Technical University of Crete
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Analyzing Data 'Boxes': Multi-way linear algebra and its applications in signal processing and communications

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Dedication

In memory of Richard Harshman († Jan. 10, 2008), who co-founded three-way analysis, and fathered PARAFAC in the early 70's.

Richard was a true gentleman.

Acknowledgments

- 3-way Students: X. Liu, T. Jiang
- 3-way Collaborators: R. Bro (Denmark), J. ten Berge, A. Stegeman (Netherlands), D. Nion (ENSEA-France & TUC-Greece)
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Contents

- 3-way arrays: similarities and differences with matrices
- Rank, and low-rank decomposition
- 3-way notation, using CDMA as example
- Uniqueness
- Algorithms
- Performance
- Application: blind speech separation
- What lies ahead & wrap-up

Applications

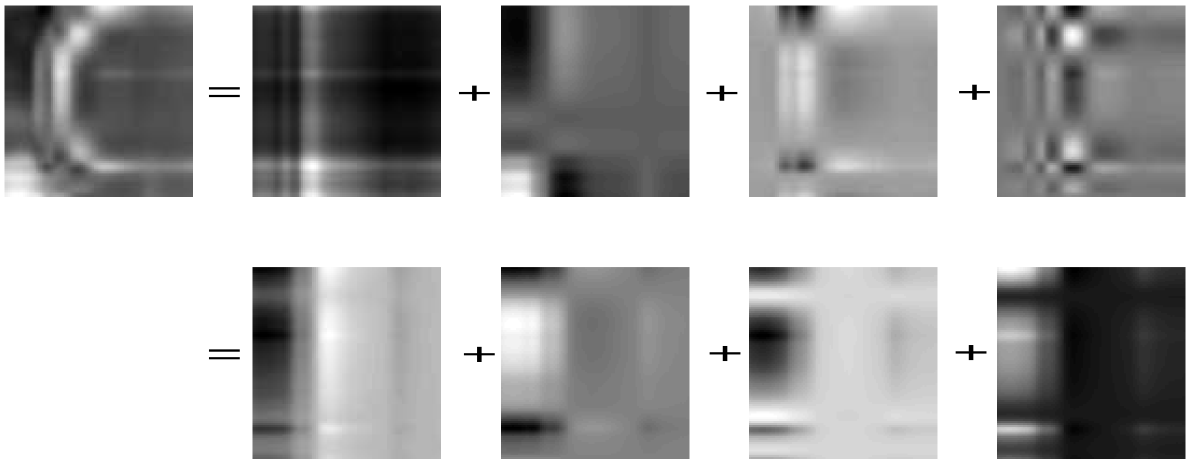
- CDMA intercept / signal intelligence
- Sensor array processing
- Multi-dimensional harmonic retrieval
- Radar
- Speech separation
- Multimedia data mining
- Chemistry
- Psychology
- Chromatography, spectroscopy, magnetic resonance ...

Matrices, Factor Analysis, Rotational Indeterminacy

$$\mathbf{X} = \mathbf{A}\mathbf{B}^T = \mathbf{a}_1\mathbf{b}_1^T + \cdots + \mathbf{a}_r\mathbf{b}_r^T \quad (r := \mathrm{rank}(\mathbf{X}))$$

$$x_{i,j} = \sum_{k=1}^{r} a_{i,k} b_{j,k}$$

$$\mathbf{X} = \mathbf{A}\mathbf{B}^T = \mathbf{A}\mathbf{M}\mathbf{M}^{-1}\mathbf{B}^T$$



Reverse engineering of soup?

☞ Can only guess recipe: $\mathbf{a}_1\mathbf{b}_1^T + \cdots + \mathbf{a}_r\mathbf{b}_r^T$

Sample from two or more Cooks!

