Decompositions of Higher-Order Tensors: Concepts and Computation

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Canonical Polyadic Decomposition

Rank: minimal number of rank-1 terms [Hitchcock, 1927]

Canonical Polyadic Decomposition (CPD): decomposition in minimal number of rank- $[Harshman '70]$, $[Carroll and Chang '70]$

- Unique under mild conditions on number of terms and differences between terms
- Orthogonality (triangularity, . . .) not required (but may be imposed)

Overview

- Basics: Rank and Canonical Polyadic Decomposition
- Conceptual advances: CPD uniqueness
- Conceptual advances: more general decompositions and variants
- Computational advances: numerical optimization

Rank-1 tensor

• Rank-1 matrix: tensor (outer) product of 2 vectors $\mathbf{u}^{(1)}$, $\mathbf{u}^{(2)}$:

$$
a_{i_1 i_2} = u_{i_1}^{(1)} u_{i_2}^{(2)}
$$

$$
A = u^{(1)} \cdot u^{(2)^T} \equiv u^{(1)} \circ u^{(2)}
$$

• Rank-1 tensor: tensor (outer) product of N vectors $\mathbf{u}^{(1)}$, $\mathbf{u}^{(2)}$, ..., $\mathbf{u}^{(N)}$:

$$
a_{i_1 i_2 \dots i_N} = u_{i_1}^{(1)} u_{i_2}^{(2)} \dots u_{i_N}^{(N)}
$$

$$
A = u^{(1)} \circ u^{(2)} \circ \dots \circ u^{(N)}
$$

Rank of a tensor

• The rank R of a matrix A is minimal number of rank-1 matrices that yield ^A in ^a linear combination.

• The rank R of an Nth-order tensor $\mathcal A$ is the minimal number of rank-1 tensors that yield A in a linear combination.

Rank and dimension

Matrices:

The rank of a $(K \times K)$ matrix is at most equal to K

Tensors:

The rank of a $(K \times K \times \ldots \times K)$ tensor can be greater than K

Partial explanation: number of free tensor parameters: K^N number of parameters in expansion: NKR

Rank and multilinear rank: $R \ge \max(R_1, R_2, \ldots, R_N)$

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Factor Analysis and Blind Source Separation

• Decompose ^a data matrix in rank-1 terms that can be interpreted E.g. statistics, telecommunication, biomedical applications, chemometrics, data analysis, . . .

$$
\mathbf{A}=\mathbf{F}\cdot\mathbf{G}^T
$$

$$
\begin{array}{c|c}\n\hline\n\end{array}\n\qquad = \begin{array}{c}\n\hline\n\end{array}\n\begin{array}{c}\n\overline{\mathbf{g}_1} \\
\hline\n\end{array}\n\begin{array}{c}\n\mathbf{g}_2 \\
\hline\n\end{array}\n\begin{array}{c}\n\mathbf{g}_1 \\
\hline\n\end{array}\n\begin{array}{c}\n\mathbf{g}_R \\
\hline\n\end{array}\n\begin{array}{c}\n\overline{\mathbf{g}_R} \\
\hline\n\end{array}
$$

- **F**: mixing matrix G: source signals
- Decompose ^a data matrix in rank-1 terms that can be interpreted

$$
\begin{array}{|c|c|}\n\hline\n\textbf{A} &=& \boxed{\textbf{g}_1} & & \textbf{g}_2 \\
\hline\n\textbf{f}_1 & & \textbf{f}_2 & & \textbf{f}_R\n\end{array}
$$

• Problem: decomposition in rank-1 terms is not unique

$$
\begin{array}{rcl} \mathbf{A} & = & (\mathbf{F}\mathbf{M}) \cdot (\mathbf{M}^{-1}\mathbf{G}^T) \\ & = & \tilde{\mathbf{F}} \cdot \tilde{\mathbf{G}}^T \end{array}
$$

What about SVD?

