. If the trend does not have a complex form, the trend is usually well separated, see Fragment 2.8.9. A slightly different approach is described in (Watson, 2016).

**Periodicity identification** The approach based on component’s periodograms can be extended to detection of harmonics (sine waves). The specific of harmonic extraction is that they produce two components in the SSA decomposition for any frequency from \((0, 0.5)\) and one component for frequency 0.5. The algorithm of recognition of paired components based on periodograms was suggested in (Vautard et al., 1992) and studied for application to exponentially-modulated harmonics in (Alexandrov & Golyandina, 2005).

Whereas the trend is as a rule well separated from the residual, pairs of components produced by different harmonics can mix if the harmonic amplitudes are close. Two SSA modifications, Iterative Oblique SSA and SSA with derivatives (see Section 2.9.2) can be applied for improving the separability before the use of component identification algorithms. In the case when the period is known in advance (for example, in the case of seasonality extraction), the periodogram approach can be applied to decomposition components separately to detect if the contribution of the known frequencies exceeds the threshold.

**Grouping** We have described approaches to identification of trend and periodic components. There is an approach to automatic grouping. This approach is in fact the application of a clustering algorithm to the matrix of weighted correlations between elementary reconstructed components. If the time series components are well separated, this approach works

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23 [https://ssa-with-r-book.github.io/02-chapter2-part2.html#fragment-289-paynsa-automatically-identified-trend](https://ssa-with-r-book.github.io/02-chapter2-part2.html#fragment-289-paynsa-automatically-identified-trend)
well, see Fragment 2.7.1. However, this way of grouping fails if groups are poorly separated.

**Use of automatic identification**  Automatic identification and batch processing have their own parameters, which can be chosen according to the assumed structure of extracted components. Therefore, these techniques work in the case of analysis of a collection of similar time series. Generally, to choose parameters of the identification procedure, a preliminary analysis of the time series should be performed in manual mode.

Note that a method of automatic identification, which calculates some measures and compares them with a threshold, can provide a helpful guess for manual grouping based on the values of considered measures.

**Signal identification** A completely different way of identification of signal components is based on the parametric model approach. If the signal is assumed to be of finite rank $r$ and is dominated, that is, the $r$ leading components correspond to the signal in the SSA decomposition, then the model (which is determined by the given rank) is usually chosen by information criteria like AIC or BIC (BIC is recommended). Information criteria need MLE estimates, whereas, as a rule, an LS estimate of the signal is constructed within low-rank approximation methods. The WLS estimate with appropriate weights is MLE if the residuals are Gaussian. See e.g. (Zvonarev & Golyandina, 2018) for construction of a fast algorithm for the WLS estimation and discussion of the parametric model and its parameters; in particular, the difference with the approach from (Usevich & Markovsky, 2014) is discussed.

Consider the simple case of white Gaussian noise. Denote $\tilde{S}(d)$ the LS estimate of the signal of length $N$ assuming the parametric model of time series of rank $d$. The number of parameters is $k = 2d$. Define $\text{RSS}(d) = \|\tilde{S}(d) - S\|^2$. Then, by definition,

$$
AIC = N \ln(\text{RSS}(d)/N) + 2k, \quad BIC = N \ln(\text{RSS}(d)/N) + k \ln N.
$$

The values of AIC/BIC can be used for the choice of $r$ in a conventional way.

Information criteria as is can be used in the SLRA statement of the problem, see Section 3.4, if the signal is of finite rank and we are able to construct its MLE estimate. In practice, signals are only approximated by series of finite rank. Even if the signal is of finite rank, the signal estimate given by SSA is generally not of finite rank and is not the LS estimate. Thus, the use of information criteria for the rank estimation is questionable in application for real-life problems.

The other general approach for automatic choice of $r$ is cross-validation, which is shortly discussed in Section 3.10. This approach is time-consuming and can be applied to long time series; moreover, the aim of this approach is to find $r$ for better forecasting/gap filling, not for signal rank estimation. However, it is suitable under much weaker assumptions about of signal/noise and therefore is applicable in practice. The R code for the choice of the signal rank $r$ by cross-validation can be found in Fragments 3.5.13–3.5.15.

