

Tensors for signal and frequency estimation in subspace-based methods: when they are useful?

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Introduction to Singular Spectrum Analysis (SSA)

SSA - family of methods for time series analysis

Problems that can be solved by SSA-related methods:

- Signal extraction
- Frequency estimation
- Smoothing and Noise reduction
- Signal decomposition (Trend and Periodicity extraction)
- Forecasting
- Missing data imputation
- Change in structure detection
- Many others. . .

SSA References

Books:

- J.Elsner and A.Tsonis. Singular Spectrum Analysis: A New Tool in Time Series Analysis, Plenum, 1996.
- N.Golyandina, V.Nekrutrin and A.Zhigljavsky. Analysis of Time Series Structure: SSA and Related Techniques, CRC Press, 2001.
- S.Sanei and H.Hassani. Singular Spectrum Analysis for Biomedical Signals, CRC Press, 2016.
- N.Golyandina, A.Korobeynikov and A.Zhigljavsky. Singular spectrum analysis with R, Springer, 2018.
- N.Golyandina and A.Zhigljavsky. Singular Spectrum Analysis for Time Series, Springer, 2013, 2020 (2nd Edition).

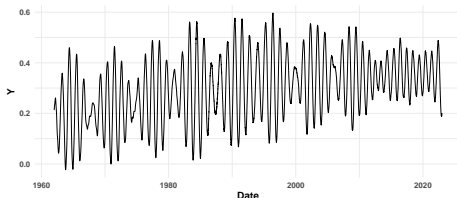
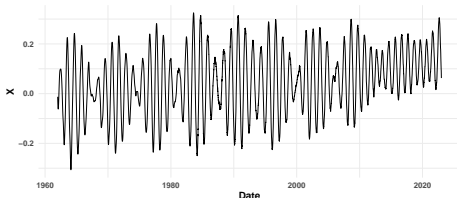
Implementations:

- R Package: Rssa
<https://CRAN.R-project.org/package=Rssa>
- Python Package: PyRssa (Python wrapper over Rssa)
<https://pypi.org/project/pyrssa/>

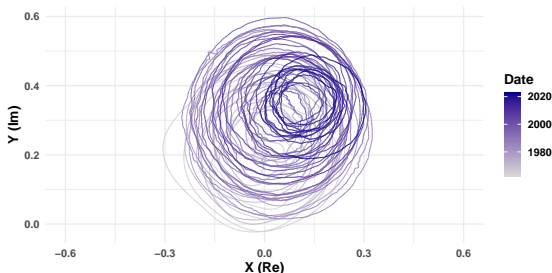
Decomposition and Estimation Example

Data: Coordinates of Earth pole motion [IERS EOP 14 C04]

Raw data:



As complex time series:

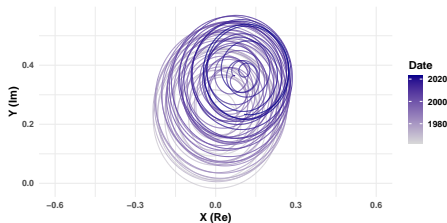


Decomposition and Estimation Example

Decomposition of time series:

- Low-frequency component + high-frequency component
- Signal + noise
- Trend + Seasonality + Noise

Extracted signal:



Signal parameters estimates:

Period (Days)	Change rate
365.41	$-5.5 \cdot 10^{-6}$
433.10	$-2.2 \cdot 10^{-5}$
$\rightarrow \infty$	$2.7 \cdot 10^{-5}$

SSA Algorithm: Embedding

Input: time series $\mathbf{X} = (x_1, x_2, \dots, x_N)$, window length L , signal rank r .

- ① **Embedding.** Constructing the L -Trajectory Hankel matrix $\mathbf{X} \in \mathbb{C}^{L \times K}$ from the series \mathbf{X} , where $K = N - L + 1$:

$$\mathbf{X} = \mathcal{T}^{(L)}(\mathbf{X}) = \begin{pmatrix} x_1 & x_2 & x_3 & \dots & x_K \\ x_2 & x_3 & x_4 & \dots & x_{K+1} \\ x_3 & x_4 & x_5 & \dots & x_{K+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_L & x_{L+1} & x_{L+2} & \dots & x_N \end{pmatrix}$$

Why not embed into a higher order array (tensor)?

