



**The Abdus Salam  
International Centre for Theoretical Physics**



**2044-8**

**Summer School and Advanced Workshop on Trends and  
Developments in Linear Algebra**

*22 June - 10 July, 2009*

**Tensor decompositions and tensors ranks: general concepts and algorithms**

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# TENSOR DECOMPOSITIONS AND TENSOR RANKS: GENERAL CONCEPTS AND ALGORITHMS

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## WHAT ARE TENSORS?

TENSOR = MULTI-INDEX ARRAY = MULTI-WAY ARRAY =  
MULTI-DIMENSIONAL MATRIX:

$$\mathbf{A} = [a_{ij\dots k}]$$

$$i \in I, \quad j \in J, \quad \dots, \quad k \in K$$

Number of different indices is *dimension*.

Indices are called also *modes*.

Cardinalities of index ranges  $I, J, \dots, K$  are *mode sizes*.

In case of dimension  $d$  and mode sizes  $n_1, n_2, \dots, n_d$ ,  
 $\mathbf{A}$  is a *tensor of size*  $n_1 \times n_2 \times \dots \times n_d$ .

Talking of tensors, tacitly assume that  $d \geq 3$ .

## TENSORS AND MATRICES

Let  $\mathbf{A} = [a_{ijklm}]$ .

Consider pairs of complementary *long indices*

$(ij)$  and  $(klm)$

$(kl)$  and  $(ijm)$

.....

Then  $\mathbf{A}$  gives rise to several matrices:

$$B_1 = [b_{(ij),(klm)}],$$

$$B_2 = [b_{(kl),(ijm)}]$$

.....

with

$$b_{(ij),(klm)} = b_{(kl),(ijm)} = \dots = a_{ijklm}$$

## MODE UNFOLDING MATRICES

$$\mathbf{A}_1 = [\mathbf{a}_{i,(jklm)}]$$

$$\mathbf{A}_2 = [\mathbf{a}_{j,(iklm)}]$$

$$\mathbf{A}_3 = [\mathbf{a}_{k,(ijlm)}]$$

$$\mathbf{A}_4 = [\mathbf{a}_{l,(ijkm)}]$$

$$\mathbf{A}_5 = [\mathbf{a}_{m,(ijkl)}]$$

Columns of unfolding matrices are called *mode vectors*.

If  $\mathbf{d} = \mathbf{3}$ , typical names are *columns, rows, fibers*.

Ranks of unfolding matrices are called *mode ranks* or *Tucker ranks*.

L. R. Tucker, Some mathematical notes on three-mode factor analysis,  
*Psychometrika*, V. 31, P. 279–311 (1966).

## TENSOR-BY-MATRIX MULTIPLICATIONS

Also called *mode contractions*.

Given a tensor  $\mathbf{A} = [a_{ijk}]$  and matrices

$$\mathbf{U} = [u_{i'i}], \quad \mathbf{V} = [v_{j'j}], \quad \mathbf{W} = [w_{k'k}],$$

define new tensors

$$\mathbf{A}^U = \mathbf{A} \times_1 \mathbf{U} = [a_{i'jk}^U]$$

$$\mathbf{A}^V = \mathbf{A} \times_2 \mathbf{V} = [a_{ij'k}^V]$$

$$\mathbf{A}^W = \mathbf{A} \times_3 \mathbf{W} = [a_{ijk'}^W]$$

as follows:

$$\begin{aligned} a_{i'jk}^U &= \sum_i u_{i'i} a_{ijk} && \Leftrightarrow \mathbf{A}_1^U = \mathbf{U} \mathbf{A}_1 \\ a_{ij'k}^V &= \sum_j v_{j'j} a_{ijk} && \Leftrightarrow \mathbf{A}_2^V = \mathbf{V} \mathbf{A}_2 \\ a_{ijk'}^W &= \sum_k w_{k'k} a_{ijk} && \Leftrightarrow \mathbf{A}_3^W = \mathbf{W} \mathbf{A}_3 \end{aligned}$$

## WHY CONTRACTIONS?

Let  $\mathbf{A} = [\mathbf{a}_{ijk}]$  be  $n \times n \times n$  and mode ranks be equal to  $r \ll n$ .  
Consider  $\mathbf{QR}$  decompositions of unfolding matrices

$$\mathbf{A}_1 = \mathbf{Q}_1 \mathbf{R}_1, \quad \mathbf{A}_2 = \mathbf{Q}_2 \mathbf{R}_2, \quad \mathbf{A}_3 = \mathbf{Q}_3 \mathbf{R}_2$$

$\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3$  are orthogonal  $n \times r$  matrices.

Define the *Tucker core* tensor  $\mathbf{G} = [\mathbf{g}_{\alpha\beta\gamma}]$   
of *contracted* size  $r \times r \times r$ :

$$\mathbf{G} = \mathbf{A} \times_1 \mathbf{Q}_1^\top \times_2 \mathbf{Q}_2^\top \times_3 \mathbf{Q}_3^\top \quad \text{i.e.} \quad \mathbf{g}_{\alpha\beta\gamma} = \sum_{i,j,k} \mathbf{a}_{ijk} \mathbf{q}_{i\alpha}^1 \mathbf{q}_{j\beta}^2 \mathbf{q}_{k\gamma}^3$$

## THEOREM

$$\mathbf{A} = \mathbf{G} \times_1 \mathbf{Q}_1 \times_2 \mathbf{Q}_2 \times_3 \mathbf{Q}_3 \quad \text{i.e.} \quad \mathbf{a}_{ijk} = \sum_{\alpha,\beta,\gamma} \mathbf{g}_{\alpha\beta\gamma} \mathbf{q}_{i\alpha}^1 \mathbf{q}_{j\beta}^2 \mathbf{q}_{k\gamma}^3$$

**IMPORTANT:**  $\mathbf{A}$  is now represented in a *contracted form*  
with only  $3nr + r^3 \ll n^3$  parameters.

## TUCKER DECOMPOSITION

Regarded as *Tensor SVD* or *Higher Order SVD*:

$$\mathbf{A} = \mathbf{G} \times_1 \mathbf{Q}_1 \times_2 \mathbf{Q}_2 \times_3 \mathbf{Q}_3 \quad \text{i.e.} \quad a_{ijk} = \sum_{\alpha, \beta, \gamma} g_{\alpha\beta\gamma} q_{i\alpha}^1 q_{j\beta}^2 q_{k\gamma}^3$$

Orthogonal matrices  $\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3$  are *Tucker factors* or *frame matrices*.

