Décompositions tensorielles et applications

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gipsa-lab

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Representation of multivariate functions

$$\boldsymbol{x} \stackrel{\text{def}}{=} [x_1, \ldots, x_D]$$

-
- Discrete case:

$$F(i,j,..,k) \sum_{r=1}^{R} \lambda_r \, g_{r1}(i) \, g_{r2}(j) \cdots g_{rD}(k)$$

- Approximation

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$$\boldsymbol{x} \stackrel{\text{def}}{=} [x_1, \ldots, x_D]$$

- Parsimony:

$$f(\boldsymbol{x}) = \sum_{r=1}^{R} \lambda_r \, g_r(\boldsymbol{x})$$

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- Separability:

$$f(\boldsymbol{x}) = \prod_{d=1}^{D} h_d(x_d)$$

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Definition (1/2)

- Order D tensor: *multi-linear* map $\mathbb{S}_1 \times \dots \mathbb{S}_m \to \mathbb{S}_{m+1} \times \dots \mathbb{S}_D$
- In this talk, $\mathbf{T}$ is an *array* with D indices, of dimension $I_2 \times I_2 \times \cdots \times I_D$
- **Examples**:
  - bilinear form: $\mathbb{S}_1 \times \mathbb{S}_2 \to \mathbb{K}$, represented by a matrix
  - linear operator: $\mathbb{S}_1 \to \mathbb{S}_2$, represented by a matrix
  - bilinear operator: $\mathbb{S}_1 \times \mathbb{S}_2 \to \mathbb{S}_3$, repres. by a 3-way array
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Definition (2/2)

- *Decomposable* tensor: $E_{ij..k} = u_i\, v_j\, \dots w_k$

$$\mathbf{E} = \boldsymbol{u} \otimes \boldsymbol{v} \otimes \dots \otimes \boldsymbol{w}$$

- **E** may be seen as the discretization of a function in D variables, with *separated variables*:

$$e(x,y,..z) = u(x)\, v(y)..w(z)$$

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Tensor vs array

If bases of linear spaces $\mathbb{S}_\ell$ are fixed, $\{\boldsymbol{e}_p^{(\ell)}, 1 \leq p \leq I_\ell\}$, then

$$\mathcal{T} = \sum_{i,j,..k} T_{ij..k}\ \boldsymbol{e}_i^{(1)} \otimes \boldsymbol{e}_j^{(2)} \otimes \ldots \otimes \boldsymbol{e}_k^{(D)}$$

where $T_{ij..k}$ are the *coordinates* of $\mathcal{T} \Rightarrow \mathcal{T}$ can be arranged in a D-way array.

Usual abuse of notation: assimilate $\mathcal{T}$ with $\mathbf{T}$.

- Array of coordinates changes multi-linearly under linear change of basis: $\mathbf{T}' = (\mathbf{A}, \mathbf{B}, \ldots, \mathbf{C}) \cdot \mathbf{T}$.
- Bases of $\mathbb{S}_\ell$ induce decomposable tensors

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Kronecker product $\otimes$

- product defined *only* between 1-way or 2-way arrays:

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\,\mathbf{B} & \dots & a_{1n}\,\mathbf{B} \\ \vdots & & \vdots \\ a_{m1}\,\mathbf{B} & \dots & a_{mn}\,\mathbf{B} \end{bmatrix}$$

- It should *not be confused* with tensor product $\otimes$.
- **Usefulness:** for convenience, an array with D indices may be stored in larger vectors or matrices. For instance:
  ➽ tensor product $\boldsymbol{a} \otimes \boldsymbol{b}$ can be stored in vector $\boldsymbol{a} \otimes \boldsymbol{b}$ or in matrix $\boldsymbol{a}\,\boldsymbol{b}^{\mathsf{T}}$. *Usual abuse of notation.*
  ➽ tensor $\boldsymbol{a} \otimes \boldsymbol{b} \otimes \boldsymbol{c}$ can be stored in matrix $(\boldsymbol{a} \otimes \boldsymbol{b})\boldsymbol{c}^{\mathsf{T}}$, or in vector $\boldsymbol{a} \otimes \boldsymbol{b} \otimes \boldsymbol{c}$, or in matrix $\boldsymbol{a}\,(\boldsymbol{b} \otimes \boldsymbol{c})^{\mathsf{T}}$, etc...

