Shaped extensions of Singular Spectrum Analysis

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Outline

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Common scheme of Singular Spectrum Analysis (SSA)

Input: time series or array (or something else) $\mathbb{X} \in \mathsf{X} \sim \mathsf{R}^N$
Parameter: embedding operator $\mathcal{T} \colon \mathsf{X} \hookrightarrow \mathsf{R}^{L \times K}$, injective, linear

Decomposition

1. Embedding
   Trajectory matrix $\mathbf{X} = \mathcal{T}(\mathbb{X})$, structured (i.e. $\mathbf{X} \in \mathsf{H} = \operatorname{image} \mathcal{T}$)
2. Singular Value Decomposition (SVD)
   $$\mathbf{X} = \sum_{k=1}^{d} \sqrt{\lambda_k} U_k V_k^{\mathrm{T}}, \ \{U_k\}_{k=1}^{d} \text{ and } \{V_k\}_{k=1}^{d} \text{ are orthonormal}$$

Reconstruction

1. Grouping: $\{1, \dots, d\} = I_1 \sqcup \dots \sqcup I_c$
   $\mathbf{X} = \mathbf{X}_{I_1} + \dots + \mathbf{X}_{I_c}$, where $\mathbf{X}_I = \sum_{k \in I} \sqrt{\lambda_k} U_k V_k^{\mathrm{T}}$
2. Projection
   Matrix $\mathbf{X}_I \xrightarrow{\mathcal{H} = \Pi^{(\mathsf{H})}}$ structured matrix $\widetilde{\mathbf{X}}_I \xrightarrow{\mathcal{T}^{-1}}$ reconstructed $\widetilde{\mathbb{X}}^{(I)}$

Output: $\mathbb{X} = \widetilde{\mathbb{X}}^{(I_1)} + \dots + \widetilde{\mathbb{X}}^{(I_c)}$

Particular SSA cases: Classical 1D-SSA

Input: time series $\mathbb{X} = (x_1, x_2, \dots, x_N)$
Parameter: L, window length; $1 < L < N$; $K = N - L + 1$

The embedding operator:

$$\mathcal{T}(\mathbb{X}) = \mathcal{T}_L(\mathbb{X}) := [X_1 : \dots : X_K] = \begin{pmatrix} x_1 & x_2 & \dots & x_{K-1} & x_K \\ x_2 & \iddots & \dots & \iddots & x_{K+1} \\ \vdots & \vdots & & \vdots & \vdots \\ x_{L-1} & \iddots & \dots & \iddots & x_{N-1} \\ x_L & x_{L+1} & \dots & x_{N-1} & x_N \end{pmatrix},$$

where the columns X_j are lagged subvectors of length L:

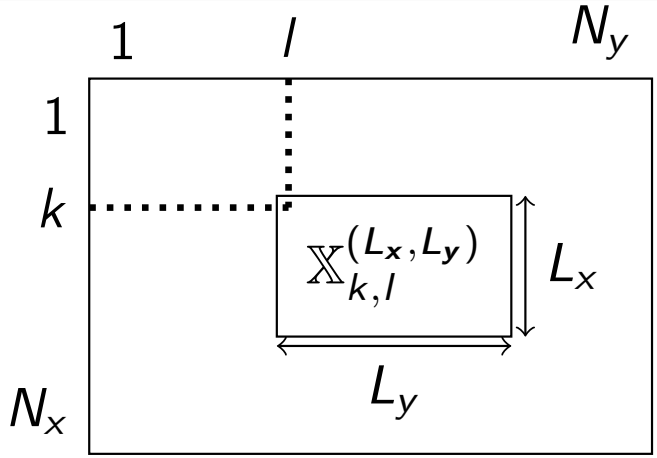
$$X_j = (x_j, x_{j+1}, \dots, x_{j+L-1})^{\mathrm{T}}$$

- $\mathsf{H} = \operatorname{image} \mathcal{T}_L$ is the set of Hankel matrices
- Projection $\Pi^{(\mathsf{H})}$ is diagonal averaging (or "hankelization")

Particular SSA cases: 2D-SSA

Input: 2D array $\mathbb{X} = \begin{pmatrix} x_{1,1} & \dots & x_{1,N_y} \\ \vdots & & \vdots \\ x_{N_x,1} & \dots & x_{N_x,N_y} \end{pmatrix}$

Parameters: window sizes L_x, L_y;
$1 < L_x < N_x$; $1 < L_y < N_y$;
$K_x = N_x - L_x + 1$; $K_y = N_y - L_y + 1$;



The embedding operator:

$$\mathcal{T}_{L_x,L_y}(\mathbb{X}) := \mathbf{X} = [X_1 : \dots : X_{K_xK_y}] \in \mathrm{R}^{L_xL_y \times K_xK_y},$$

where the columns X_j are vectorizations of shifted $L_x \times L_y$ subarrays:

$$X_{k+(l-1)K_x} = \mathrm{vec}(\mathbb{X}_{k,l}^{(L_x,L_y)})$$

- $\mathrm{H} = \mathrm{image}\,\mathcal{T}_{L_x \times L_y}$ is the set of Hankel-block-Hankel matrices
- Projection $\Pi^{(\mathrm{H})}$ is "block-hankelization" (also averaging)