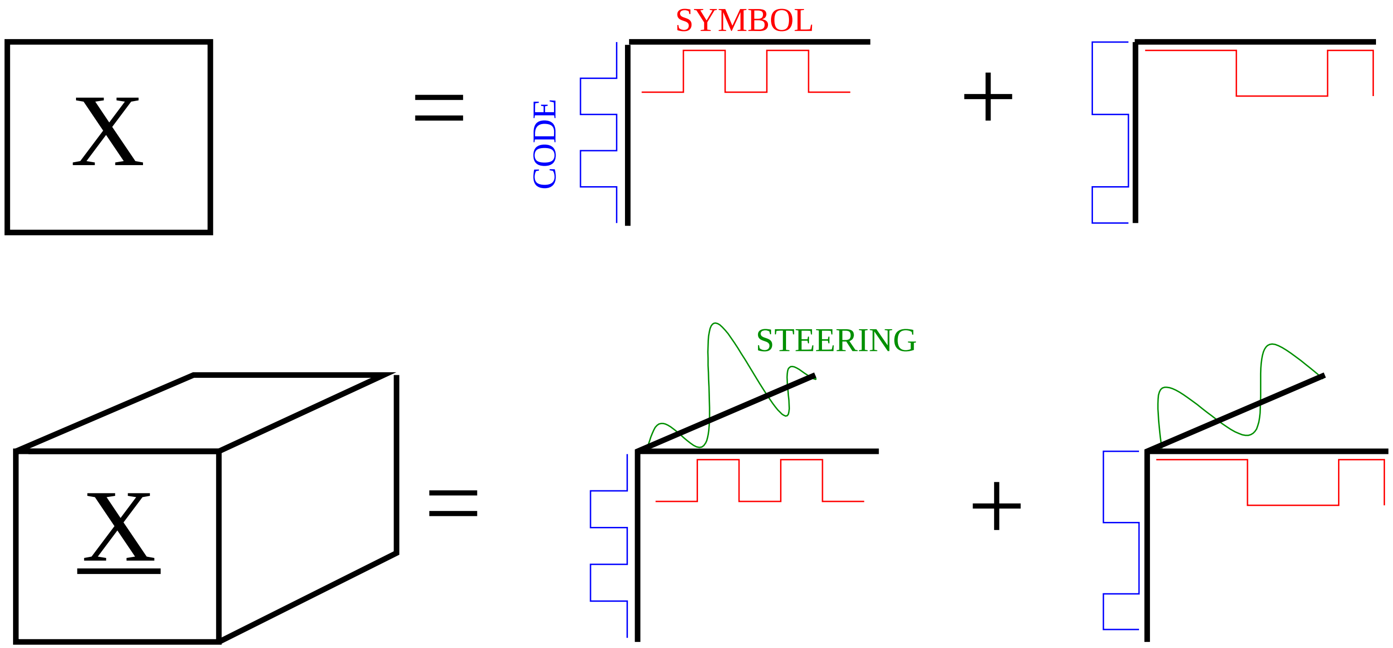
☞ Left: $\mathbf{a}_1\mathbf{b}_1^T + \cdots + \mathbf{a}_r\mathbf{b}_r^T$; right: $1.2 \times \mathbf{a}_1\mathbf{b}_1^T + \cdots + 0.87 \times \mathbf{a}_r\mathbf{b}_r^T$

☞ Same ingredients, different proportions $\hookrightarrow$ recipe!

Three-Way Arrays

- Two-way arrays, AKA matrices: $\mathbf{X} := [x_{i,j}] : (I \times J)$
- Three-way arrays: $[x_{i,j,k}] : (I \times J \times K)$
- CDMA w/ Rx Ant array @ baseband: chip $\times$ symbol $\times$ antenna

Take-Home Point



☞ Fact 1: Low-rank matrix (2-way array) decomposition not unique for rank > 1

☞ Fact 2: Low-rank 3- and higher-way array decomposition (PARAFAC) is unique under certain conditions

Three-Way vs Two-Way Arrays - Similarities

- Rank := smallest number of rank-one "factors" ("terms" is probably better) for exact additive decomposition (same concept for both 2-way and 3-way)
- Two-way rank-one factor: rank-one MATRIX outer product of 2 vectors (containing all double products)
- Three-way rank-one factor: rank-one 3-WAY ARRAY outer product of 3 vectors (containing all triple products) - same concept