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Terminology

Let the array $\{T_{ij..k}\}$ associated with tensor $\mathcal{T}$.

- *Order* D of $\mathcal{T}$: # of its *ways* or *modes*
- There are D *dimensions*
- *Cubic* if all dimensions equal
- *Symmetric*: $T_{ij..k} = T_{\sigma(ij..k)}$, $\forall \sigma$ permutation
  e.g. derivatives of a multivariate scalar function
- *Diagonal*: $T_{ij..k} = 0$ unless $i = j = \cdots = k$.

NB: avoid words such as "super-symmetric" or "super-diagonal".

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Decomposable tensor of order $D = 3$

- Take $$\boldsymbol{v} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$
- Then $\boldsymbol{v}^{\otimes 3} \stackrel{\text{def}}{=} \boldsymbol{v} \otimes \boldsymbol{v} \otimes \boldsymbol{v} \rightarrow$ can be represented by
$$\boldsymbol{v}\,(\boldsymbol{v} \otimes \boldsymbol{v})^{\mathsf{T}} = \left[\begin{array}{cc|cc} 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 \end{array}\right]$$
- It is symmetric, and decomposable

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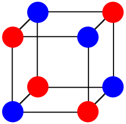

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Claude Elwood Shannon (1916-2001)

Frank Lauren Hitchcock (1875-1957)

Canonical Polyadic decomposition (CP) 1/2

- Every tensor **T** can be written as a sum of decomposable tensors *[Hitchcock'27]*:

$$\mathbf{T} = \sum_{r=1} \lambda_r \, \mathbf{E}(r)$$

- *Rank* of **T** = is the minimal $R(\mathbf{T})$ of necessary terms
- Decomposable $\Leftrightarrow$ rank 1
- $\mathbf{E}(r)$ normalised (scale uniqueness), $\lambda_r \in \mathbb{R}^+$
- Special tensors (positive, symmetric..) $\Rightarrow$ different rank definition!

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Canonical Polyadic decomposition (CP) 2/2

- Explicity writing of CP:

$$\mathbf{T} = \sum_{r=1}^{R} \lambda_r \underbrace{\boldsymbol{u}^{(1)}(r) \otimes \boldsymbol{u}^{(2)}(r) \otimes \ldots \otimes \boldsymbol{u}^{(D)}(r)}_{\mathbf{E}(r)} \tag{1}$$

- CP is *one* possible extension of SVD
- CP is unique if pairs $\{\lambda_r, \mathbf{E}(r)\}$ are uniquely determined, even if $\mathbf{E}(r)$ can be written in different manners (unimodulus scale indeterminacy).

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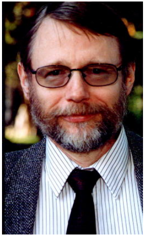
Towards a unique terminology?

- Minimal *Polyadic Form* *[Hitchcock'27]*
- *Canonical decomposition* *[Weinstein'84, Carroll'70, Chiantini-Ciliberto'06, Comon'00, Khoromskij, Tyrtyshnikov]*
- *Parafac* *[Harshman'70, Sidiropoulos'00]*
- *Optimal computation* *[Strassen'83]*
- Minimum-length *additive decomposition* (AD) *[Iarrobino'96]*

Suggestion:

- *Canonical Polyadic decomposition (CP)* *[Comon'08, Grasedyk, Espig...]*
- *CP* does also already stand for Candecomp/Parafac *[Bro'97, Kiers'98, tenBerge'04...]*

Psychometrics



Richard A. Harshman
(1970)

J. Douglas Carroll
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Tucker decomposition

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$$T_{ijk} = \sum_{pqr} A_{ip}\, B_{jq}\, C_{kr}\; G_{pqr}$$

where tensor $\mathcal{G}$ is at most as big as $\mathcal{T}$

- This decomposition is not unique $\rightarrow$ it can be used for compression, but *not* for identification
- **HOSVD (2000)** One can impose matrices **A**, **B** and **C** to be unitary, and core tensor $\mathcal{G}$ to be *all orthogonal*, i.e. its matrix slices to be orthogonal.