Note: $\mathrm{R}^{L_x \times L_y} \sim \mathrm{R}^{L_xL_y}$, *thus any singular vector U can be considered as $L_x \times L_y$ array $\mathbb{U}$*

2D-SSA example: Gentlemen

Eigenvectors

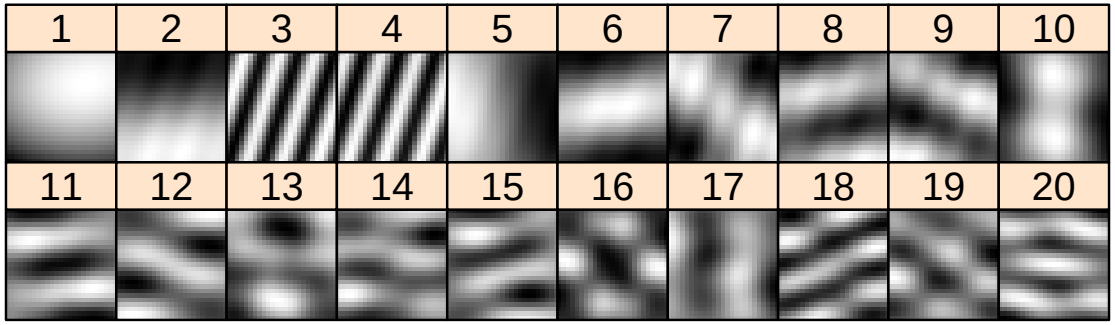


Figure: Gentlemen, 2D-SSA: Eigenarrays, $(L_x, L_y) = (25, 25)$

Reconstructions

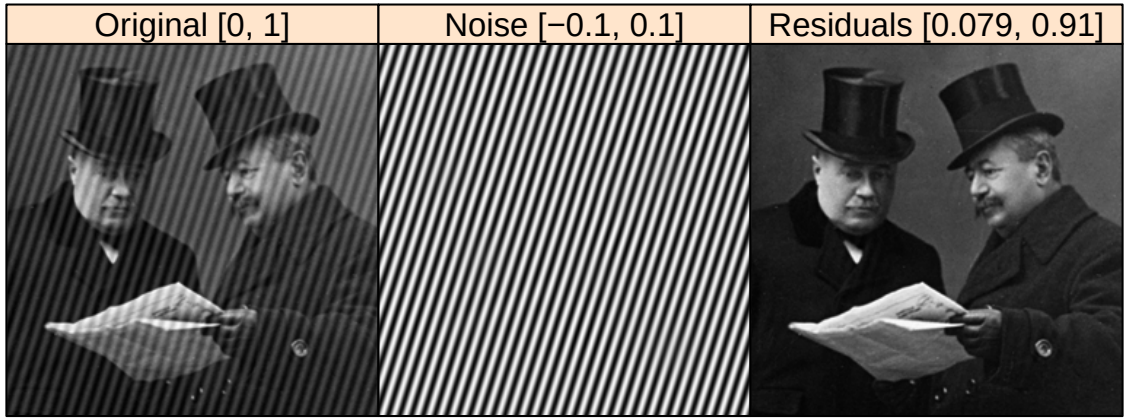


Figure: Gentlemen, 2D-SSA: Separated periodic noise, $(N_x, N_y) = (256, 256)$, $(L_x, L_y) = (25, 25)$, $I = \{3, 4\}$