### THEOREM

Rows in each of unfolding matrices for the Tucker core can be made *orthogonal* and arranged in *length-decreasing order*.

Row lengths of unfoldings for  $\mathbf{G}$  = singular values of unfoldings for  $\mathbf{A}$ .

PROOF is easy via SVD of unfolding matrices:

$$\text{if } \mathbf{A}_1 = \mathbf{Q}_1 \mathbf{\Sigma}_1 \mathbf{V}_1 \text{ then } (\mathbf{A} \times_1 \mathbf{Q}_1^\top)_1 = \mathbf{\Sigma}_1 \mathbf{V}_1.$$

Same for other modes.



# TUCKER APPROXIMATIONS

$$\mathbf{a}_{ijk} \approx \sum_{\alpha, \beta, \gamma} \mathbf{g}_{\alpha\beta\gamma} \mathbf{q}_{i\alpha}^1 \mathbf{q}_{j\beta}^2 \mathbf{q}_{k\gamma}^3$$

## APPLICATIONS:

- Multi-way Principal Component Analysis  
(senior frame matrices are most informative).
- Tensor data compression  
(ignore small and get to reduced Tucker ranks  $\ll$  mode sizes).
- New generation of numerical algorithms  
with [all data in the Tucker format](#).  
Enjoy linear and even sublinear complexity in total size of data  
(could be petabytes).

I. Oseledets, D. Savostyanov, E. Tyrtyshnikov,  
*Linear algebra for tensor problems*, submitted to *Computing* (2008).

G. Beylkin, M. Mohlenkamp, Algorithms for numerical analysis in  
high dimensions, *SIAM J. Sci. Comput.*, 26 (6), pp. 2133-2159 (2005).

## CANONICAL DECOMPOSITION

$$a_{ij\dots k} = \sum_{t=1}^{\rho} u_{it} v_{jt\dots} w_{kt}$$

Minimal  $\rho = \mathbf{tRank}$  is called *canonical rank* or *tensor rank* of  $\mathbf{A}$ .

### THEOREM

Let mode ranks be equal to  $r$ . Then

$$r \leq \mathbf{tRank}(\mathbf{A}) \leq r^2.$$

## CANONICAL APPROXIMATIONS

$$a_{ij\dots k} \approx \sum_{t=1}^{\rho} u_{it} v_{jt\dots} w_{kt}$$

play same compression role as Tucker.

Could be better but not necessarily!

## TENSOR RANKS IN COMPLEXITY THEORY

In the “row-by-column” rule for multiplication of  $n \times n$  matrices we have  $n^2$  multiplications. Can we reduce this number?

$$\begin{bmatrix} c_1 & c_2 \\ c_3 & c_4 \end{bmatrix} = \begin{bmatrix} a_1 & a_2 \\ a_3 & a_4 \end{bmatrix} = \begin{bmatrix} b_1 & b_2 \\ b_3 & b_4 \end{bmatrix}$$

$$c_k = \sum_{i=1}^n \sum_{j=1}^n h_{ijk} a_i b_j$$

Let  $\rho =$  tensor rank of  $h_{ijk}$  and canonical decomposition read

$$h_{ijk} = \sum_{t=1}^{\rho} u_{it} v_{jt} w_{kt} \Rightarrow$$

$$c_k = \sum_{t=1}^{\rho} w_{kt} \left( \sum_{i=1}^n u_{it} a_i \right) \left( \sum_{j=1}^n v_{jt} b_j \right)$$

**Now we have  $\rho$  multiplications!**

If  $n = 2$  then  $\rho = 7$  (Strassen, 1965).

By recursion  $\Rightarrow$  only  $O(n^{\log_2 7})$  multiplications for arbitrary  $n$ .

## TUCKER VS CANONICAL FOR MATRICES

$$a_{ij} = \sum_{\alpha=1}^r \sum_{\beta=1}^r g_{\alpha\beta} q_{i\alpha}^1 q_{j\beta}^2 \Leftrightarrow A = Q_1 G Q_2^\top$$

Tucker = a *pseudo-skeleton* decomposition of  $A$ .

$$a_{ij} = \sum_{t=1}^{\rho} u_{it} v_{jt} \Leftrightarrow A = UV^\top$$

Canonical = a *skeleton* or *dyadic* decomposition of  $A$ .

Tensor (canonical) rank seems to be a true generalization of the matrix rank concept.

However, tensor rank for dimension  $\geq 3$  and matrix rank have *noticably different properties*.

# KRONECKER PRODUCT REPRESENTATION

Tucker decomposition:

$$\mathbf{A} = \sum_{\alpha, \beta, \gamma} g_{\alpha\beta\gamma} \mathbf{u}_{\alpha} \otimes \mathbf{v}_{\beta} \otimes \mathbf{w}_{\gamma}$$

Canonical decomposition:

$$\mathbf{A} = \sum_t \mathbf{u}_t \otimes \mathbf{v}_t \otimes \mathbf{w}_t$$

## KRUSKAL (ESSENTIAL) UNIQUENESS

Minimal canonical decomposition

$$\mathbf{A} = \sum_t \mathbf{u}_t \otimes \mathbf{v}_t \otimes \mathbf{w}_t$$

is said to be *essentially unique* if

$$\sum_t \mathbf{u}_{it} \otimes \mathbf{v}_{jt} \otimes \mathbf{w}_{kt} = \sum_t \bar{\mathbf{u}}_{it} \otimes \bar{\mathbf{v}}_{jt} \otimes \bar{\mathbf{w}}_{kt}$$

implies that, upon some reordering,

$$\begin{aligned} \mathbf{u}_t &|| \bar{\mathbf{u}}_t, & \mathbf{v}_t &|| \bar{\mathbf{v}}_t, & \mathbf{w}_t &|| \bar{\mathbf{w}}_t, \\ ||\mathbf{u}_t \otimes \mathbf{v}_t \otimes \mathbf{w}_t|| &= & ||\bar{\mathbf{u}}_t \otimes \bar{\mathbf{v}}_t \otimes \bar{\mathbf{w}}_t||. \end{aligned}$$

Matrix skeleton (dyadic) decomposition is **NOT ESSENTIALLY UNIQUE**.

This becomes an obstacle in Principal Component Analysis, e.g. in **separation of signals**.

Despite that, **tensors possess ESSENTIAL UNIQUENESS** (under mild assumptions).