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Link with SVD

Matrix SVD, $\mathbf{M} = (\mathbf{U},\mathbf{V}) \cdot \mathbf{\Sigma}$, may be extended in at least two ways to tensors

- **Keep orthogonality:** Tucker, HOSVD

$$\mathcal{T} = (\mathbf{U},\mathbf{V},\mathbf{W}) \cdot \mathcal{C}$$

$\mathcal{C}$ is $R_1 \times R_2 \times R_3$: *multilinear rank* $= (R_1,R_2,R_3)$

- **Keep diagonality:** Canonical Polyadic decomposition (CP)

$$\mathcal{T} = (\mathbf{A},\mathbf{B},\mathbf{C}) \cdot \mathcal{L}$$

$\mathcal{L}$ is $R \times R \times R$ diagonal: $= R$

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$$\mathcal{T} = (\mathbf{U},\mathbf{V},\mathbf{W}) \cdot \mathcal{C}$$

$\mathcal{C}$ is $R_1 \times R_2 \times R_3$: *multilinear rank* $= (R_1,R_2,R_3)$

- **Keep diagonality:** Canonical Polyadic decomposition (CP)

$$\mathcal{T} = (\mathbf{A},\mathbf{B},\mathbf{C}) \cdot \mathcal{L}$$

$\mathcal{L}$ is $R \times R \times R$ diagonal: *rank* $= R$.

CP uniqueness: Kruskal 1/2

The *Kruskal rank* of a matrix **A** is the largest number k_A, such that *any* subset of k_A columns is linearly independent.

CP uniqueness: Kruskal 2/2

Sufficienty condition ensuring uniqueness of CP
[Kruskal'77, Sidiropoulos-Bro'00, Landsberg'09, Rhodes'10]:

Theorem CP unique up to scale factors if R is smaller than the so-called *de Kruskal*'s bound:

$$2R + D - 1 \leq \sum_{d=1}^{D} \mathrm{krank}\{\mathbf{U}^{(d)}\} \tag{2}$$

➡ Bound smaller than *expected rank* $\Rightarrow$ $\exists$ *better bound*, in almost sure sense...

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Approximation

- Presence of additive noise with continuous pdf (rank is generic)
- Choose a smaller rank: redices noise and restores uniqueness

$$\inf_{\substack{\lambda_r,\,\mathbf{E}(r)\\ decomposables}} ||\mathbf{T} - \sum_{r=1}^{R} \lambda_r\, \mathbf{E}(r)||^2 \qquad (3)$$

- But *ill posed* problem: the set of tensors with rank at most R is closed only if $R = 1$ or $R = R_{max}$!

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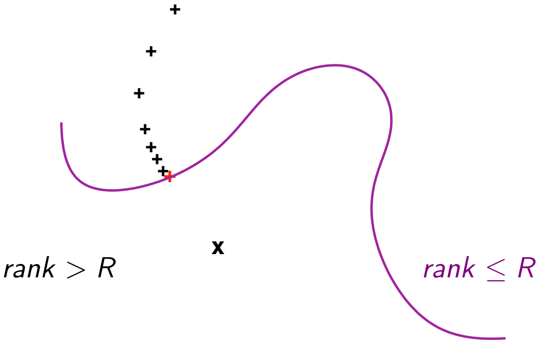
Rang frontière (Border rank)

T a un *rang frontière* $\underline{R} = \underline{rank}\{\mathbf{T}\}$ ssi il est limite de tenseurs de rang $\underline{R}$, et pas limite de tenseurs de rang plus faible
[Bini'79, Schönhage'81, Strassen'83, Likteig'85]