SSA Algorithm: Decomposition, Grouping, Reconstruction

- ② **Decomposition.** Constructing the singular value decomposition (SVD) of the matrix \mathbf{X} : $\mathbf{X} = \sum_{j=1}^{\text{rank } \mathbf{X}} \sqrt{\lambda_j} U_j V_j^H = \sum_{j=1}^{\text{rank } \mathbf{X}} \hat{\mathbf{X}}_j$ where H denotes Hermitian conjugation, U_j and V_j are left and right singular vectors of \mathbf{X} , $\sqrt{\lambda_j}$ — its singular values in descending order.
- ③ **Grouping.** Grouping the terms $\hat{\mathbf{X}}_j$ from the decomposition related to the signal: $\mathbf{S} = \sum_{j=1}^r \hat{\mathbf{X}}_j = \Pi_r \mathbf{X}$, where Π_r is the projector onto the space of matrices with rank not greater than r .
- ④ **Reconstruction.** Applying projection onto the space of Hankel matrices: $\tilde{\mathbf{S}} = \Pi_{\mathcal{H}} \hat{\mathbf{S}}$, and return to the series form: $\tilde{\mathbf{S}} = (\mathcal{T}^{(L)})^{-1} (\tilde{\mathbf{S}})$

Definition

Series X has rank $d < N/2$ in terms of SSA, if the rank of its L -trajectory matrix equals d for any L such that $d \leq \min(L, N - L + 1)$.

If such d exists, then X is called a series of finite rank.

If the signal S is a series of finite rank, then it is generally recommended to use $\text{rank}(S)$ as parameter r in the SSA method

Series rank examples

- rank of S with $s_n = A \exp(\alpha n)$, $\alpha \in \mathbb{C}$, equals 1
- rank of S with $s_n = A \sin(2\pi\omega n + \varphi)$, $0 < \omega < 1/2$, equals 2

Signal Model

What we consider a signal $S = (s_1, s_2, \dots, s_N)$:

- The trajectory matrix $\mathbf{S} = \mathcal{T}^{(L)}(S)$ is rank-deficient (\implies the time series is of some finite rank: $\text{rank}(\mathbf{S}) = r$)
- Any signal S can be represented in the form of a finite sum:

$$s_n = \sum_j p_j(n) \exp(\alpha_j n + i2\pi\omega_j n),$$

where $p_j(n)$ is a polynomial in n

- Real case:

$$s_n = \sum_j p_j(n) \exp(\alpha_j n) \sin(2\pi\omega_j n + \varphi_j),$$

ESPRIT method estimates factors α_j and frequencies ω_j

ESPRIT Algorithm: General Idea

Consider a signal S with elements s_n :

$$s_n = \sum_{j=1}^2 \exp(\alpha_j n + i(2\pi\omega_j n + \varphi_j)) = A_1 z_1^n + A_2 z_2^n$$

where $A_j = \exp(i\varphi_j)$, $z_j = \exp(\alpha_j + i2\pi\omega_j)$

Signal subspace basis is given by

$$\mathbf{M} = \begin{pmatrix} z_1 & z_2 \\ z_1^2 & z_2^2 \\ \vdots & \vdots \\ z_1^L & z_2^L \end{pmatrix} \Rightarrow \overline{\mathbf{M}} = \underline{\mathbf{M}} \begin{pmatrix} z_1 & \\ & z_2 \end{pmatrix} \Rightarrow \underline{\mathbf{M}}^- \overline{\mathbf{M}} = \begin{pmatrix} z_1 & \\ & z_2 \end{pmatrix}$$

where $\overline{\mathbf{M}}$ denotes \mathbf{M} without the first row, $\underline{\mathbf{M}}$ — without the last row
 $\underline{\mathbf{M}}^-$ denotes the pseudoinverse of $\underline{\mathbf{M}}$