Outline

Problem: non-rectangular arrays & edge effects

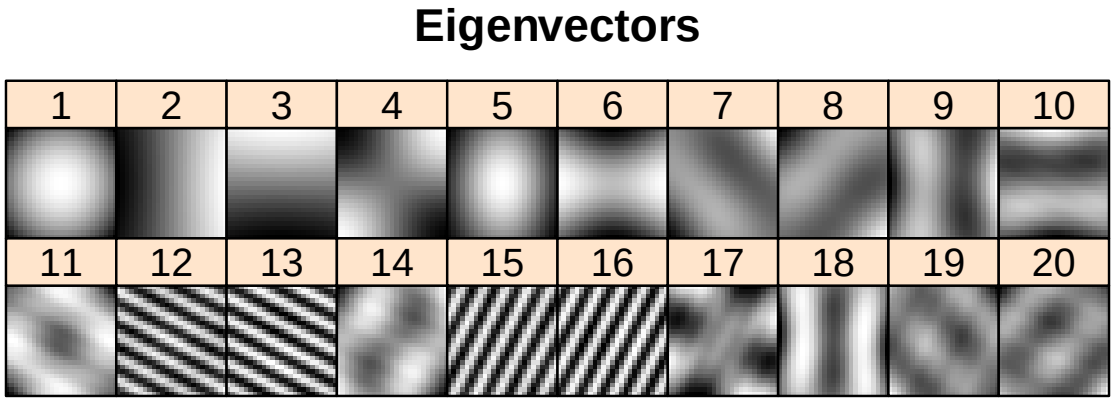


Figure: Mars, 2D-SSA: Eigenarrays, $(L_x, L_y) = (25, 25)$

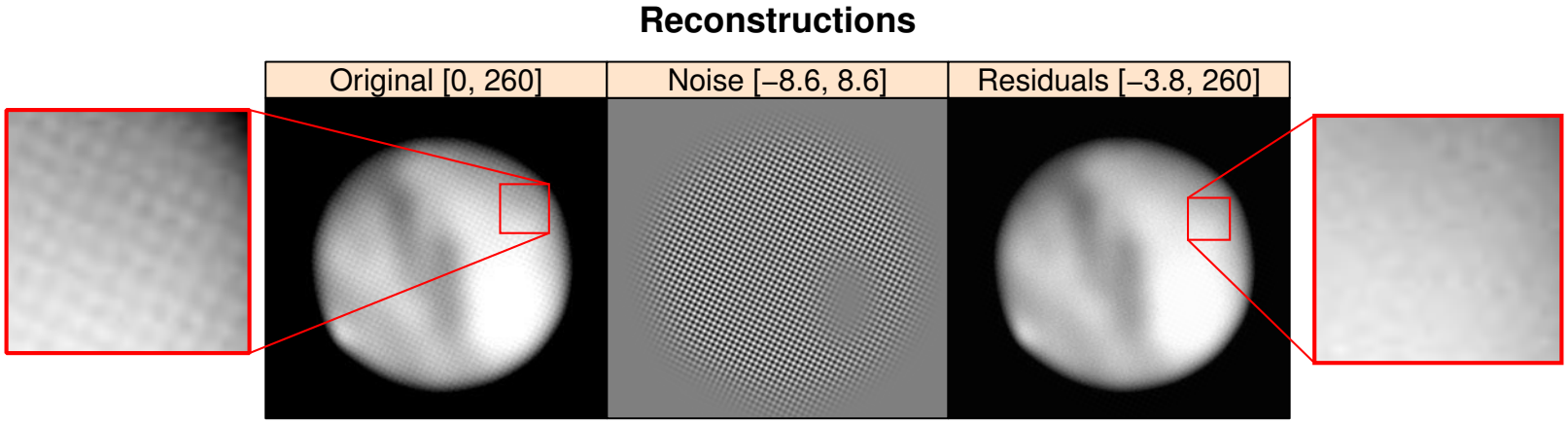
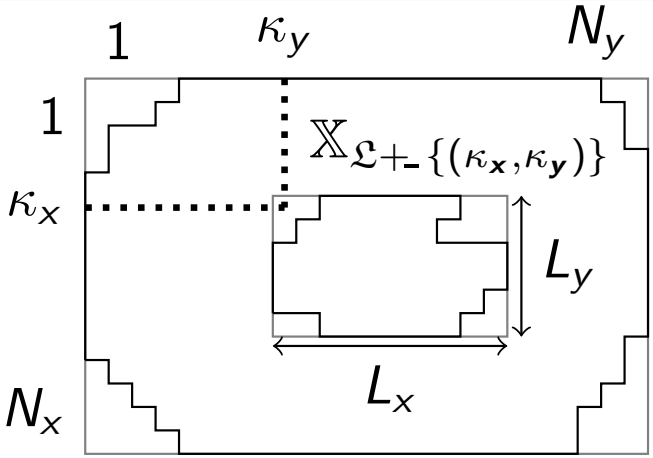


Figure: Mars, 2D-SSA: Separated periodic noise, $(N_x, N_y) = (258, 275)$, $(L_x, L_y) = (25, 25)$, $I = \{12, 13, 15, 16\}$

Let's develop "shaped" SSA, by analogy with shaped filters

New method: Shaped 2D-SSA

Input: $\mathfrak{N}$-shaped array $\mathbb{X} = \mathbb{X}_{\mathfrak{N}} = (x_\eta)_{\eta\in\mathfrak{N}}$, where $\mathfrak{N} = \{\eta_1, \dots, \eta_N\} \subseteq \{1, \dots, N_x\} \times \{1, \dots, N_y\}$
Parameter: window shape $\mathfrak{L} = \{\ell_1, \dots, \ell_L\} \subseteq$
$\subseteq \{1, \dots, L_x\} \times \{1, \dots, L_y\}$



The embedding operator:

$$\mathcal{T}_{\mathfrak{L}}(\mathbb{X}) := \mathbf{X} = [X_1 : \cdots : X_K] \in \mathsf{R}^{L\times K},$$

where columns $X_j = (x_{\ell_i +\!\!- \kappa_j})_{i=1}^{L}$ are vectorizations of shifted $\mathfrak{L}$-shaped arrays $\mathbb{X}_{\mathfrak{L}+\!\!-\{\kappa_j\}} = (x_\eta)_{\eta\in\mathfrak{L}+\!\!-\{\kappa_j\}}$

And $\mathfrak{K}$ is the set of all possible origin positions for $\mathfrak{L}$-shaped windows:

$$\mathfrak{K} = \{\kappa_1, \dots, \kappa_K\} = \{\kappa \in \mathsf{N}^2 \mid \mathfrak{L} +\!\!- \{\kappa\} \subseteq \mathfrak{N}\},$$

where $\cdot +\!\!- \eta$ means shape shift by vector η: $\mathfrak{A} +\!\!- \eta := \{\alpha + \eta - 1 \mid \alpha \in \mathfrak{A}\}$