Three-Way vs Two-Way Arrays - Differences

- Two-way $(I \times J)$: row-rank = column-rank = rank $\leq \min(I, J)$;
- Three-way: row-rank $\neq$ column-rank $\neq$ "tube"-rank $\neq$ rank
- Two-way: rank(randn(I,J))=min(I,J) w.p. 1;
- Three-way: rank(randn(2,2,2)) is a RV (2 w.p. 0.3, 3 w.p. 0.7)
- 2-way: rank insensitive to whether or not underlying field is open or closed ($\mathbb{R}$ versus $\mathbb{C}$); 3-way: rank sensitive to $\mathbb{R}$ versus $\mathbb{C}$
- 3-way: Except for loose bounds and special cases [Kruskal; J.M.F. ten Berge], general results for maximal rank and typical rank sorely missing for decomposition over $\mathbb{R}$; theory more developed for decomposition over $\mathbb{C}$ [Burgisser, Clausen, Shokrollahi, *Algebraic complexity theory*, Springer, Berlin, 1997]

Khatri-Rao Product

☞ Column-wise Kronecker Product:

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 5 & 10 \\ 15 & 20 \\ 25 & 30 \end{bmatrix}, \quad \mathbf{A} \odot \mathbf{B} = \begin{bmatrix} 5 & 20 \\ 15 & 40 \\ 25 & 60 \\ 15 & 40 \\ 45 & 80 \\ 75 & 120 \end{bmatrix}$$

$$vec(\mathbf{A}\mathbf{D}\mathbf{B}^T) = (\mathbf{B} \odot \mathbf{A})\mathbf{d}(\mathbf{D})$$

$$\mathbf{A} \odot (\mathbf{B} \odot \mathbf{C}) = (\mathbf{A} \odot \mathbf{B}) \odot \mathbf{C}$$

LRD of Three-Way Arrays: Notation

- Scalar: [CDMA: (i, j, k, f): (Rx, symbol, chip, user)]

$$x_{i,j,k} = \sum_{f=1}^{F} a_{i,f} b_{j,f} c_{k,f}, \quad i = 1, \cdots, I, \; j = 1, \cdots, J, \; k = 1, \cdots, K$$

- Slabs:

$$\mathbf{X}_k = \mathbf{A}\mathbf{D}_k(\mathbf{C})\mathbf{B}^T, \; k = 1, \cdots, K$$

- Matrix:

$$\mathbf{X}^{(KJ \times I)} = (\mathbf{B} \odot \mathbf{C})\mathbf{A}^T$$

- Vector:

$$\mathbf{x}^{(KJI)} := vec\left(\mathbf{X}^{(KJ \times I)}\right) = (\mathbf{A} \odot (\mathbf{B} \odot \mathbf{C}))\,\mathbf{1}_{F \times 1} = (\mathbf{A} \odot \mathbf{B} \odot \mathbf{C})\,\mathbf{1}_{F \times 1}$$

LRD of N-Way Arrays: Notation

- Scalar:

$$x_{i_1,\cdots,i_N} = \sum_{f=1}^{F} \prod_{n=1}^{N} a_{i_n,f}^{(n)}$$

- Matrix:

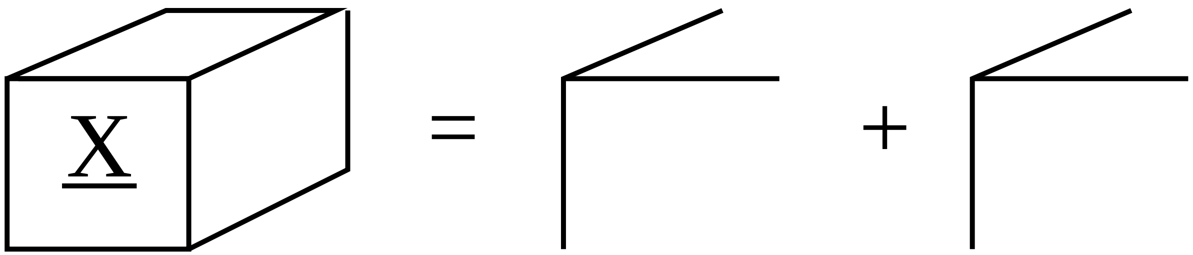
$$\mathbf{X}^{(I_1 I_2 \cdots I_{N-1} \times I_N)} = \left(\mathbf{A}^{(N-1)} \odot \mathbf{A}^{(N-2)} \odot \cdots \odot \mathbf{A}^{(1)}\right) \left(\mathbf{A}^{(N)}\right)^T$$