Input: same as in SSA: \mathbf{X} , L , r

① **Embedding.** $\mathbf{X} = \mathcal{T}^{(L)}(\mathbf{X})$

② **Decomposition.** $\mathbf{X} = \sum_{j=1}^{\text{rank } \mathbf{X}} \sqrt{\lambda_j} U_j V_j^H$, $\mathbf{U}_r = [U_1 : U_2 : \dots : U_r]$

③ **Estimation.** Finding eigenvalues z_j of matrix $\underline{\mathbf{U}}_r^- \overline{\mathbf{U}}_r$

From $z_j = \exp(\alpha_j + i2\pi\omega_j)$ parameters α_j and ω_j can be found

Multi-Channel Time Series, MSSA

$$\mathbf{X} = (\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \dots, \mathbf{X}^{(P)}), \quad \mathbf{X}^{(p)} = (x_1^{(p)}, x_2^{(p)}, \dots, x_N^{(p)}) - \text{channels}$$

The only change in the algorithms — Embedding step:

$$\mathbf{X} = \mathcal{T}_{\text{MSSA}}^{(L)}(\mathbf{X}) = [\mathbf{X}^{(1)} : \mathbf{X}^{(2)} : \dots : \mathbf{X}^{(P)}],$$

$$\mathbf{X}^{(p)} = \mathcal{T}^{(L)}(\mathbf{X}^{(p)})$$

When to choose MSSA over SSA for each channel:

- All channels have “similar” structure
- “Supporting” channels with lower noise level

MSSA Trajectory Matrix

$$\mathbf{X} = (\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \dots, \mathbf{X}^{(P)}), \quad \mathbf{X}^{(p)} = (x_1^{(p)}, x_2^{(p)}, \dots, x_N^{(p)})$$

$$\mathbf{X} = \mathcal{T}_{\text{MSSA}}^{(L)}(\mathbf{X}) =$$

$$\left(\underbrace{\begin{pmatrix} x_1^{(1)} & x_2^{(1)} & x_3^{(1)} & \dots & x_K^{(1)} \\ x_2^{(1)} & x_3^{(1)} & x_4^{(1)} & \dots & x_{K+1}^{(1)} \\ x_3^{(1)} & x_4^{(1)} & x_5^{(1)} & \dots & x_{K+2}^{(1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_L^{(1)} & x_{L+1}^{(1)} & x_{L+2}^{(1)} & \dots & x_N^{(1)} \end{pmatrix}}_{\mathbf{X}^{(1)}} \left| \underbrace{\begin{pmatrix} x_1^{(2)} & x_2^{(2)} & x_3^{(2)} & \dots & x_K^{(2)} \\ x_2^{(2)} & x_3^{(2)} & x_4^{(2)} & \dots & x_{K+1}^{(2)} \\ x_3^{(2)} & x_4^{(2)} & x_5^{(2)} & \dots & x_{K+2}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_L^{(2)} & x_{L+1}^{(2)} & x_{L+2}^{(2)} & \dots & x_N^{(2)} \end{pmatrix}}_{\mathbf{X}^{(2)}} \right| \dots \right)$$

But why limit yourself to matrices?
Matrix is just a 2D tensor

Introducing Tensors to the Algorithm

Basic SSA: Time series $\mathbf{X} \mapsto$ Matrix $\mathbf{X} \mapsto \text{SVD}(\mathbf{X})$
Tensor SSA: Time series $\mathbf{X} \mapsto$ Tensor $\mathcal{X} \mapsto \underbrace{\text{TD}(\mathcal{X})}_{\text{Some Tensor Decomposition}}$

Tensor SVD Generalizations:

- Higher-Order SVD (HOSVD)
- Canonical Polyadic Decomposition (CPD)
- T-SVD
- $(L_r, L_r, 1)$ -Decomposition