- $\mathsf{H} = \operatorname{image} \mathcal{T}_{\mathfrak{L}}$ is the set of quasi-Hankel matrices
- Projection $\Pi^{(\mathsf{H})}$ is "quasi-hankelization" (again, averaging)

Note: $\mathsf{R}^{\mathfrak{L}} \sim \mathsf{R}^{L}$, *thus any singular vector U can be considered as $\mathfrak{L}$-shaped subarray $\mathbb{U}$*

Real life examples: Mars

Eigenvectors

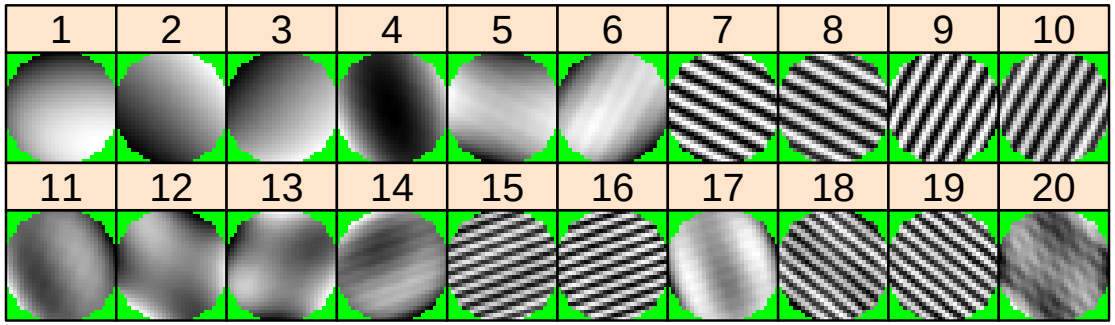


Figure: Mars, ShSSA: Eigenarrays, $\mathfrak{L}$ is circle of radius 15

Reconstructions

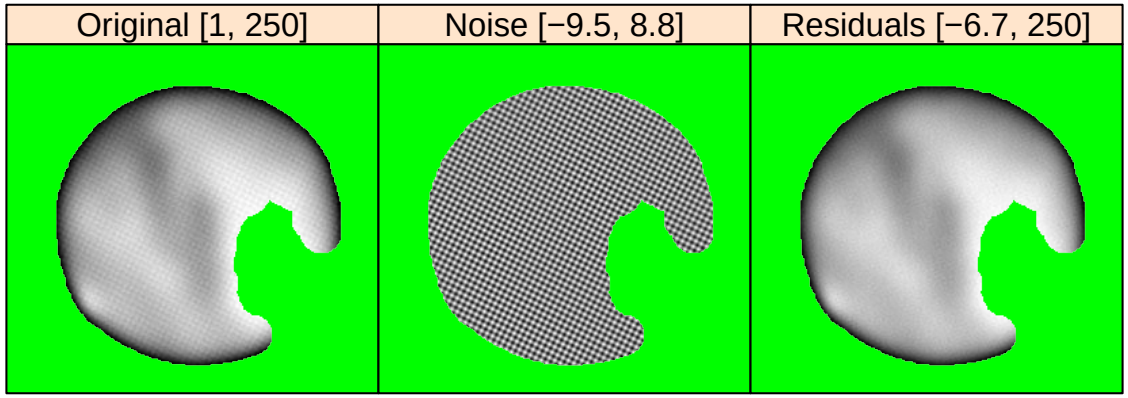


Figure: Mars: Separated period noise, $\mathfrak{L}$ is circle of radius 15, $I = \{7, 8, 9, 10\}$