## INDEPENDENT COMPONENT RECONSTRUCTION

EXAMPLE (De Lathauwer) where the PCA fails.

Assume we need to separate two independent zero-mean signals

$$x_1(t) = \sqrt{2} \sin t, \quad x_2(t) = \begin{cases} 1 & \text{if } k\pi \leq t < k\pi + \pi/2, \\ -1 & \text{if } k\pi + \pi/2 \leq t < k\pi + \pi, \end{cases}$$

defined on the interval  $0 \leq t \leq 4\pi$  and mixed by a matrix

$$A = \begin{pmatrix} -1 & -3\sqrt{3} \\ 3\sqrt{3} & -5 \end{pmatrix}.$$

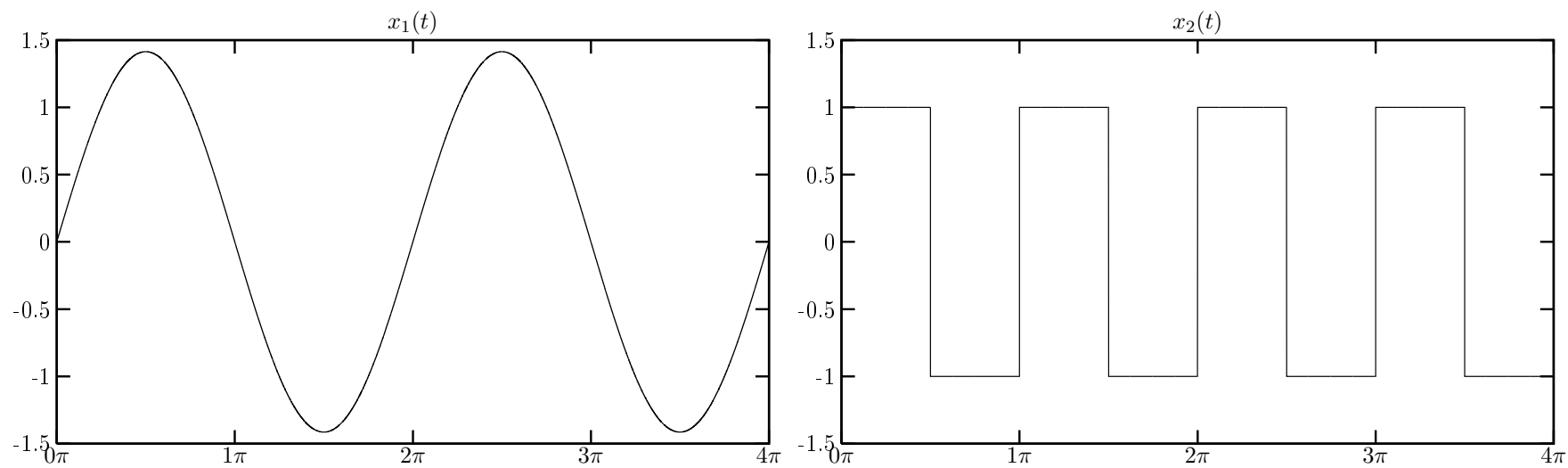


FIG. 1. Signals to be separated.

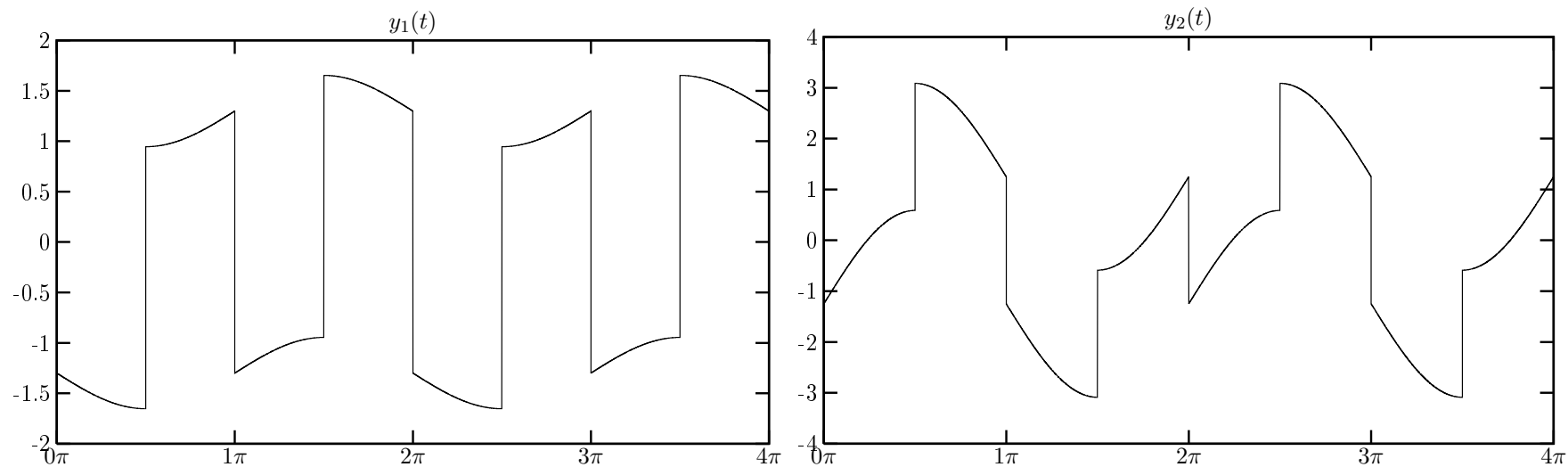


Fig. 2. Observations of linearly mixed signals.