Reminder: Trajectory Matrix

- Single-Channel:

$$\mathcal{T}^{(L)}(\mathbf{X}) = \begin{pmatrix} x_1 & x_2 & x_3 & \dots & x_K \\ x_2 & x_3 & x_4 & \dots & x_{K+1} \\ x_3 & x_4 & x_5 & \dots & x_{K+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_L & x_{L+1} & x_{L+2} & \dots & x_N \end{pmatrix}$$

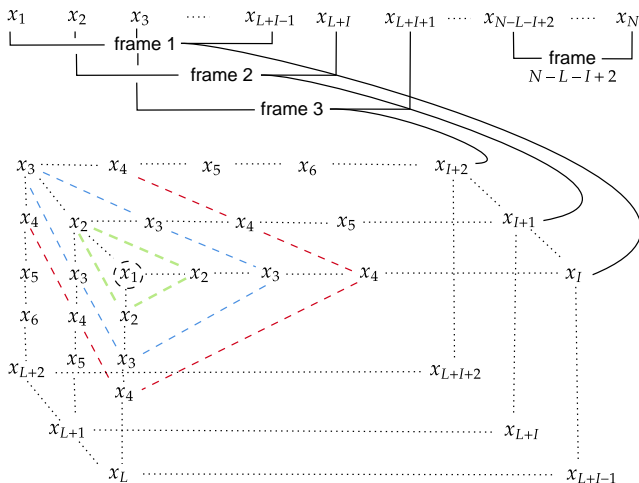
- Multi-Channel:

$$\mathcal{T}_{\text{MSSA}}^{(L)}(\mathbf{X}) = \left(\begin{array}{cccc|cccc|c} x_1^{(1)} & x_2^{(1)} & \dots & x_K^{(1)} & x_1^{(2)} & x_2^{(2)} & \dots & x_K^{(2)} & \dots \\ x_2^{(1)} & x_3^{(1)} & \dots & x_{K+1}^{(1)} & x_2^{(2)} & x_3^{(2)} & \dots & x_{K+1}^{(2)} & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \dots \\ x_L^{(1)} & x_{L+1}^{(1)} & \dots & x_N^{(1)} & x_L^{(2)} & x_{L+1}^{(2)} & \dots & x_N^{(2)} & \dots \end{array} \right)$$

Mapping Single-Channel Time Series to a Tensor

$$\mathbf{X} = (x_1, x_2, \dots, x_N)$$

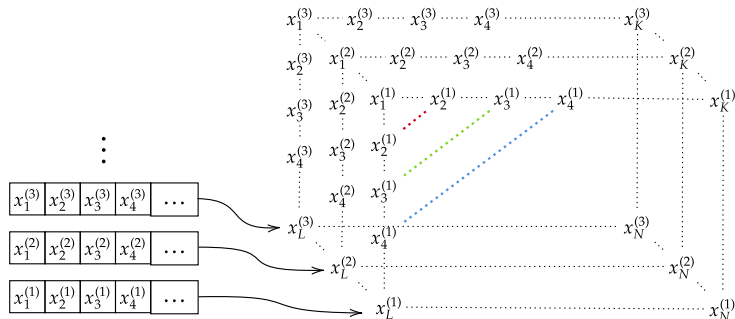
$$\mathbf{X} \mapsto \mathcal{T}_{\text{T-SSA}}^{(I,L)}(\mathbf{X}) = \mathcal{X} \in \mathbb{C}^{I \times L \times K}, K = N - I - L + 2$$



Mapping Multi-Channel Time Series to a Tensor

$$\mathbf{X} = (\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \dots, \mathbf{X}^{(P)}), \mathbf{X}^{(p)} = (x_1^{(p)}, x_2^{(p)}, \dots, x_N^{(p)})$$

$$\mathbf{X} \mapsto \mathcal{T}_{\text{T-MSSA}}^{(L)}(\mathbf{X}) = \mathcal{X} \in \mathbb{C}^{P \times L \times K}, K = N - L + 1$$



Some Tensor Decompositions

Unlike in matrix case, there exist several definitions of tensor ranks and SVD generalizations based on them.