- Vector:

$$\mathbf{x}^{(I_1 \cdots I_N)} := vec\left(\mathbf{X}^{(I_1 I_2 \cdots I_{N-1} \times I_N)}\right) =$$

$$\left(\mathbf{A}^{(N)} \odot \mathbf{A}^{(N-1)} \odot \mathbf{A}^{(N-2)} \odot \cdots \odot \mathbf{A}^{(1)}\right) \mathbf{1}_{F \times 1}$$

Uniqueness



☞ [Kruskal, 1977], $N = 3, \mathbb{R}$: $k_{\mathbf{A}} + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2F + 2$
k-rank= maximum r such that *every* r columns are linearly independent ($\leq$ rank)

☞ [Sidiropoulos *et al*, IEEE TSP, 2000]: $N = 3$, $\mathbb{C}$

☞ [Sidiropoulos & Bro, J. Chem., 2000]: any N, $\mathbb{C}$:
$\sum_{n=1}^{N} k - ranks \geq 2F + (N - 1)$

Key-I

☞ Kruskal's Permutation Lemma [Kruskal, 1977]: Consider $\mathbf{A}$ ($I \times F$) having no zero column, and $\bar{\mathbf{A}}$ ($I \times \bar{F}$). Let $w(\cdot)$ be the *weight* (# of nonzero elements) of its argument. If for any vector $\mathbf{x}$ such that

$$w(\mathbf{x}^H \bar{\mathbf{A}}) \leq F - r_{\bar{\mathbf{A}}} + 1,$$

we have

$$w(\mathbf{x}^H \mathbf{A}) \leq w(\mathbf{x}^H \bar{\mathbf{A}}),$$

then $F \leq \bar{F}$; if also $F \geq \bar{F}$, then $F = \bar{F}$, and there exist a permutation matrix $\mathbf{P}$ and a non-singular diagonal matrix $\mathbf{D}$ such that $\mathbf{A} = \bar{\mathbf{A}}\mathbf{P}\mathbf{D}$.

☞ Easy to show for a pair of square nonsingular matrices (use rows of pinv); but the result is very deep and difficult for fat matrices - see [Jiang & Sidiropoulos, TSP:04], [Stegeman & Sidiropoulos, LAA:07]

Key-II

☞ Property: [Sidiropoulos & Liu, 1999; Sidiropoulos & Bro, 2000]

If $k_{\mathbf{A}} \geq 1$ and $k_{\mathbf{B}} \geq 1$, then it holds that

$$k_{\mathbf{B}\odot\mathbf{A}} \geq \min(k_{\mathbf{A}} + k_{\mathbf{B}} - 1, F),$$

whereas if $k_{\mathbf{A}} = 0$ or $k_{\mathbf{B}} = 0$

$$k_{\mathbf{B}\odot\mathbf{A}} = 0$$

Is Kruskal's Condition Necessary?

- Long-held conjecture (Kruskal'89): Yes
- ten Berge & Sidiropoulos, *Psychometrika*, 2002: Yes for $F \in \{2,3\}$, no for $F > 3$
- Jiang & Sidiropoulos '03: new insights that explain part of the puzzle: E.g., for $r_{\mathbf{C}} = F$, the following condition has been proven to be *necessary and sufficient*:

  No linear combination of two or more columns of $\mathbf{A} \odot \mathbf{B}$ can be written as KRP of two vectors

P-a.s. uniqueness results

- de Lathauwer ’03 - SIAM JMAA ’06 (cf. Jiang & Sidiropoulos ’03): Decomposition is a.s. unique provided

$$min(K, IJ) \geq F \;\; and \;\; F(F-1) \leq \frac{1}{2} I(I-1)J(J-1)$$

- Far better than previously known in many cases of practical interest

Algorithms

- SVD/EVD or TLS 2-slab solution (similar to ESPRIT) in some cases (but conditions for this to work are restrictive)
- Workhorse: ALS [Harshman, 1970]: LS-driven (ML for AWGN), iterative, initialized using 2-slab solution or multiple random cold starts
- ALS $\longrightarrow$ monotone convergence, usually to global minimum (uniqueness), close to CRB for $F << IJK$