Comparison: shaped vs non-shaped

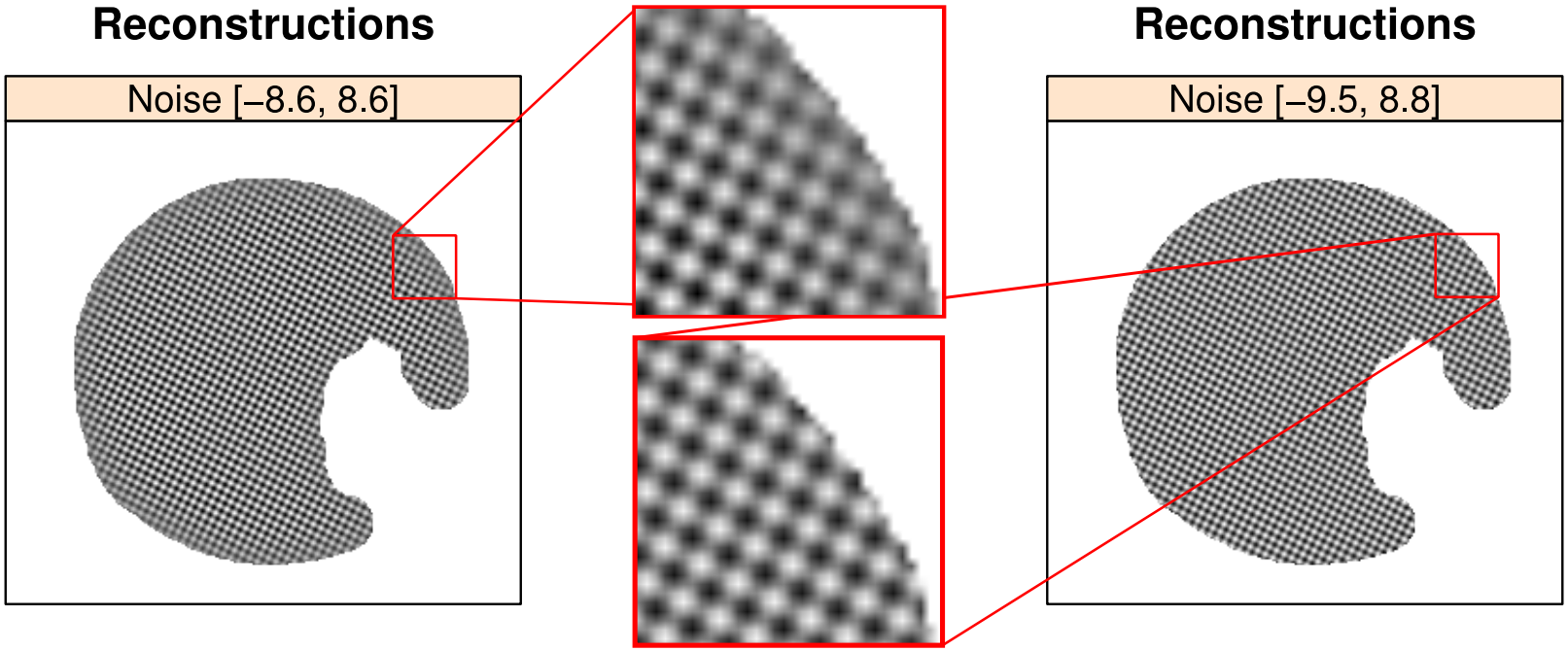


Figure: Left: cutted image of periodic noise from rectangular SSA; right: image of periodic noise from Shaped SSA

Outline

Problem: circular topology

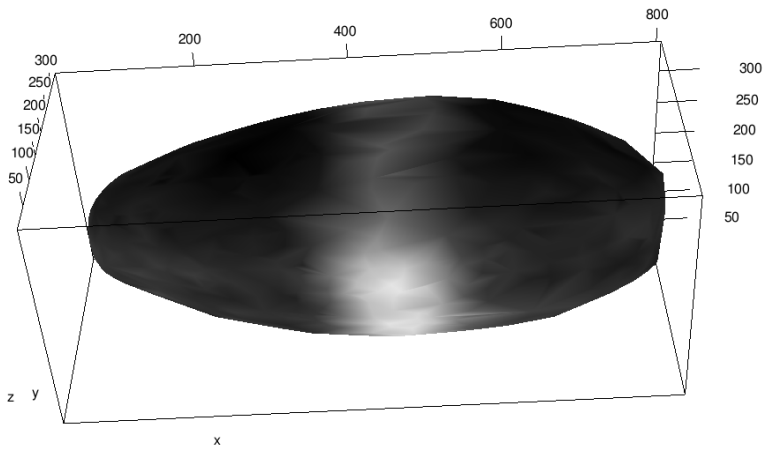
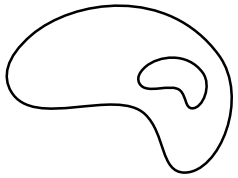
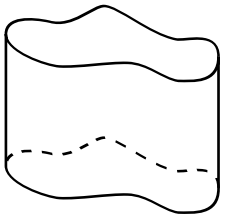


Figure: Drosophila, 3d intensity plot, "Krüppel" gene

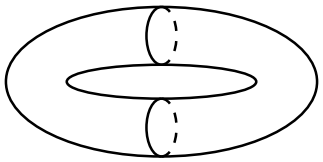
Three topology cases:



(a) Planar topology ($T_x = T_y = \infty$)



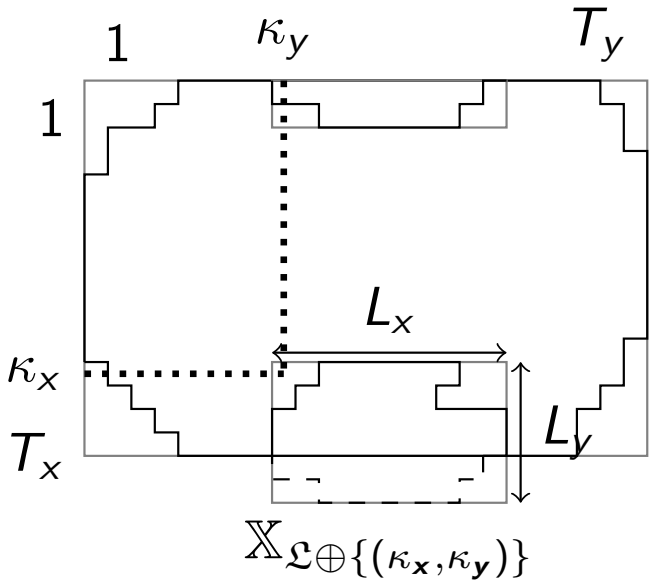
(b) Cylindrical topology ($T_x \neq \infty$; $T_y = \infty$)