Exemple dans le cas symétrique

Soient $\boldsymbol{u}$ et $\boldsymbol{v}$ deux vecteurs non colinéaires.
On pose $\mathbf{T}_0$ *[Comon et al.'08]*:

$$\mathbf{T}_0 = \boldsymbol{u} \otimes \boldsymbol{u} \otimes \boldsymbol{u} \otimes \boldsymbol{v} + \boldsymbol{u} \otimes \boldsymbol{u} \otimes \boldsymbol{v} \otimes \boldsymbol{u} + \boldsymbol{u} \otimes \boldsymbol{v} \otimes \boldsymbol{u} \otimes \boldsymbol{u} + \boldsymbol{v} \otimes \boldsymbol{u} \otimes \boldsymbol{u} \otimes \boldsymbol{u}$$

Alors la suite $\mathbf{T}_\varepsilon = \frac{1}{\varepsilon}\left[(\boldsymbol{u} + \varepsilon\, \boldsymbol{v})^{\otimes 4} - \boldsymbol{u}^{\otimes 4}\right]$ est de rang 2,

Mais $\mathbf{T}_\varepsilon \to \mathbf{T}_0$ quand $\varepsilon \to 0$

➽ Donc $\text{rank}\{\mathbf{T}_0\} = 4$, et $\underline{\text{rank}}\{\mathbf{T}_0\} = 2$

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Une idée simple

Dans notre exemple, 2 causes:

- certains $\{\lambda_p, \lambda_q\} \to \infty$
- certaines colonnes $\{\boldsymbol{u}^{(d)}(p), \boldsymbol{u}^{(d)}(q)\}$ tendent à être colinéaires dans la CP (1):

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Approches du problème mal posé

1. Imposer l'*orthogonalité* entre les vecteurs $\boldsymbol{u}^{(d)}(r)$ *[Comon'92]*
2. Imposer l'*orthogonalité* entre les tenseurs $\mathbf{E}(r)$ *[Kolda'01]*
3. Empêcher la divergence en imposant une *contrainte de norme* *[Paatero'00]* $\Leftrightarrow$ borner les λ_r
4. Tenseurs non négatifs: imposer la *non négativité* à chaque terme de la CP *[Lim-Comon'09]* $\rightarrow$ "rang non négatif"
5. Pour chaque d, imposer un *angle minimal* entre les vecteurs $\boldsymbol{u}^{(d)}(r)$ *[Lim-Comon'10, Comon-Lim'11]*
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Cohérence

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Condition suffisante d'existence et d'unicité (1/2)

- **Théorème 1 (Existence)** Si

$$\mathrm{rank}\{\mathbf{T}\} < \prod_{d=1}^{D} \mu_d^{-1}$$

alors l'*Inf* est atteint.

Condition suffisante d'existence et d'unicité (2/2)

- **Théorème 2 (Existence et unicité)** Si

$$\left(\prod_{d=1}^{D} \mu_d\right)^{1/D} \leq \frac{D}{2R+D-1}$$

alors la meilleure approximation de rang R existe et est unique, à des facteurs d'échelle de module 1 près.

Référence: arxiv:1212.6663

Applications

1. Analyse de facteurs
2. Sonar, Radar, Télécommunications, Traitement d'antenne
3. Imagerie EEG, ECG
4. Environnement: tenseurs à éléments positifs
5. Complexité arithmétique
6. Compression
7. Codage espace-temps (CDMA)

Tenseurs symétriques

8. Statistiques: cumulants d'ordre supérieur à 2
9. Filtrage de Volterra, compression

Fin

Spectrométrie fluorescente

Mélange inconnu de R solutés

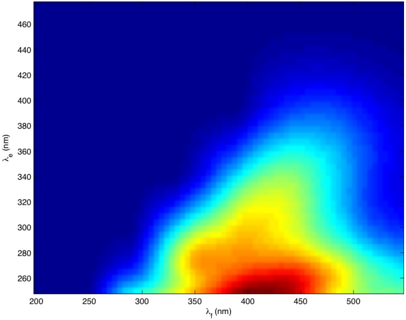
Loi de Beer-Lambert pour de faibles concentrations:

$$I(\lambda_f,\lambda_e,k) = I_o \sum_{\ell=1}^{R} \gamma_\ell(\lambda_f)\,\epsilon_\ell(\lambda_e)\,c_{k,\ell}$$

$\gamma_\ell(\lambda_f)$: spectre de fluorescence
$\epsilon_\ell(\lambda_e)$: spectre d'absorbance
$c_{k,\ell}$: concentration