Algorithms

- ALS is based on matrix view:

$$\mathbf{X}^{(KJ \times I)} = (\mathbf{B} \odot \mathbf{C})\mathbf{A}^T$$

- Given interim estimates of **B**, **C**, solve for conditional LS update of **A**:

$$\mathbf{A}_{CLS} = \left((\mathbf{B} \odot \mathbf{C})^{\dagger} \mathbf{X}^{(KJ \times I)} \right)^T$$

- Similarly for the CLS updates of **B**, **C** (symmetry); repeat in a circular fashion until convergence in fit (guaranteed)

Algorithms

- ALS initialization matters, not crucial for heavily over-determined problems
- Alt: rank-1 updates possible [Kroonenberg], but inferior
- COMFAC (Tucker3 compression), G-N, Levenberg, ATLD, DTLD, ESPRIT-like,...
- G-N converges faster than ALS, but it may fail
- In general, no “algebraic” solution like SVD
- Possible if e.g., a subset of columns in A is known [Jiang & Sidiropoulos, JASP 2003]; or under very restrictive rank conditions

Robust Regression Algorithms

- Laplacian, Cauchy-distributed errors, outliers
- Least Absolute Error (LAE) criterion: optimal (ML) for Laplacian, robust across α-stable
- Similar to ALS, each conditional matrix update can be shown equivalent to a LP problem $\longrightarrow$ alternating LP [Vorobyov, Rong, Sidiropoulos, Gershman, 2003]
- Alternatively, very simple element-wise updating using *weighted median filtering* [Vorobyov, Rong, Sidiropoulos, Gershman, 2003]
- Robust algorithms perform well for Laplacian, Cauchy, and not far from optimal in the Gaussian case

CRBs for the PARAFAC model

- Dependent on how scale-permutation ambiguity is resolved
- Real i.i.d. Gaussian, 3-way, Complex circularly symmetric i.i.d. Gaussian, 3-way & 4-way [Liu & Sidiropoulos, TSP 2001]
- Compact expressions for complex 3-way case & asymptotic CRB when one mode length goes to infinity [Jiang & Sidiropoulos, JASP/SMART:04]
- Laplacian, Cauchy [Vorobyov, Rong, Sidiropoulos, Gershman, TSP:04] - scaled versions of the Gaussian CRB; scaling parameter only dependent on noise pdf