(c) Toroidal topology ($T_x \neq \infty$; $T_y \neq \infty$)

New method: Circular Shaped 2D-SSA

Input: topology characteristics $T_x, T_y \in \mathsf{N} \cup \{\infty\}$, $\mathfrak{N}$-shaped array $\mathbb{X} = \mathbb{X}_{\mathfrak{N}} = (x_\eta)_{\eta \in \mathfrak{N}}$, where $\mathfrak{N} = \{\eta_1, \dots, \eta_N\} \subseteq \{1, \dots, T_x\} \times \{1, \dots, T_y\}$
Parameter: window shape $\mathfrak{L} = \{\ell_1, \dots, \ell_L\} \subseteq$
$\subseteq \{1, \dots, L_x\} \times \{1, \dots, L_y\}$



The embedding operator:

$$\mathcal{T}_{\mathfrak{L}}(\mathbb{X}) := \mathbf{X} = [X_1 : \cdots : X_K] \in \mathsf{R}^{L \times K},$$

where columns $X_j = (x_{\ell_i +\!\!- \kappa_j})_{i=1}^{L}$ are vectorizations of shifted $\mathfrak{L}$-shaped arrays

And $\mathfrak{K}$ is the set of all possible origin positions for $\mathfrak{L}$-shaped windows:

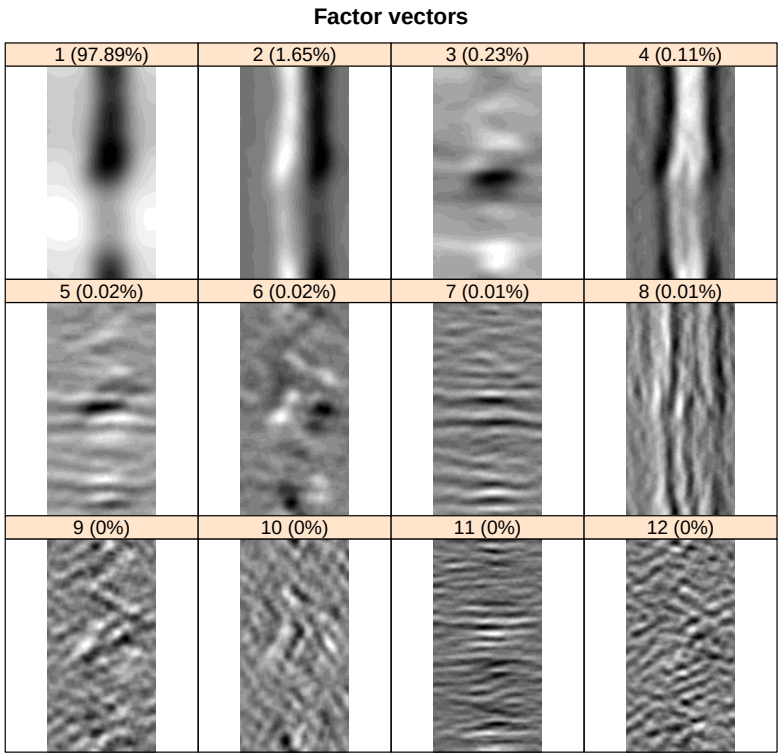
$$\mathfrak{K} = \{\kappa_1, \dots, \kappa_K\} = \{\kappa \in \mathsf{N}^2 \mid \mathfrak{L} \oplus \{\kappa\} \subseteq \mathfrak{N}\},$$

where $\cdot \oplus \eta$ means cycled shape shift by vector η:

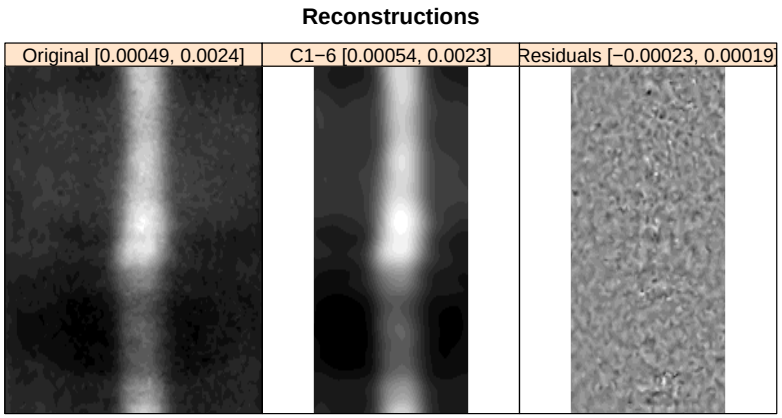
$$\mathfrak{A} \oplus \eta := \{((\alpha_x + \eta_x - 2) \bmod T_x + 1, (\alpha_y + \eta_y - 2) \bmod X_y + 1) \mid \alpha \in \mathfrak{A}\}$$