Definition (Tensor rank)

Tensor \mathcal{A} has rank 1, if there exist vectors B , C and D such that $\mathcal{A} = B \circ C \circ D$, where \circ denotes an outer product.

Tensor \mathcal{A} has rank R , if it can be represented as a sum of R rank-1 tensors: $\mathcal{A} = \sum_{i=1}^R \mathcal{B}_i$, $\text{rank}(\mathcal{B}_i) = 1$, and such R is minimal.

The representation of a tensor as a sum of R rank-1 tensors is called **Canonical Polyadic Decomposition (CPD)**.

- Considered for signal extraction in [Kouchaki, Sanei (2013)]
- Does not provide any form of orthogonality of components
- Requires to know the tensor rank in advance
- No connection between signal SSA-rank and the rank of a trajectory tensor

Some tensor decompositions

Definition

n -mode vectors of a tensor \mathcal{A} are vectors obtained from \mathcal{A} by varying the index of the n -th direction and keeping the other indices fixed (analog of rows and columns of a matrix).

n -rank of a tensor \mathcal{A} , denoted by $R_n = \text{rank}_n(\mathcal{A})$, is the dimension of the linear space spanned by the n -mode vectors.

HOSVD: $\mathcal{A} = \sum_{i=1}^{R_1} \sum_{l=1}^{R_2} \sum_{k=1}^{R_3} z_{ilk} U_i^{(1)} \circ U_l^{(2)} \circ U_k^{(3)}$

- Considered for signal parameter estimation in [Papy et al. (2005)], [Papy et al. (2009)]
- Provides orthogonality of components
- Does not require any prior knowledge about tensor n -ranks
- There is a proven connection between number of components and signal SSA-rank

Higher-Order SVD. Higher-Order Orthogonal Iterations

$$\text{SVD}(\mathbf{X}) = \sum_{j=1}^{\text{rank}(\mathbf{X})} \sqrt{\lambda_j} U_j V_j^H$$

$$\text{HOSVD}(\mathcal{X}) = \sum_{i=1}^{\text{rank}_1(\mathcal{X})} \sum_{l=1}^{\text{rank}_2(\mathcal{X})} \sum_{k=1}^{\text{rank}_3(\mathcal{X})} z_{ilk} U_i^{(1)} \circ U_l^{(2)} \circ U_k^{(3)}$$

- $\tilde{\mathbf{X}} = \sum_{j=1}^R \dots \Rightarrow \left\| \mathbf{X} - \tilde{\mathbf{X}} \right\|_F = \min_{\text{rank}(\hat{\mathbf{X}}) \leq R} \left\| \mathbf{X} - \hat{\mathbf{X}} \right\|_F$
- $\tilde{\mathcal{X}} = \sum_{i=1}^{R_1} \sum_{l=1}^{R_2} \sum_{k=1}^{R_3} \dots \Rightarrow \left\| \mathcal{X} - \tilde{\mathcal{X}} \right\|_F \geq \min_{\text{rank}_m(\hat{\mathcal{X}}) \leq R_m} \left\| \mathcal{X} - \hat{\mathcal{X}} \right\|_F$

Truncation of SVD is optimal, but truncation of HOSVD is not

Iterative algorithm for finding optimal approximation – HOOI

T-SSA, T-MSSA and T-ESPRIT with HOSVD

Input: time series X , window length: (I, L) for single-channel or L for multi-channel, signal ranks (r_1, r_2, r_3) , d — estimation dimension for HO-ESPRIT.