Performance

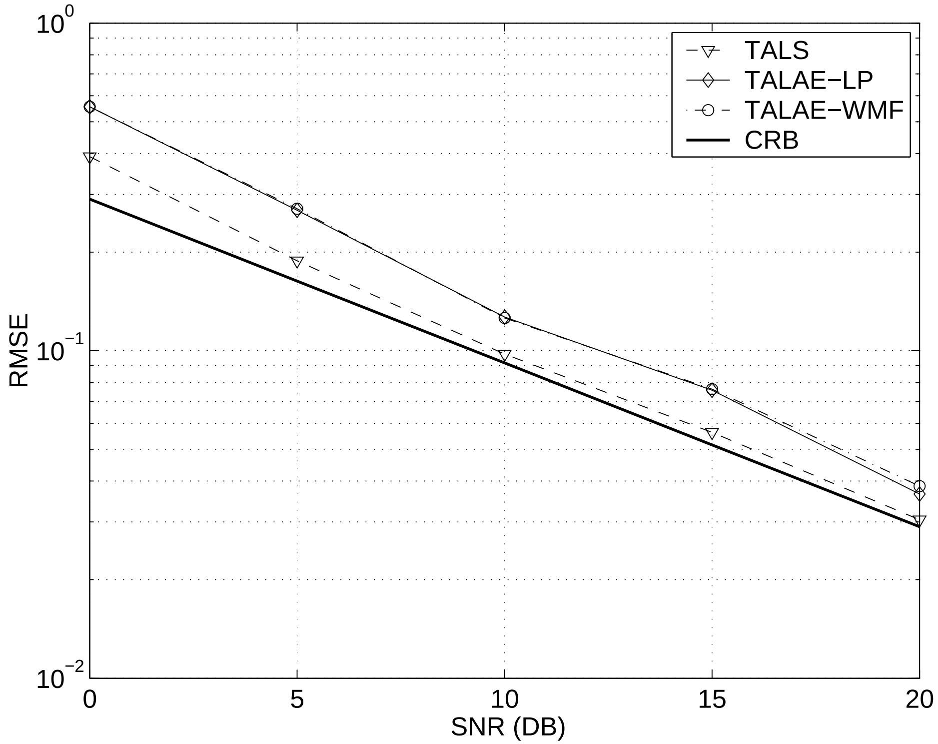


Figure 1: RMSEs versus SNR: Gaussian noise, $8 \times 8 \times 20$, $F = 2$

Performance

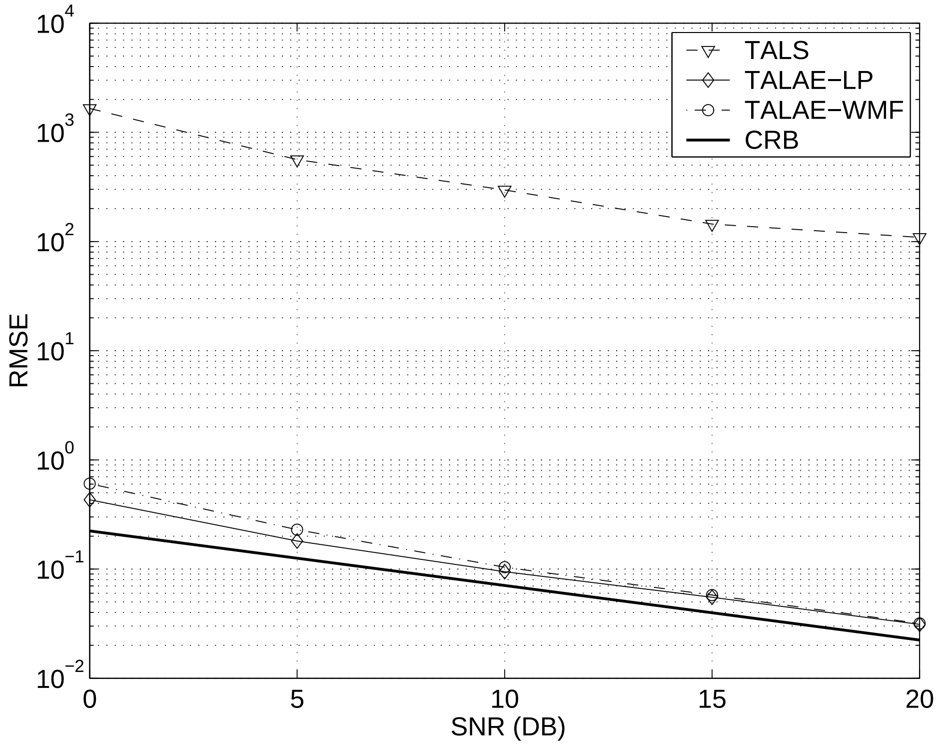


Figure 2: RMSEs versus SNR: Cauchy noise, $8 \times 8 \times 20$, $F = 2$

Performance

☞ ALS works well in AWGN because it is ML-driven, and with 3-way data it is easy to get to the large-samples regime: e.g., $10 \times 10 \times 10 = 1000$

☞ Performance is worse (and further from the CRB) when operating close to the identifiability boundary; but ALS *works* under model identifiability conditions only, which means that at high SNR the parameter estimates are still accurate

☞ Main shortcoming of ALS and related algorithms is the high computational cost

☞ For difficult datasets, so-called *swamps* are possible: progress towards convergence becomes extremely slow