- $\mathsf{H} = \operatorname{image} \mathcal{T}_{\mathfrak{L}}$ is the set of partially circulant quasi-Hankel matrices
- Projection $\Pi^{(\mathsf{H})}$ is "quasi-hankelization" (and again, averaging)

Real life example: drosophila embryo



(d) Drosophila, factor vectors



(e) Drosophila, reconstruction and residuals

Figure: Drosophila, Circular SSA, cylindrical case ($T_x = N_x$ and $T_y = \infty$).
The data are downloaded from the BDTNP archive,
the file "v5_s11643-28no06-04.pca", gene "Krüppel".
Middle part from 20% to 80% of the embryo length was processed.
Interpolation step is 0.5% and both window sizes are 10% of the embryo length

Outline

2D-ESPRIT for shaped array

Parametric model: corrupted finite-rank array:
$(\mathbb{S})_{l,n} = \sum_{k=1}^{r} A_k \mu_k^l \nu_k^n, \quad A_k, \mu_k, \nu_k \in \mathrm{C}\backslash\{0\}$
$\mathbb{X} = \mathbb{S} + \mathbb{R}$, where $\mathbb{R}$ is noise or another signal

Problem: estimate nonlinear parameters $\{(\mu_k, \nu_k)\}_{k=1}^{r}$

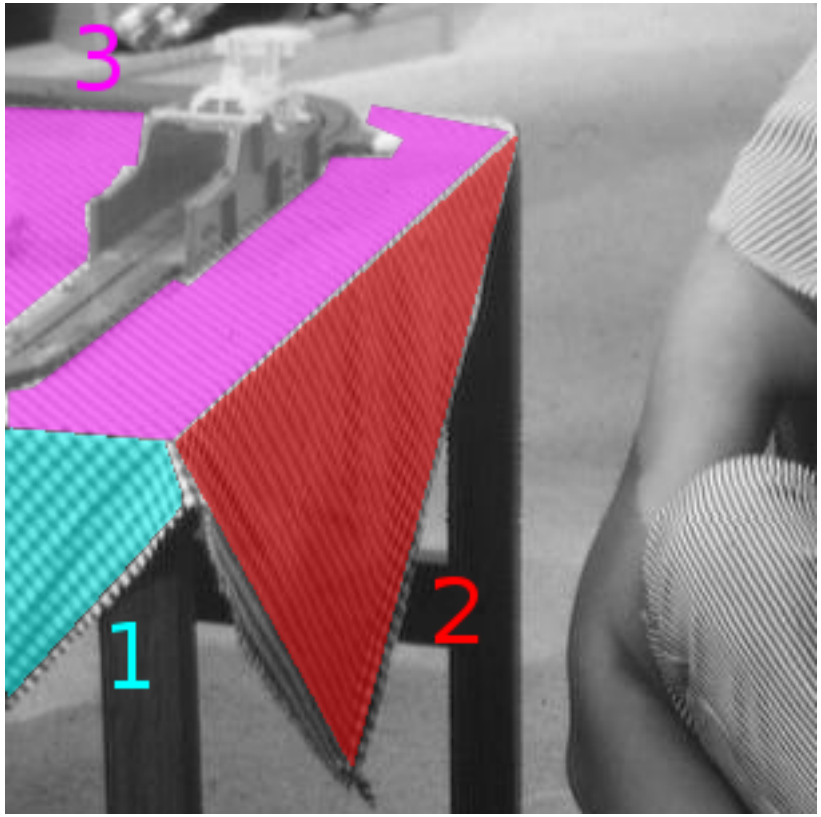
Algorithm rectangular 2D-ESPRIT (Rouquette and Najim, 2001):

1. **Estimation of the signal subspace:** Get the basis $\mathbb{U}_{i_1}, \ldots, \mathbb{U}_{i_r}$ of an estimate of signal subspace (e.g. from SSA)
2. **Construction of truncated matrices:**
   $\mathbf{P}_x = [\mathrm{vec}\,(\underline{\mathbb{U}_{i_1}}) : \cdots : \mathrm{vec}\,(\underline{\mathbb{U}_{i_r}})]$, $\mathbf{Q}_x = [\mathrm{vec}\,(\overline{\mathbb{U}_{i_1}}) : \cdots : \mathrm{vec}\,(\overline{\mathbb{U}_{i_r}})]$,
   $\mathbf{P}_y = [\mathrm{vec}\,(\mathbb{U}_{i_1}|) : \cdots : \mathrm{vec}\,(\mathbb{U}_{i_r}|)]$, $\mathbf{Q}_y = [\mathrm{vec}\,(|\mathbb{U}_{i_1}) : \cdots : \mathrm{vec}\,(|\mathbb{U}_{i_r})]$,
   where $(\underline{\cdot})$, $(\overline{\cdot})$, $(\cdot|)$, $(|\cdot)$ denote the array without last row, first row last column and first column respectively
3. **Construction of shift matrices:** Approximate solution of $\mathbf{P}_x\mathbf{M}_x \approx \mathbf{Q}_x$ and $\mathbf{P}_y\mathbf{M}_y \approx \mathbf{Q}_y$ in LS- or TLS-sense
4. **Estimation of the parameters:** EVD-decomposition of $\mathbf{M}_x$ and $\mathbf{M}_y$, eigenvalues $\widehat{\mu}_i$ and $\widehat{\nu}_j$ is an estimates of the parameters