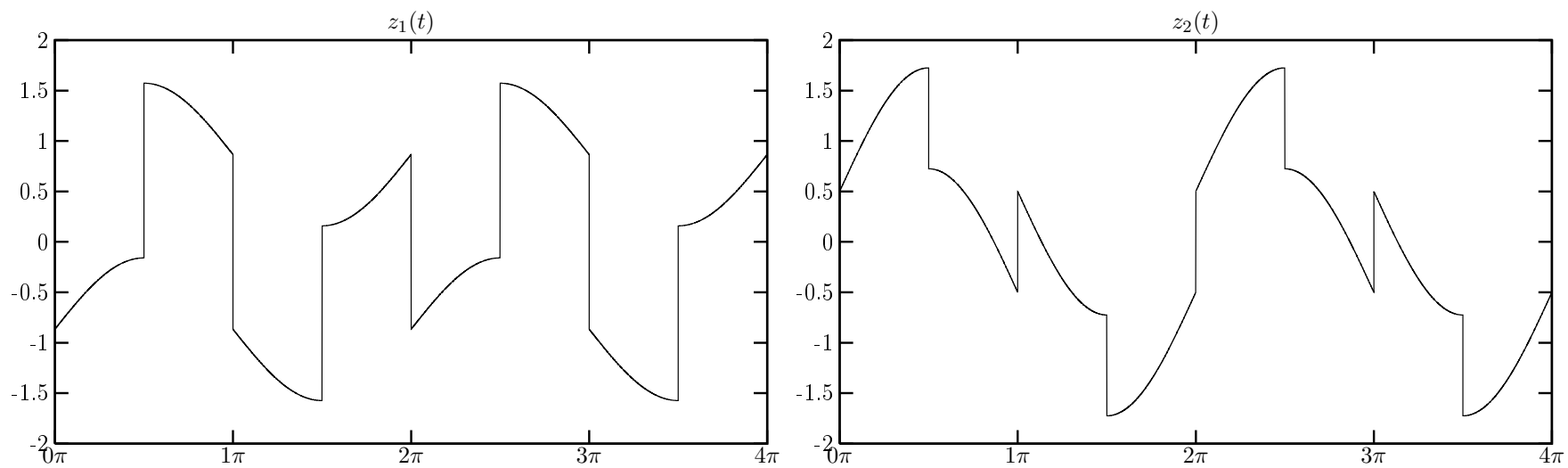


FIG. 3. Separation results produced by the PCA.

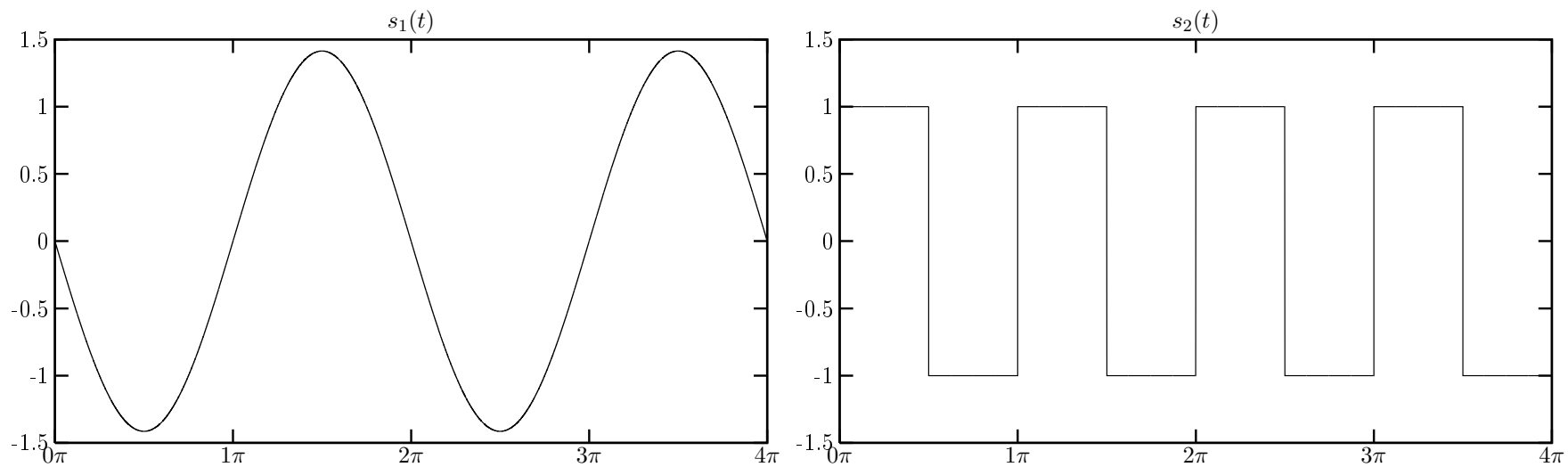


FIG. 4. Separation results of the tensor technique.