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24. https://ssa-with-r-book.github.io/01-chapter2-part1.html#fragment-271-white-dwarf-auto-grouping-by-clustering

25. https://ssa-with-r-book.github.io/03-chapter3.html#fragment-3513-functions-for-the-search-of-optimal-parameters
3.15 SSA and machine learning

SSA can be called principal component analysis (PCA) for time series. Therefore, the use of SSA in many cases is similar to the use of PCA (SVD) for multivariate data. In (Golyandina et al., 2018, Section 1.7.3) one can find a brief review of papers, where SSA together with some other methods (SVM, SVR, NN among others) are used in machine learning.

4 Implementation of SSA

4.1 Software and fast implementation

At the moment, there are a lot of different implementations of SSA. Let us enumerate several of them:

1. the general-purpose interactive ‘Caterpillar’-SSA software (http://gistatgroup.com, Windows);
2. the interactive software oriented mainly on climatic applications, SSA-MTM Toolkit for spectral analysis and its commercial extension kSpectra Toolkit, interactive (http://www.atmos.ucla.edu/tcd/ssa, Unix, Mac);
3. the commercial statistical software SAS, which includes SSA to its econometric extension SAS/ETS®;
4. the R package Rssa, a cross-platform implementation of the main SSA procedures, extensively developed (http://cran.r-project.org/web/packages/Rssa).

Fast effective algorithms are implemented in the Rssa package, where the complexity (in flops) is dropped from $O(N^3)$ down to $O(kN \log N + k^2N)$; here $N$ is the series length, $k$ is the number of calculated eigentriples. Briefly, the approach is based on the Lanczos algorithm and on computing the vector multiplication through Fast Fourier Transform applied for calculation of convolutions (Korobeynikov, 2010; Golyandina et al., 2015).

Note that the SSA decomposition implemented in Rssa does not take into consideration if the data were updated (if new data were appended to the time series). That is, application of SSA to updated data adds twice the computational cost. There are different approaches for updating the SVD. However, it is still unanswered question whether an algorithm for updating SSA can be faster than the current implementation of SSA.

Let us finally remark that reasonings about the computational cost of SSA-related methods, which are reported in the literature, can be irrelevant; e.g., the sources can use only the information known on the publication date. Let us give some examples. In many papers, SSA is considered as a very time-consuming method because of the used SVD expansion; in particular, in some past papers, the method ESPRIT is called time-consuming (with computational cost $O(N^3)$ as the time series length tends to infinity). However, the method implementation in Rssa is much faster.

Another example is the SSA vector forecasting. In (Golyandina et al., 2001), this method is called very time-consuming in comparison with the SSA recurrent forecasting. In Rssa, the implementation of the SSA vector forecasting (Golyandina et al., 2015) is even faster.
than that of the recurrent one. On the other hand, this does not mean that the recurrent forecasting cannot be done faster in next implementations.

One more example is related to mathematical issues. In SSA and especially in MSSA, the understanding that for the original trajectory matrix and for the transposed one the SVD decompositions are in fact the same can help to considerably decrease computational costs by choosing the case, which is less time-consuming for the used numerical algorithm.

4.2 An example of calculations in Rssa

Let us demonstrate how fast the computations in Rssa are performed. For the time series length $N = 1000000$ and the window length $L = 500000$, the reconstruction of a sine wave signal based on two leading components is executed in a few seconds:

```r
> library("Rssa")
> N <- 1000000
> signal <- sin((1:N)*2*pi/10)
> ts <- signal + 10*rnorm(1:N)
> system.time(s <- ssa(ts, L = N/2, svd.method = "auto", neig = 2))
user  system  elapsed
 1.19    0.16    1.34
> system.time(rec <- reconstruct(s, groups = list(sig = 1:2)))
user  system  elapsed
 0.55    0.13    0.67
> max(abs(signal-rec$sig))
[1] 0.0515102
```

5 Conclusion

As the readers can see, even a brief description of SSA-related themes composes a very large paper. Therefore, it is very difficult to conclude this advanced review paper. Summing up, we want to express the hope that the paper can help researchers from different scientific areas to understand SSA both deeper and in a flexible manner and to successfully incorporate SSA to their research together with other methods.

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