This talk: from rectangular to shaped arrays

Real life example: Barbara's cloth

(a) Barbara, whole image



(b) Barbara, table with enumerated subimages

Real life example: Barbara's cloth

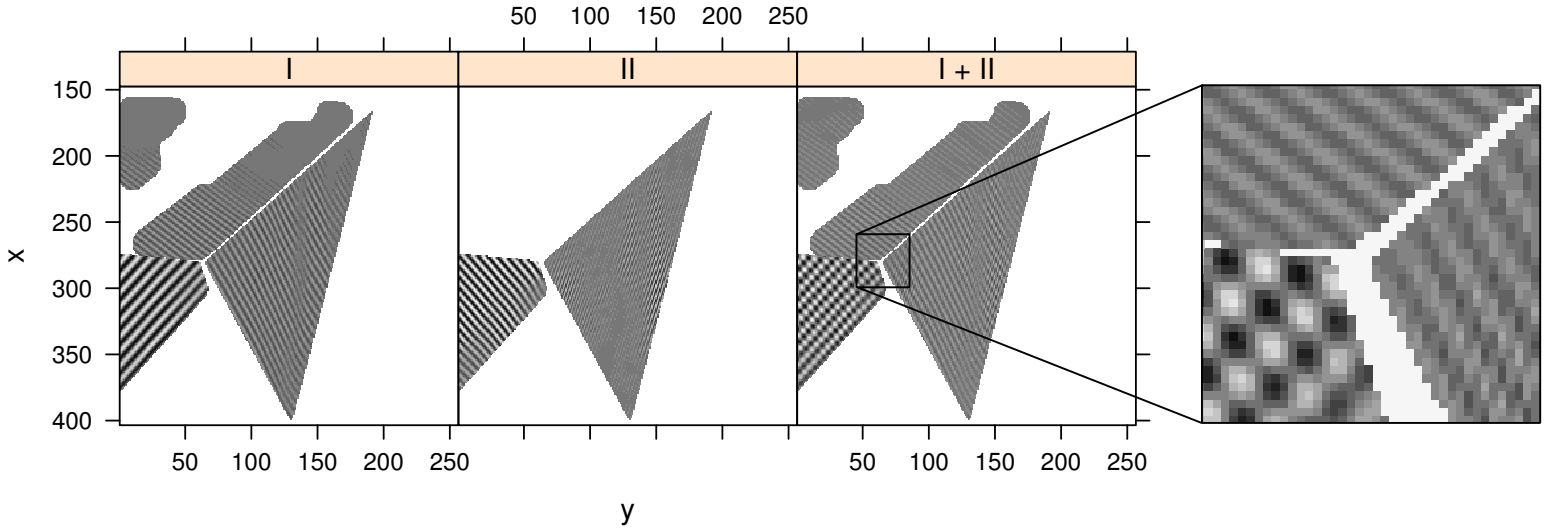


Figure: Barbara's table: reconstructions of texture.
$I_{\mathrm{I}} = \{2, 3\}$, $I_{\mathrm{II}} = \{4, 5\}$ (if present)

Table: Barbara, ESPRIT periods and rates

Part	t_x	t_y	Width	$\alpha,^\circ$	Rate_x	Rate_y
1	8.1	6.9	5.2	50	−0.0066	−0.0061
1	11.0	10.1	7.4	47	−0.0022	−0.0064
2	9.7	5.0	4.4	63	−0.0031	−0.0075
2	7.2	2.6	2.5	70	0.0025	0.017
3	5.1	6.8	4.1	37	0.0054	−0.0046

Outline

Efficient implementation

Main ideas:

1. The truncated SVD calculated by Lanczos methods is used, since only a number of leading SVD components correspond to the signal (ν-`TRLan` and `PROPACK` libraries are used)
2. In Lanczos methods, only multiplication of $\mathbf{X}$ (and $\mathbf{X}^{\mathrm{T}}$) by a vector is needed. Due to quasi-Hankel structure it can be implemented via FFT (`FFTW` library is used)
3. At the Reconstruction step, hankelization or quasi-hankelization of a matrix of rank 1 can be also implemented via FFT

Total complexity: $\mathcal{O}(rN \log N)$

`R` **implementation:**
`R` package "Rssa": `http://cran.r-project.org/web/packages/Rssa/`

Article:
N. Golyandina, A. Korobeynikov, A. Shlemov and K. Usevich (2014): *"Multivariate and 2D Extensions of Singular Spectrum Analysis with the* Rssa *Package"*, accepted to "Journal of Statistical Software"

Outline

Conclusions

- An extension of SSA (shaped SSA) was proposed for decomposition of shaped images including circular and toroidal topology
- An extension of 2D-ESPRIT method for parameter estimation in the signal-plus-noise model was described
- An efficient publicly available implementation is provided
- The algorithms and their implementation can be easily extended to higher dimensions

Thanks for your attention!