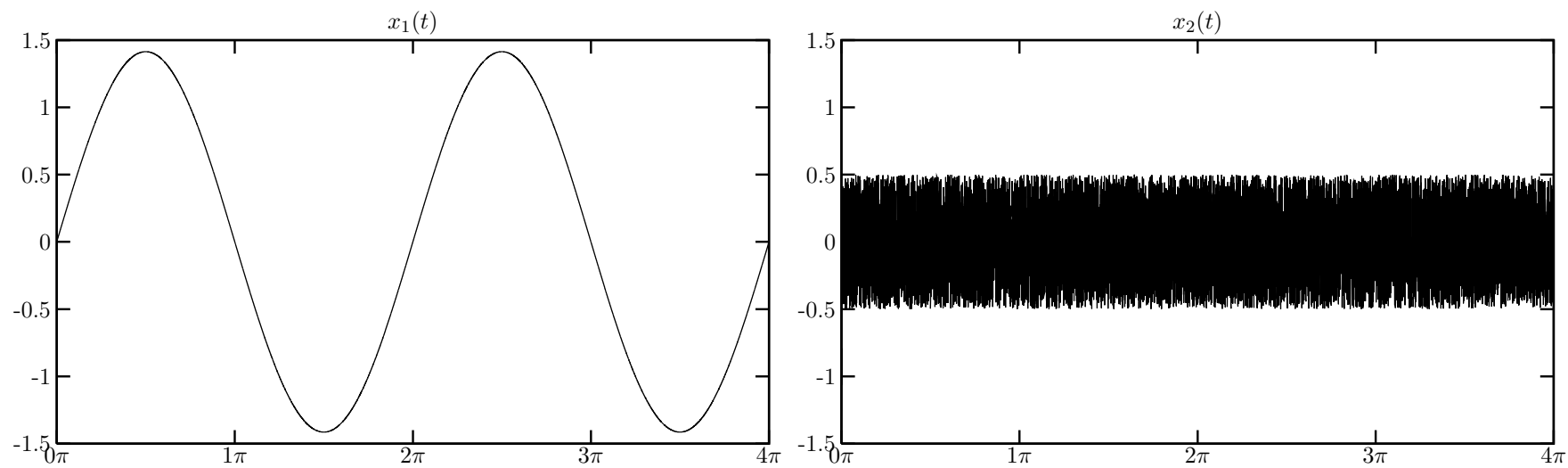


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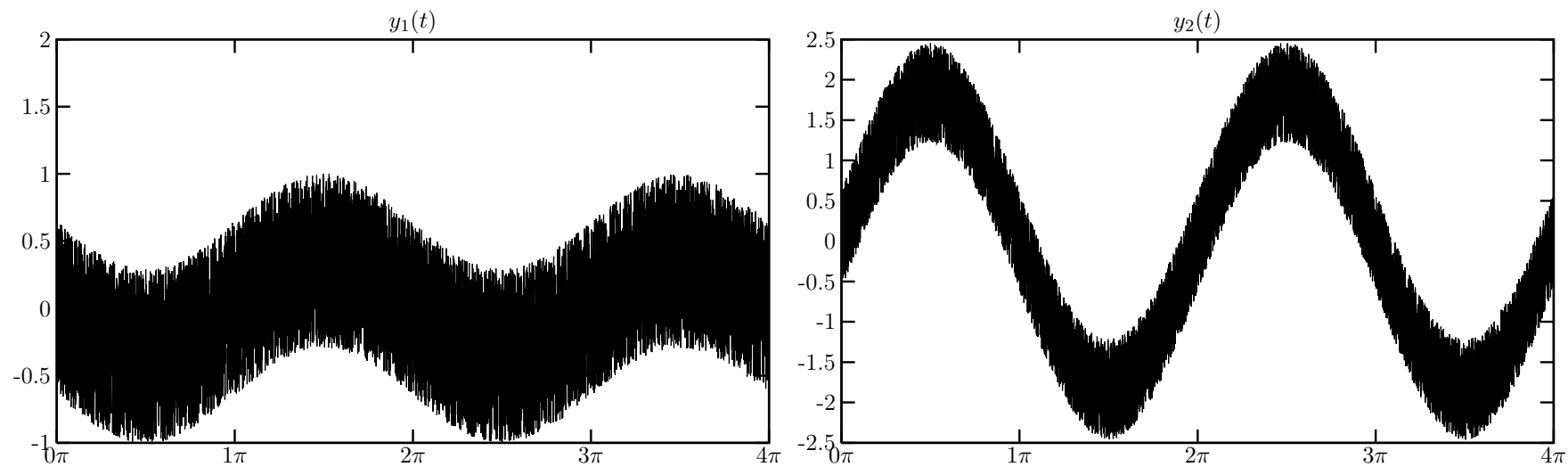


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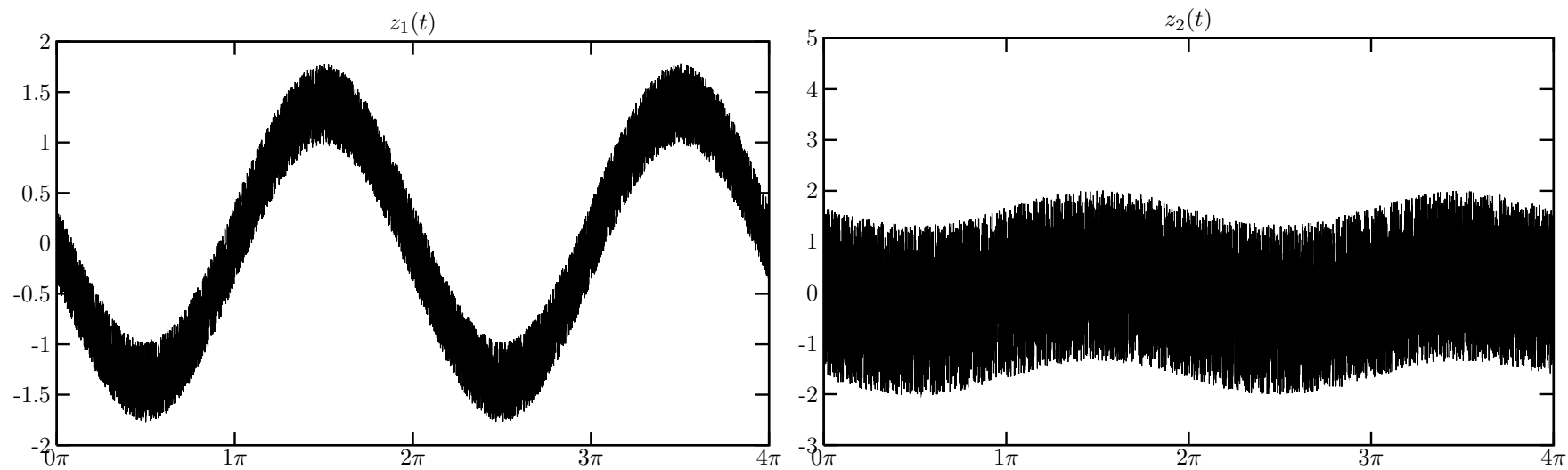


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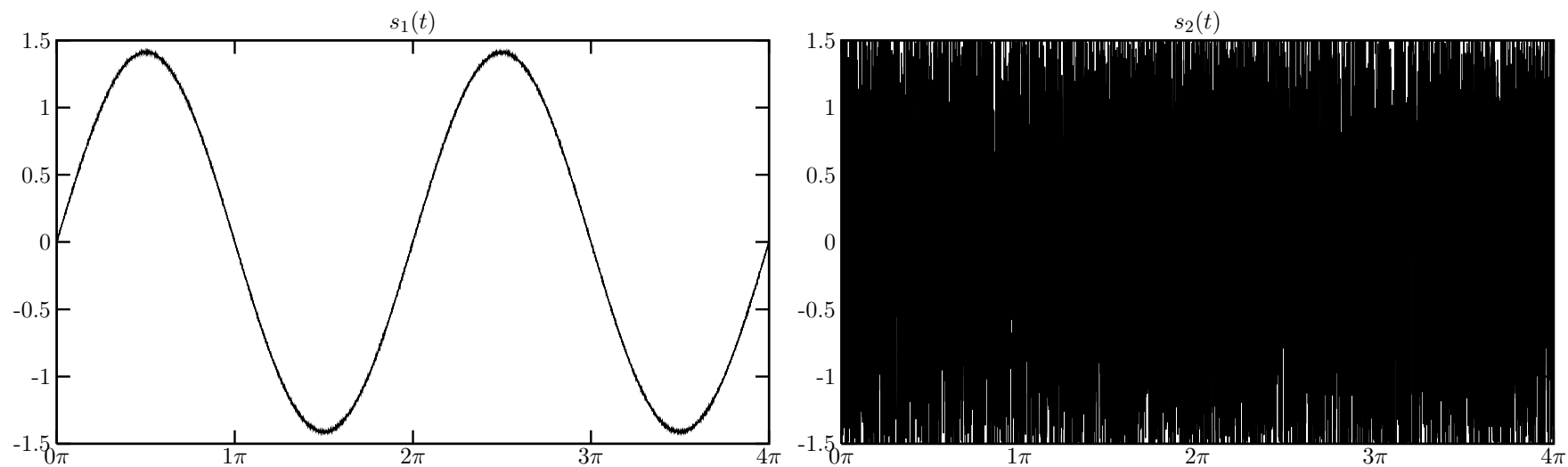