Demo: Blind speech separation

- Frequency-domain vs time-domain methods
- Joint diagonalization (symmetric PARAFAC / INDSCAL) per frequency bin
- Exploits time variation in speaker powers: $\mathbf{R}_k(f) = \mathbf{A}(f)\mathbf{D}_k\mathbf{A}^H(f)$
- Frequency-dependent permutation problem is key
- How to ensure consistency (“string together”) across bins
- Engineering! - not science ...
- We now have *very competitive* solution
- Joint work with D. Nion, K. Mokios, A. Potamianos `http://www.telecom.tuc.gr/~nikos/BSS_Nikos.html`

Adaptive PARAFAC

☞ Nion & Sidiropoulos 2008, IEEE TSP, submitted

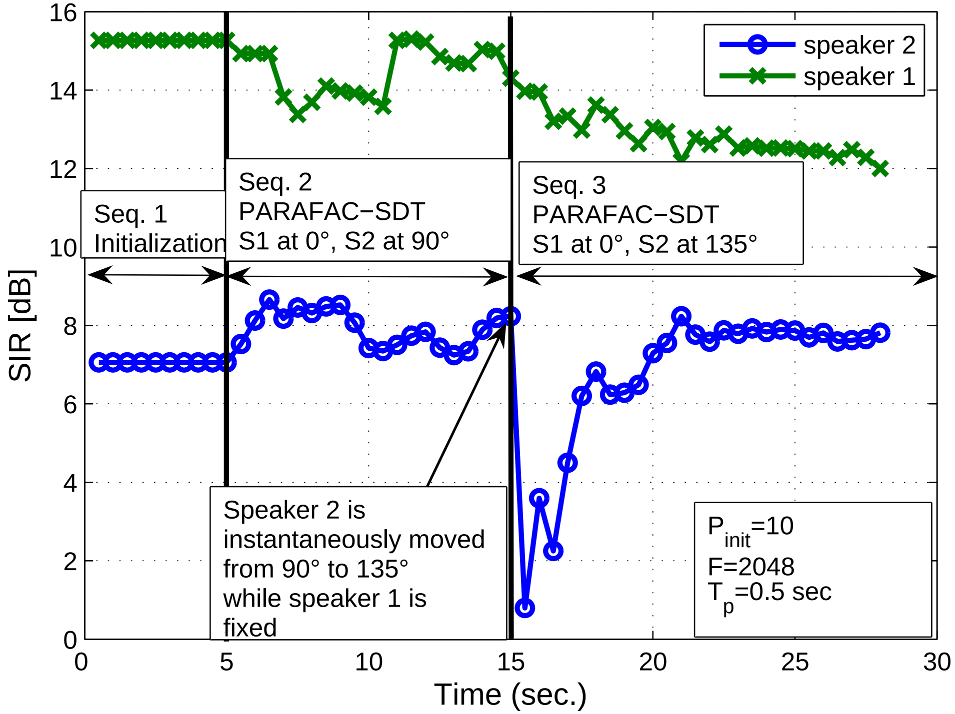


Figure 3: Blind speaker separation and tracking

Adaptive PARAFAC

☞ MIMO radar

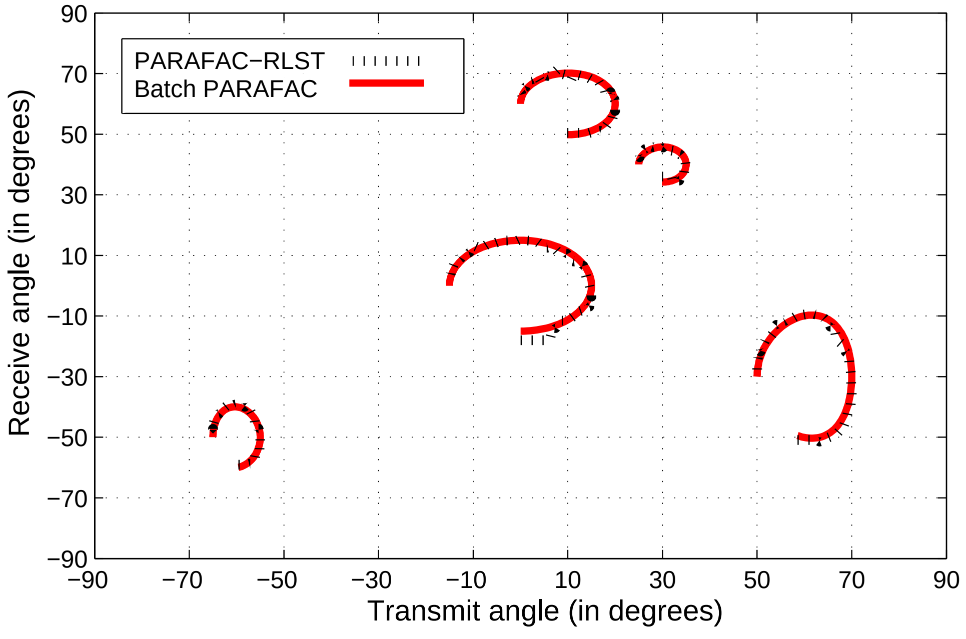


Figure 4: Trajectory tracking

Adaptive PARAFAC

☞ Complexity

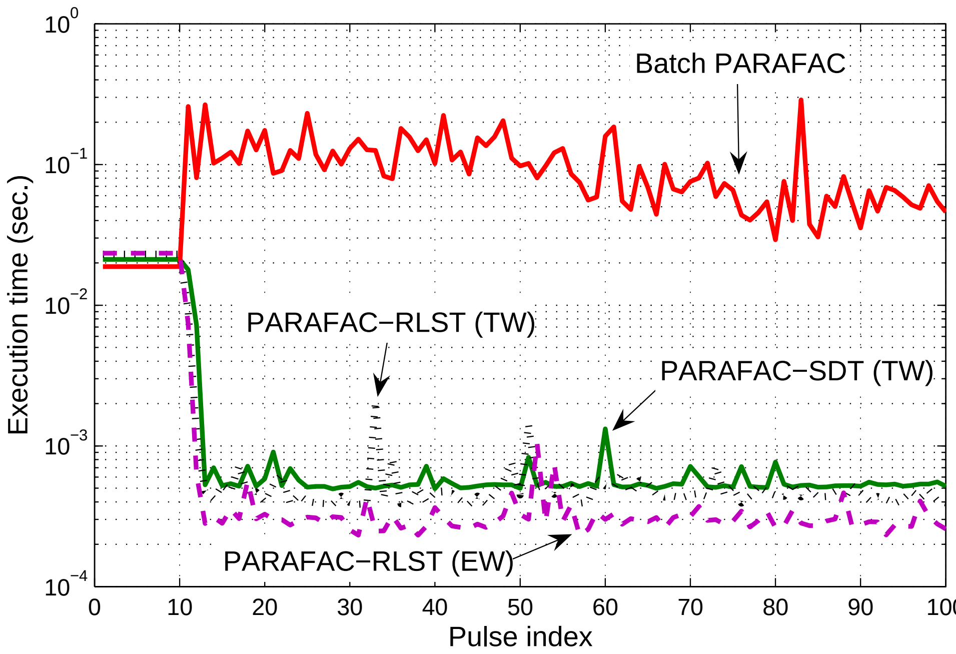


Figure 5: Execution time

Learn more - tutorials, bibliography, papers, software,...

- Group homepage (Nikos Sidiropoulos):
  `www.telecom.tuc.gr/~nikos`
- 3-way group at KVL/DK (Rasmus Bro):
  `http://www.models.kvl.dk/users/rasmus/` and
  `http://www.models.kvl.dk/courses/`
- 3-Mode Company (Peter Kroonenburg):
  `http://www.leidenuniv.nl/fsw/three-mode/3modecy.htm`
- Hard-to-find original papers (Richard Harshman):
  `http://publish.uwo.ca/~harshman/`
- 3-way workshop: TRICAP every 3 years, since '97; 2006, Chania-Crete Greece; 2009, Pyrenees Spain.

What lies ahead & wrap-up

- Take home point: $(N > 3)$-way arrays *are* different; low-rank models unique, have many applications
- Major challenges: Rank & uniqueness: i) rank detection; ii) necessary & sufficient conditions, esp. for higher-way models; iii) uniqueness under application-specific constraints
- Major challenges: Algorithms: Faster at small performance loss; incorporation of application-specific constraints
- New exciting applications: Yours!

Preaching the Gospel of 3-Way Analysis

☞ Thank you!