① Embedding.	Single-channel	$X \mapsto \mathcal{T}_{\text{T-SSA}}^{(I,L)}(X) = \mathcal{X}$
	Multi-channel	$X \mapsto \mathcal{T}_{\text{T-MSSA}}^{(L)}(X) = \mathcal{X}$

② **Decomposition & Approximation.** Using (r_1, r_2, r_3)
 $\mathcal{X} \mapsto \text{Trunc}(\text{HOSVD}(\mathcal{X})) = \tilde{\mathcal{S}}$ or $\mathcal{X} \mapsto \text{HOOI}(\mathcal{X}) = \tilde{\mathcal{S}}$

③ **Reconstruction or Estimation.**

- **Reconstruction.** $S = \mathcal{T}^{-1} \left(\Pi_{\mathcal{H}_T}(\tilde{\mathcal{S}}) \right)$, $\Pi_{\mathcal{H}_T}$ — projector onto the space of Hankel tensors
- **Estimation.** Finding eigenvalues z_j of matrix $\underline{U}^{-} \overline{U}$, where $\underline{U} = \underline{U}_d = \left[U_1^{(d)} : U_2^{(d)} : \dots : U_{r_d}^{(d)} \right]$. From $z_j = \exp(\alpha_j + i2\pi\omega_j)$ factors α_j and frequencies ω_j of the signal can be found

Single-Channel Series Comparison

$$x_n = e^{\alpha_1 n} e^{2\pi i \omega_1 n} + e^{\alpha_2 n} e^{2\pi i \omega_2 n} + \zeta_n$$

ζ_n — Complex white gaussian noise, $D(\zeta_n) = 0.04^2$, $\omega_1 = 0.2$, $\omega_2 = 0.22$, $\alpha_1 = \alpha_2 = 0$ (same results for $\alpha_1 = \alpha_2 < 0$ and $\alpha_1 < \alpha_2 < 0$).

RMSE results with respect to parameters choice:

- Parameters estimation

	Best	Worst	Mean
T-ESPRIT	0.0012	0.0033	0.0016
ESPRIT	0.0013	0.0140	0.0031

T-method is better

- Signal extraction

	Best	Worst	Mean
T-SSA	0.019	0.024	0.020
SSA	0.018	0.031	0.021

T-method is worse with optimal parameter choice.

Multi-Channel Series Comparison

$$x_n^{(m)} = a_1^{(m)} e^{2\pi i \omega_1 n} + a_2^{(m)} e^{2\pi i \omega_2 n} + \zeta_n^{(m)},$$

$\zeta_n^{(m)}$ — Complex white gaussian noise, $D(\zeta_n^{(m)}) = 0.2^2$,
 $\omega_1 = 0.2, \omega_2 = 0.22$

RMSE results with respect to parameters choice:

- Parameters estimation

	Best	Worst	Average
T-M-ESPRIT	5.33e-04	9.99e-04	6.16e-04
M-ESPRIT	5.36e-04	1.80e-03	7.13e-04

T-method is better

- Signal extraction

	Best	Worst	Average
T-MSSA	0.065	0.068	0.066
MSSA	0.066	0.152	0.086

T-method is better

Dstack Modifications

Possible problem for ESPRIT: components with close frequencies can mix into one in the presence of noise. Solution: using Dstack mapping.

Consider $\mathbf{X} = (x_1, x_2, \dots, x_N)$, $M = \lfloor N/D \rfloor$, then

$$\text{Dstack}_D(\mathbf{X}) = \mathcal{D}_D(\mathbf{X}) = \left[\begin{array}{c|c|c|c} x_1 & x_2 & \dots & x_D \\ x_{D+1} & x_{D+2} & \dots & x_{2D} \\ x_{2D+1} & x_{2D+2} & \dots & x_{3D} \\ \vdots & \vdots & \dots & \vdots \\ x_{(M-1)D+1} & x_{(M-1)D+2} & \dots & x_{MD} \end{array} \right]$$

$\underbrace{\hspace{10em}}_{\mathbf{X}_D^{(1)}}$

$\underbrace{\hspace{10em}}_{\mathbf{X}_D^{(2)}}$

$\underbrace{\hspace{10em}}_{\mathbf{X}_D^{(D)}}$

Dstack-SSA	$\mathbf{X} \mapsto \mathbf{X} = \mathcal{T}_{\text{MSSA}}^{(L)}(\mathcal{D}_D(\mathbf{X}))$
Dstack-T-SSA	$\mathbf{X} \mapsto \mathcal{X} = \mathcal{T}_{\text{T-MSSA}}^{(L)}(\mathcal{D}_D(\mathbf{X}))$