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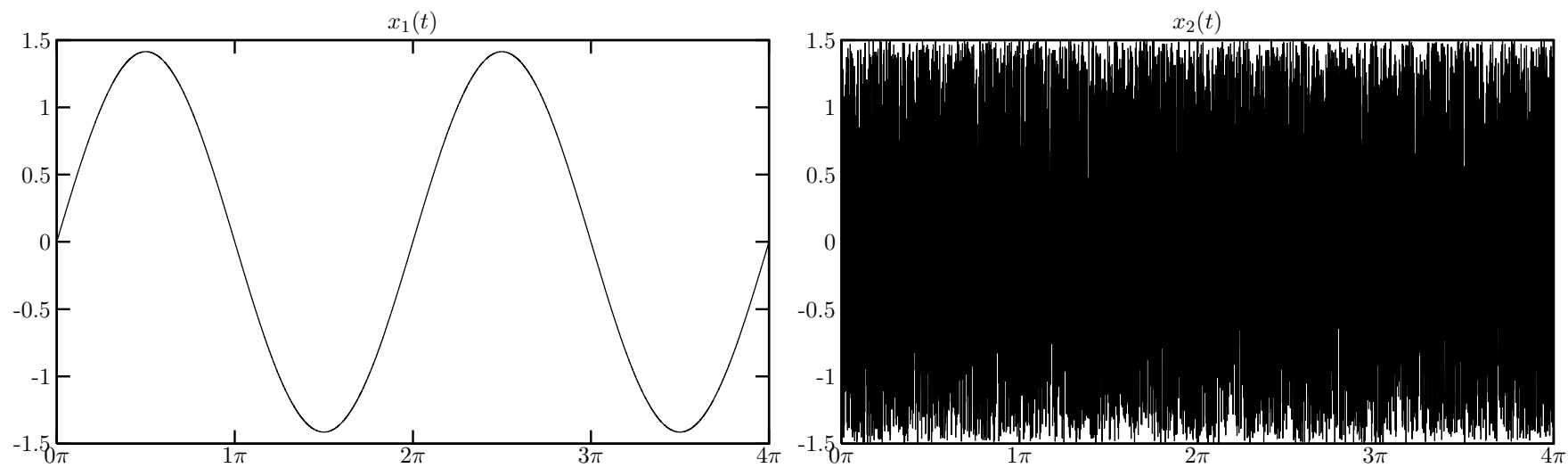


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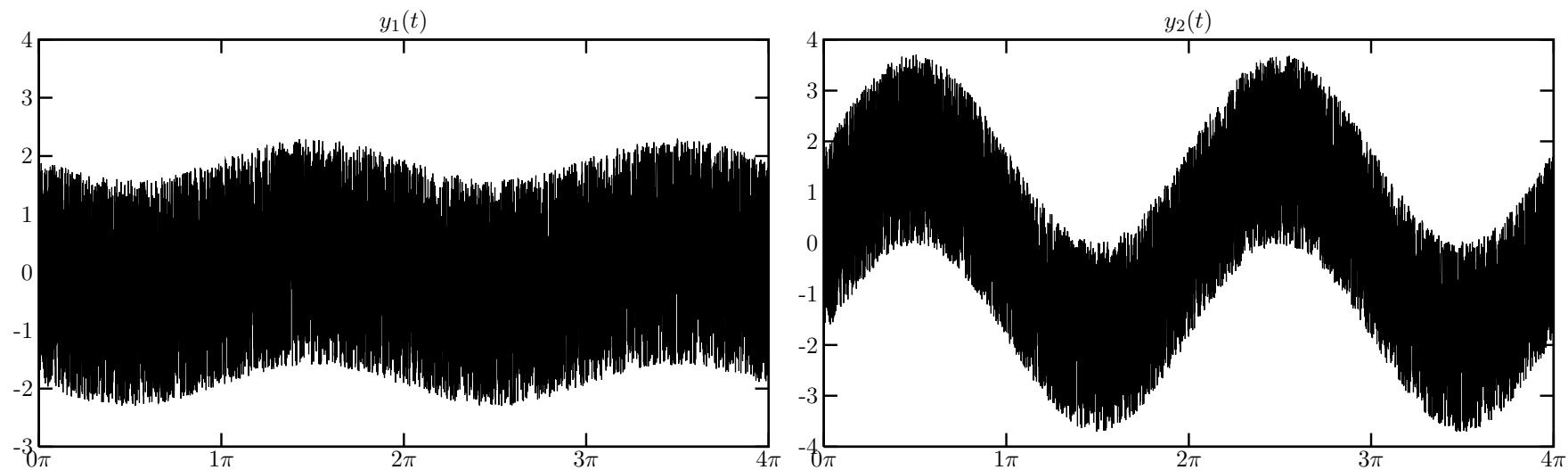