- SVD is unique
- ... thanks to orthogonality constraints

$$
\mathbf{A} = \mathbf{U} \cdot \mathbf{S} \cdot \mathbf{V}^T = \sum_{r=1}^R s_{rr} \mathbf{u}_r \mathbf{v}_r^T
$$

^U, ^V orthogonal, ^S diagonal

- Whether these constraints make sense, depends on the application
- SVD is great for dimensionality reduction best rank-R approximation \leftarrow truncated SVD

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Uniqueness: Kruskal's Theorem

Rank: at least one set of $r_{\rm A}$ columns is independent

K-rank: every set of k_A columns is independent $(k_\mathrm{A}\leqslant r_\mathrm{A})$ $(k_\mathrm{A}+1$ is spark)

Theorem:

 $k_{\rm A}+k_{\rm B}+k_{\rm C}\geq 2R+2$

 $\rightarrow r_{\mathcal{T}} = R$ and CPD is unique

[Kruskal '77]

Generic: $\mathbf{A}(I\times R) = \mathbf{B}(J\times R) - \mathbf{C}(K\times R)$ CPD is unique for R bounded by I, J, K as in

 $\min(I, R) + \min(J, R) + \min(K, R) \geqslant 2R + 2$

New conditions

Kruskal-type corollary:

Let at least two of the following conditions hold:

$$
\begin{cases}\nk_{\mathbf{A}} + r_{\mathbf{B}} + r_{\mathbf{C}} \ge 2R + 2\\ \nr_{\mathbf{A}} + k_{\mathbf{B}} + r_{\mathbf{C}} \ge 2R + 2\\ \nr_{\mathbf{A}} + r_{\mathbf{B}} + k_{\mathbf{C}} \ge 2R + 2\n\end{cases}
$$

 $\rightarrow r_{\mathcal{T}} = R$ and CPD is unique

[Domanov, DL '12]

Uniqueness: C has full column rank

CPD: $\mathcal{T} = \sum_{r=1}^R \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r \in \mathbb{C}^{I \times J \times K}$ e.g. C-mode is sample mode

$$
\mathbf{T}_{[1,2;3]} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^T \in \mathbb{C}^{IJ \times K}
$$

Khatri-Rao product second compound matrices:

$$
\mathbf{U} = C_2(\mathbf{A}) \odot C_2(\mathbf{B}) \in \mathbb{C}^{\frac{I(I-1)}{2} \times \frac{I(I-1)}{2} \times \frac{R(R-1)}{2}}
$$

$$
u_{i_1 i_2 j_1 j_2 r_1 r_2} = \begin{vmatrix} a_{i_1 r_1} & a_{i_2 r_1} \\ a_{i_1 r_2} & a_{i_2 r_2} \end{vmatrix} \cdot \begin{vmatrix} b_{j_1 r_1} & b_{j_2 r_1} \\ b_{j_1 r_2} & b_{j_2 r_2} \end{vmatrix}
$$

$$
1 \leq i_1 < i_2 \leq I \quad 1 \leq j_1 < j_2 \leq J \quad 1 \leq r_1 < r_2 \leq R
$$

Theorem: if ^U and ^C have full column rank, then CPD is unique

(proof is constructive)

[Jiang and Sidiropoulos, '04], [DL '06]

Uniqueness: ^C has full column rank (2)

Theorem: if $U \in \mathbb{C}$ $I(I-1)$ 2 $\frac{J(J-1)}{2}{\times}\frac{R(R-1)}{2}$ and $\mathbf{C}\in\mathbb{C}^{K\times R}$ have full column rank, then CPD is unique

Generic: CPD is unique for R bounded by I, J, K as in

$$
\frac{I(I-1)}{2} \frac{J(J-1)}{2} \ge \frac{R(R-1)}{2} \quad \text{and} \quad K \ge R
$$

Approximately: $\frac{IJ}{\sqrt{2}} \geq R$ $K \geq R$

Compare to Kruskal:

 $\min(I, R) + \min(J, R) \ge R + 2$ and $K \ge R$

Recent results

Unifying theory

Constructive proof

Algorithm for Kruskal's condition (and beyond)

[Domanov, DL, '12], [Domanov, DL, '13]

Overview

- Basics: Rank and Canonical Polyadic Decomposition
- Conceptual advances: CPD uniqueness
- Conceptual advances:
	- Block terms
	- Coupled decompositions
	- Constraints
- Computational advances: numerical optimization

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Decomposition in rank- $(L,L,1)$ terms

Unique under mild conditions

[DL '08]

Decomposition in rank- (R_1,R_2,R_3) terms

Unique under mild conditions

Rank-1 term \sim data atom Block term \sim data molecule

[DL '08]

Constraints

Not needed for uniqueness in tensor case

.