Undersampling: $\omega \mapsto \hat{\omega} = D\omega \implies |\omega| \leq \frac{1}{2D}$ is required

Single-Channel Series Comparison with Dstack

$$x_n = \cos(2\pi\omega_1 n) + \cos(2\pi\omega_2 n) + \xi_n$$

$\omega_1 = 0.02$, $\omega_2 = 0.0205$, ξ_n — white gaussian noise, $D(\xi_n) = \sigma^2$

RMSE results with respect to parameters choice:

- Parameters estimation, $\sigma = 0.2$

	Best	Worst	Average
ESPRIT	4.98e-05	5.66e-05	5.32e-05
Dstack-ESPRIT	5.30e-05	7.63e-05	6.24e-05
T-Dstack-ESPRIT	5.40e-05	6.24e-05	5.86e-05

T-method
is worse

- Parameters estimation, $\sigma = 0.6$

	Best	Worst	Average
ESPRIT	0.101	0.138	0.115
Dstack-ESPRIT	0.009	0.011	0.010
T-Dstack-ESPRIT	0.003	0.005	0.004

T-method is better

Single-Channel Series Comparison with Dstack

$$x_n = \cos(2\pi\omega_1 n) + \cos(2\pi\omega_2 n) + \xi_n$$

$\omega_1 = 0.02$, $\omega_2 = 0.0205$, ξ_n — white gaussian noise, $D(\xi_n) = \sigma^2$

RMSE results with respect to parameters choice:

- Signal extraction, $\sigma = 0.2$

	Best	Worst	Average
SSA	0.020	0.021	0.021
Dstack-SSA	0.052	0.066	0.057
T-Dstack-SSA	0.050	0.052	0.051

T-method is worse

- Signal extraction, $\sigma = 0.6$

	Best	Worst	Average
SSA	0.086	0.095	0.090
Dstack-SSA	0.175	0.208	0.189
T-Dstack-SSA	0.175	0.179	0.178

T-method is worse

Conclusions

- Using High-Order SVD tensor decompositions instead of matrix SVD appears to be a more natural extension of the tensor that serves signal ranks. However, even in this case, truncation is not optimal for approximation, and ranks in different directions may differ.
- HO-SSA is a natural extension of SSA, as are HO-M-SSA (signal extraction) and HO-ESPRIT and HO-M-ESPRIT (frequency estimation).
- For optimal parameters, the accuracy of the tensor and matrix SSA/ESPRIT versions is comparable. The advantage of tensor-based methods is that they are generally less dependent on parameter choice (the worst and best parameter sets provide errors of the same order). However, the drawback is the complexity of tensor decompositions.
- The HO-extension has fewer advantages for extracting one-dimensional signals. Therefore, this usage is not recommended.
- Tensor methods using Dstack mapping can be useful for estimating parameters in the presence of strong noise.

$$\mathcal{X} \in \mathbb{C}^{I \times L \times K}, \mathbf{X} \in \mathbb{C}^{\hat{L} \times \hat{K}}, I < L < K, \hat{L} < \hat{K}, \\ I + L + K = N + 2, \hat{L} + \hat{K} = N + 1$$

- **SVD**(\mathbf{X}):
 $O(\hat{L}^2 \hat{K})$,
or $O(r \hat{L} \hat{K})$ if only need r -rank approximation,
or $O(rN \log(N))$ if \mathbf{X} is Hankel
- **HOSVD**(\mathcal{X}):
 $O(ILKN)$,
or $O(ILK(r_1 + r_2 + r_3))$ if only need (r_1, r_2, r_3) -rank approximation,
or $O((r_1 + r_2 + r_3)I(L + K) \log(L + K))$ if \mathcal{X} is Hankel