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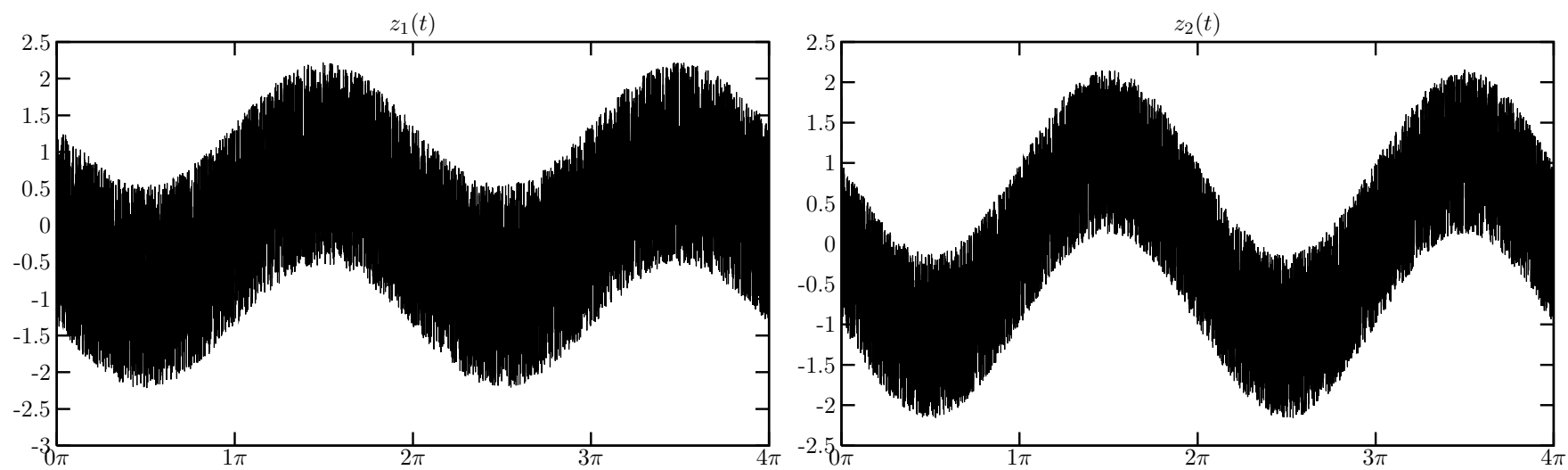


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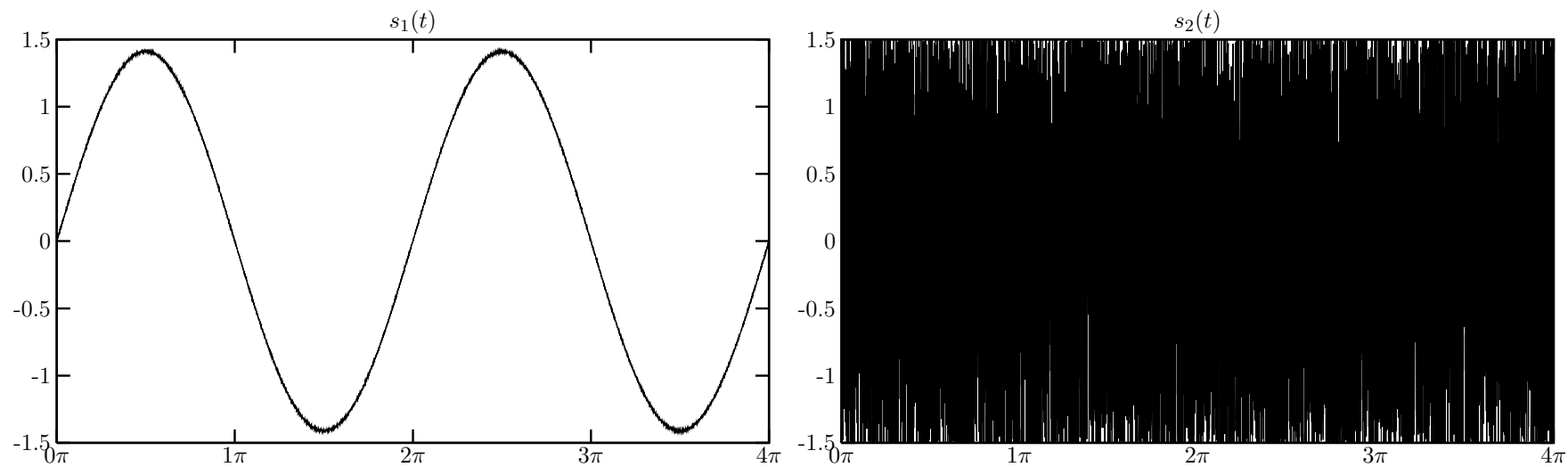


FIG. 4. Separation results of the tensor technique.

## KRUSKAL (ESSENTIAL) UNIQUENESS

Canonical decomposition

$$\mathbf{A} = \sum_{t=1}^{\rho} \mathbf{u}_t \otimes \mathbf{v}_t \otimes \mathbf{w}_t$$

is defined by matrices with  $\rho$  columns:

$$\mathbf{U} = [\mathbf{u}_{it}], \quad \mathbf{V} = [\mathbf{v}_{jt}], \quad \mathbf{W} = [\mathbf{w}_{kt}].$$

A matrix is said to have *Kruskal rank*  $\mathbf{r}$  if  $\mathbf{r}$  is the maximal number s.t. any  $\mathbf{r}$  columns are linearly independent.

### KRUSKAL THEOREM

Let the Kruskal ranks for  $\mathbf{U}, \mathbf{V}, \mathbf{W}$  coincide with their ranks and

$$\mathbf{rankU} + \mathbf{rankV} + \mathbf{rankW} \geq 2\rho + 2.$$

Then this canonical decomposition is essentially unique.

J. B. Kruskal, Three-way arrays: rank and uniqueness for 3-way and n-way arrays, *Linear Algebra Appl.*, 18, pp. 95–138 (1977).

## SIMULTANEOUS DIAGONALIZATION

Tensor decomposition of an  $n \times n \times n$  tensor

$$a_{ijk} = \sum_{t=1}^{\rho} u_{it} v_{jt} w_{kt}$$

means simultaneous diagonalization of  $n$  slice matrices

$$M_k = [a_{ijk}] = U \begin{bmatrix} w_{k1} & & \\ & \cdots & \\ & & w_{k\rho} \end{bmatrix} V^T$$

$U$  and  $V$  are  $n \times \rho$

## RELATED SIMULTANEOUS EIGENVALUE PROBLEM

$$M_k x = \lambda_k y$$

## **2 × 2 × 2 TENSORS**

When tensor rank is equal to 2?

If so, we have simultaneously

$$\mathbf{M}_1 = \mathbf{U}\mathbf{W}_1\mathbf{V}$$

$$\mathbf{M}_2 = \mathbf{U}\mathbf{W}_2\mathbf{V}$$

If  $\mathbf{M}_2$  is nonsingular, it follows that

$$\mathbf{M}_1\mathbf{M}_2^{-1} = \mathbf{U}\mathbf{D}\mathbf{U}^{-1}, \quad \mathbf{D} = \mathbf{W}_1\mathbf{W}_2^{-1} \text{ is a diagonal matrix.}$$

### **EXAMPLE**

$$\mathbf{M}_1 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \mathbf{M}_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Tensor with slices  $\mathbf{M}_1, \mathbf{M}_2$  must be of tensor rank  $\geq 3$ .