Thèse Jean-Philip Royer (soutenance avril 2013)

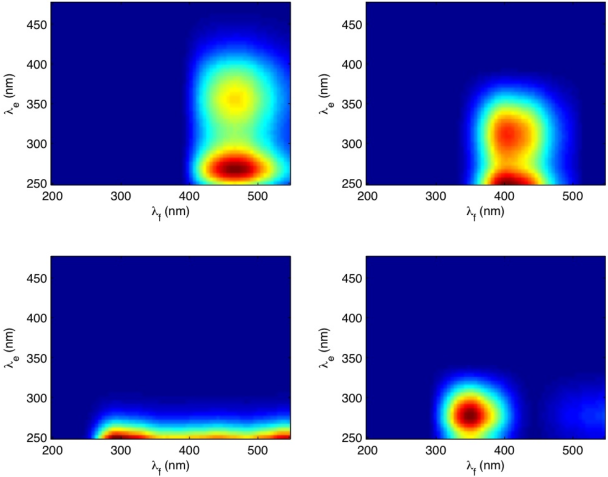
Mélange de 4 solutés (une concentration est représentée)



Fin

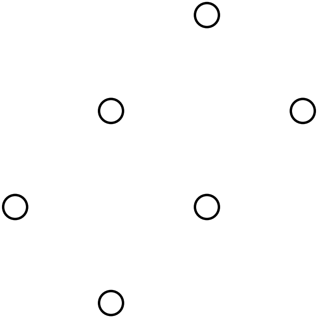
Thèse Jean-Philip Royer (soutenance avril 2013)

Résultat obtenu avec $R = 4$



Antennes structurées (1/3)

Diversité d'espace: invariance par translation



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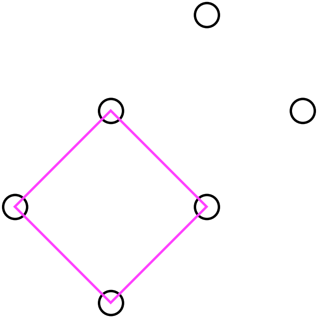

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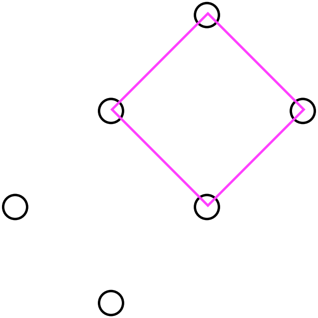

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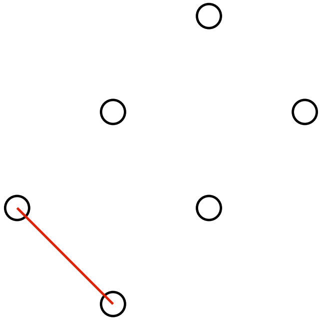

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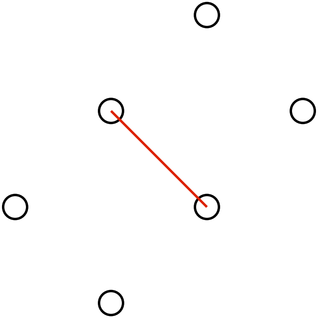

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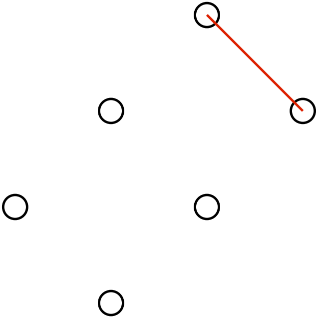

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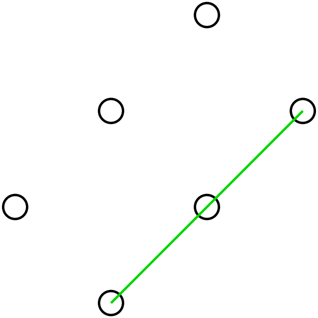