Pro: relaxed uniqueness conditions easier interpretation no degeneracy (NN, orthogonality) higher accuracy

Depending on type of constraints, lower or higher computational cost

Coupled matrix/tensor decompositions

One or more matrices

One or more tensors

Symmetric and nonsymmetric

One or more factors shared (or parts of factors, or generators)

Constraints (orthogonal, nonnegative, exponential, constant modulus, polynomial, rational, Toeplitz, Hankel, . . .)

Data fusion

Overview

- Basics: Rank and Canonical Polyadic Decomposition
- Conceptual advances: CPD uniqueness
- Conceptual advances: more general decompositions and variants
- Computational advances:
	- Optimization of complex variables
	- Numerical optimization
	- Exact line and plane search
	- Framework for (constrained) coupled decompositions

Between linear and nonlinear: numerical computation of tensor decompositions

Laurent Sorber, Marc Van Barel and Lieven De Lathauwer

KU LEUVEN

Introduction

What are tensors?

Tensor decompositions

Uniqueness & applications

Complex Optimization

Complex Taylor series

Algorithms and software

Computing tensor decompositions

Tensor optimization

Exact line and plane search

KU LEUVEN

What are tensors?

Tensor decompositions

Uniqueness & applications

[Complex Optimization](#page-26-0)

Complex Taylor series Algorithms and software

Tensor optimization

Exact line and plane search

minimize $f(\mathbf{x})$
 $\mathbf{x} \in \mathbb{R}^n$

\blacktriangleright f is not differentiable w.r.t. z

No real-valued functions are analytic in complex $z!$

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Defacto solution is to minimize $f(z_R)$ **where** $z_R := \begin{bmatrix} Re\{z\} \\ Im\{z\} \end{bmatrix}$ $Im{z}$]︃

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Defacto solution is to minimize $f(z_R)$ **where** $z_R := \begin{bmatrix} Re\{z\} \\ Im\{z\} \end{bmatrix}$

 $Im{z}$]︃

 \blacktriangleright Alternatively, use complex optimization [S, VB, DL]

Consider

$$
\begin{bmatrix} z \\ \overline{z} \end{bmatrix} = \begin{bmatrix} \mathbb{I} & \mathbb{I}i \\ \mathbb{I} & -\mathbb{I}i \end{bmatrix} \cdot \begin{bmatrix} \text{Re}\{z\} \\ \text{Im}\{z\} \end{bmatrix}
$$

$$
z_C = J \cdot z_R
$$

Consider

$$
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$$

$$
z_C = J \cdot z_R
$$

and define the complex gradient as

$$
\frac{\partial f}{\partial z_C} := J^{-T} \cdot \frac{\partial f}{\partial z_R} = \frac{1}{2} \left[\frac{\frac{\partial f}{\partial \text{Re}\{z\}} - \frac{\partial f}{\partial \text{Im}\{z\}} i}{\frac{\partial f}{\partial \text{Re}\{z\}} + \frac{\partial f}{\partial \text{Im}\{z\}} i \right] =: \begin{bmatrix} \frac{\partial f}{\partial z} \\ \frac{\partial f}{\partial \overline{z}} \end{bmatrix}
$$

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$$
Real Taylor series

$$
f(\boldsymbol{z}^{(k)}) + \boldsymbol{p}_{R}^{\mathsf{T}}
$$

$$
\frac{\partial f(\mathbf{z}^{(k)})}{\partial \mathbf{z}_R} + \mathbf{p}_R^{\mathsf{T}} \qquad \qquad \frac{\partial^2 f(\mathbf{z}^{(k)})}{\partial \mathbf{z}_R \partial \mathbf{z}_R^{\mathsf{T}}}
$$

 p_R

Real Taylor series

$$
f(\mathbf{z}^{(k)}) + \mathbf{p}_R^{\mathsf{T}} \cdot \mathbf{J}^{\mathsf{T}} \mathbf{J}^{-\mathsf{T}} \cdot \frac{\partial f(\mathbf{z}^{(k)})}{\partial \mathbf{z}_R} + \mathbf{p}_R^{\mathsf{T}} \cdot \mathbf{J}^{\mathsf{T}} \mathbf{J}^{-\mathsf{T}} \cdot \frac{\partial^2 f(\mathbf{z}^{(k)})}{\partial \mathbf{z}_R \partial \mathbf{z}_R^{\mathsf{T}}} \cdot \mathbf{J}^{\mathsf{T}} \mathbf{J}^{-\mathsf{T}} \cdot \mathbf{p}_R
$$