### **COROLLARY**

Tensor rank for a tensor of size  $2 \times 2 \times 2$  can be greater than **2**.

It cannot exceed 4, but can it be greater than 3?



## PRESERVATION OF TENSOR RANK

### LEMMA

Tensor rank is invariant under mode contractions by nonsingular matrices.

### COROLLARY 1.

Tensor rank calculation for general  $\mathbf{2} \times \mathbf{2} \times \mathbf{2}$  tensor reduces to a particular case of tensor with slices

$$\mathbf{M}_1 = \begin{bmatrix} * & \mathbf{0} \\ \mathbf{0} & * \end{bmatrix}, \quad \mathbf{M}_2 = \begin{bmatrix} * & * \\ * & * \end{bmatrix}.$$

### COROLLARY 2.

Maximum of tensor ranks for  $\mathbf{2} \times \mathbf{2} \times \mathbf{2}$  tensors is equal to 3.

## TENSOR RANK DEPENDS ON THE SUBFIELD

It does not happen for matrices!

However, for tensor over  $\mathbb{R}$  tensor ranks over  $\mathbb{R}$  and  $\mathbb{C}$  may differ.

PROOF.

Consider  $2 \times 2 \times 2$  tensor with slices

$$M_1 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad M_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Matrix  $M_1 M_2^{-1}$  has eigenvalues  $\pm\sqrt{-1}$ .

Hence, it cannot be diagonalized by a real similarity  $\Rightarrow$   
tensor rank over  $\mathbb{R}$  is equal to 3.

But tensor rank over  $\mathbb{C}$  is 2.

## RANK INSTABILITY

- Matrix rank can be made larger by arbitrarily small perturbation, but cannot be made smaller.  
The same for Tucker ranks.
- Tensor (canonical) rank *may decrease* by an arbitrary small perturbation, at least for some tensors.

**EXAMPLE** (could be 3D Laplacian)

$$\mathbf{a} \otimes \mathbf{a} \otimes \mathbf{b} + \mathbf{a} \otimes \mathbf{b} \otimes \mathbf{a} + \mathbf{b} \otimes \mathbf{a} \otimes \mathbf{a} =$$

$$\begin{aligned} \mathbf{a} \otimes (\mathbf{a} + \varepsilon \mathbf{b}) \otimes (\mathbf{b} + \varepsilon^{-1} \mathbf{a}) + (\mathbf{b} - \varepsilon^{-1} \mathbf{a}) \otimes \mathbf{a} \otimes \mathbf{a} \\ + \varepsilon \mathbf{a} \otimes \mathbf{b} \otimes \mathbf{b} \end{aligned}$$

Notice large numbers in a lower-rank tensor.

## DIFFICULTY

Best approximation to a given tensor by tensors of a prescribed tensor rank *may not exist*.

## BEST TENSOR APPROXIMATIONS

### THEOREM 1.

For a tensor of canonical rank  $\rho$ ,  
best approximations of rank  $\mathbf{1}$  and rank  $\rho$  always exist.

*Is it possible to produce an example of tensor with non-existence  
of best approximations of any rank strictly in between of  $\mathbf{1}$  and  $\rho$ ?*

### THEOREM 2.

Best approximations of a prescribed tensor rank and a predetermined upper bound on moduli of the factor entries always exist.

### THEOREM 3.

Best approximations of a prescribed tensor rank with nonnegativity constraint for all entries of factors always exist.

## GENERIC RANKS

A minimal finite set  $\mathcal{R}(n_1, \dots, n_d) = \{r_s\}$  of positive integers s.t. tensors with tensor ranks from this set are dense in the set of all tensor of size

$$n_1 \times \dots \times n_d$$

is said to consist of *generic ranks* for  $n_1 \times \dots \times n_d$  tensors.

Real  $2 \times 2 \times 2$  tensors has generic ranks 2 and 3.

**2** in  $\sim 79\%$  and **3** in  $\sim 21\%$  cases.

The set of complex  $2 \times 2 \times 2$  tensors has generic rank 2.

### THEOREM (HYPOTHESIS?)

For complex tensors there is a single value of generic rank (depending on size).

### HYPOTHESIS (THEOREM?)

For real tensors there could be onle two possible generic ranks (depending on size).

## ALTERNATING LEAST SQUARES

R. A. Harshman,

Foundations of the Parafac procedure: models and conditions for an explanatory multimodal factor analysis, *UCLA Working Papers in Phonetics*, 16: 1–84 (1970).

Given  $\mathbf{A}$ , find an optimal canonical decomposition with factor matrices  $\mathbf{U}, \mathbf{V}, \mathbf{W}$  with prescribed number of columns.

ALS reads

- Freeze  $\mathbf{V}, \mathbf{W}$  and substitute  $\mathbf{U}$  with the best LS fit.
- Freeze  $\mathbf{U}, \mathbf{W}$  and do the same with  $\mathbf{V}$ .
- Freeze  $\mathbf{U}, \mathbf{V}$  and do the same with  $\mathbf{W}$ .
- Repeat until convergence.

Convergence theory?

## ONE STEP OF ALS

With  $\mathbf{U}$  and  $\mathbf{V}$  frozen, find  $\mathbf{W}$  from the LS problem

$$\sum_{t=1}^{\rho} \mathbf{u}_{it} \mathbf{v}_{jt} \mathbf{w}_{kt} \stackrel{\text{LS}}{=} \mathbf{a}_{ijk}.$$

In the matrix form, find vectors of size  $\rho$

$$\mathbf{x}_k = \begin{bmatrix} \mathbf{w}_{k1} \\ \dots \\ \mathbf{w}_{k\rho} \end{bmatrix}$$

solving

$$\mathbf{U} \square \mathbf{V} \stackrel{\text{LS}}{=} \mathbf{b}_k \equiv \begin{bmatrix} \mathbf{a}_{11k} \\ \mathbf{a}_{12k} \\ \dots \\ \mathbf{a}_{nnk} \end{bmatrix}$$

$$\mathbf{U} \square \mathbf{V} = [\mathbf{u}_1 \otimes \mathbf{v}_1, \dots, \mathbf{u}_\rho \otimes \mathbf{v}_\rho] \quad (\text{Khartri-Rao product})$$