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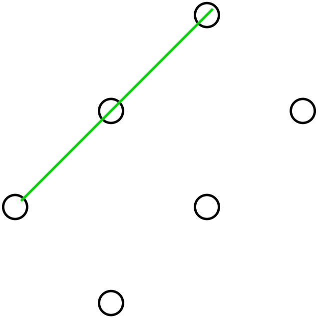

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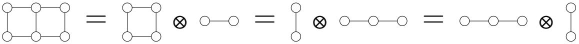

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- **Exemple 3**

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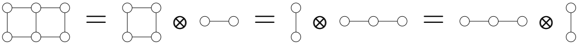

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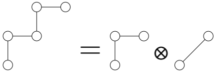

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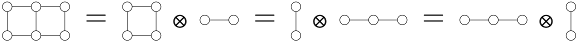

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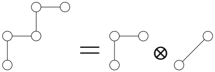

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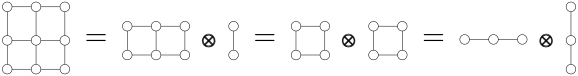

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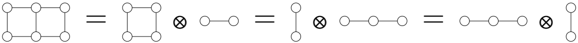

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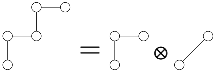

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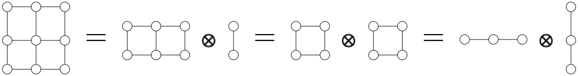

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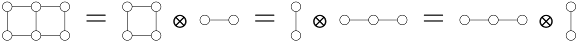

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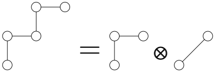

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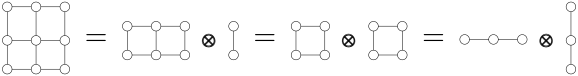

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Structured sensor arrays (3/3)

For narrow-band 3-dimensional transmission in the far field, we have

Definition A sensor array is resolvent w.r.t. direction $\boldsymbol{v}$ if two sensors are less than $\lambda/2$ apart in direction $\boldsymbol{v}$.

Theorem 4 If a subarray is resolvent w.r.t. 3 linearly independent directions, then $\mu_1 = 1$ if and only if two source paths have the same direction of arrival.

Polarization diversity

For narrow-band 3-dimensional transmission in the far field of polarized waves, we can build a $N \times 6 \times T$ tensor, where the second mode represents polarization.

Theorem 5 $\mu_2 = 1$ if and only if two source paths have the same orientation and ellipticity polarization angles, and the same direction of arrival.

Conclusion

One can localize *and* estimate source paths signals if *at least one* on the conditions below is satisfied:

- low correlation between paths
- minimal angular separation between DoA's
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For matrices:

1. Rank cannot exceed dimensions
2. CP is not unique (SVD imposes orthogonality)
3. Rank is the same in real and complex fields
4. Rank of symmetric matrix is the same if CanD is symmetric

For tensors:

1. Rank can largely exceed dimensions
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For matrices:

1. Rank cannot exceed dimensions
2. CP is not unique (SVD imposes orthogonality)
3. Rank is the same in real and complex fields
4. Rank of symmetric matrix is the same if CanD is symmetric

For tensors:

1. Rank can largely exceed dimensions
2. CP is almost surely unique for subgeneric ranks
3. Rank may be different in real and complex fields
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Matrices vs. Tensors (2)

For matrices:

5. Matrices with entries drawn randomly have maximal rank
6. Maximal rank equals generic rank
7. The set of matrices of rank at most r is closed, $\forall r$
8. subtracting the best rank-1 approximate decreases rank by 1

For tensors:

5. Generic rank is not maximal in most cases
6. Maximal rank still unknown for most order/dimensions
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   - Approximation problem ill-posed!
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Further readings

Free-access references:

1. "Tensors, usefulness and unexpected properties," Keynote SSP'09, Cardiff. *hal-00417258*
2. "Tensor Decompositions, Alternating Least Squares and other Tales," *Jour. Chemometrics*, Aug. 2009. *hal-00410057*
3. "Blind Multilinear Identification", Dec 2012. *arxiv:1212.6663*

L'ignorance est la condition nécessaire du bonheur des hommes, et il faut reconnaître que le plus souvent, ils la remplissent bien.
Anatole France (1844-1924)