Real Taylor series

$$
f(\mathbf{z}^{(k)}) + \mathbf{p}_R^{\mathsf{T}} \cdot \mathbf{J}^{\mathsf{T}} \mathbf{J}^{-\mathsf{T}} \cdot \frac{\partial f(\mathbf{z}^{(k)})}{\partial \mathbf{z}_R} + \mathbf{p}_R^{\mathsf{T}} \cdot \mathbf{J}^{\mathsf{T}} \mathbf{J}^{-\mathsf{T}} \cdot \frac{\partial^2 f(\mathbf{z}^{(k)})}{\partial \mathbf{z}_R \partial \mathbf{z}_R^{\mathsf{T}}} \cdot \mathbf{J}^{\mathsf{T}} \mathbf{J}^{-\mathsf{T}} \cdot \mathbf{p}_R
$$

Complex Taylor series

$$
f(z^{(k)}) + \boldsymbol{p}_C^{\mathsf{T}} \cdot \frac{\partial f(z^{(k)})}{\partial z_C} + \boldsymbol{p}_C^{\mathsf{T}} \cdot \frac{\partial^2 f(z^{(k)})}{\partial z_C \partial z_C^{\mathsf{T}}} \cdot \boldsymbol{p}_C
$$

Complex Optimization Toolbox (COT) for MATLAB esat.kuleuven.be/sista/cot

- \triangleright Generalized nonlinear optimization minf_lbfgs.minf_lbfgsdl.minf_ncg
- \triangleright Generalized nonlinear least squares nls_gndl nls_lm nls_gncgs nlsb_gndl
- \triangleright Complex differentiation and Moré-Thuente line search deriv, ls_mt

What are tensors?

Tensor decompositions

Uniqueness & applications

Complex Taylor series

Algorithms and software

[Computing tensor decompositions](#page-41-0)

Tensor optimization

Exact line and plane search

$$
\underset{z\,\in\,\mathbb{C}^n}{\text{minimize}}\ \frac{1}{2}\|\mathcal{M}(z)-\mathcal{T}\|_F^2
$$

where M is multilinear

minimize $\frac{1}{2} \|\mathcal{F}(z)\|_{\text{F}}^2$

where F is multilinear

- \triangleright canonical polyadic decomposition (CPD),
- \blacktriangleright low multilinear rank approximation (LMLRA),
- \blacktriangleright block term decompositions (BTD),
- \blacktriangleright support tensor machines (STM),
- \triangleright coupled tensor-matrix factorizations (CTMF),

CPD of a $9 \times 9 \times 9 \times 9 \times 9$ tensor of rank 11

The step is computed as

$$
p^*=-H^{-1}g
$$

 $f(z,\overline{z}) := \frac{1}{2} \|\mathcal{F}(z)\|_{\text{F}}^2$ is the objective function $\boldsymbol{g}:=2\frac{\partial f}{\partial \overline{z}}$ is the scaled conjugate cogradient $H :=$ is (an approximation of) the complex Hessian

Where H is

 \triangleright a diagonal plus low-rank matrix in quasi-Newton

$$
\blacktriangleright \, J^H J \text{ in NLS and } J := \frac{\partial \mathcal{F}}{\partial z^T}
$$

- \triangleright However, NLS is expensive in both memory and flop/iteration
	- \blacktriangleright $N l^2$ times more memory than ALS
	- \blacktriangleright N^2R^2 times more flop/iteration than ALS

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- Exploit rank-one and diagonal block structure in $J^H J$ to obtain a fast inexact NLS algorithm [S,VB,DL]
	- \triangleright Same memory cost as ALS
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- Exploit rank-one and diagonal block structure in $J^H J$ to obtain a fast inexact NLS algorithm [S,VB,DL]
	- \triangleright Same memory cost as ALS
	- \triangleright Same flop/iteration as ALS for large tensors
- \triangleright Additional benefits (compared to ALS)
	- \blacktriangleright Almost "embarrassingly" parallel Can theoretically achieve peak performance on GPUs
	- \triangleright Robust performance on difficult decompositions

[Algorithm performance comparison](#page-51-0)

Tensorlab — a MATLAB toolbox for tensor decompositions esat.kuleuven.be/sista/tensorlab

- \blacktriangleright Elementary operations on tensors Multicore-aware and profiler tuned
- \blacktriangleright Tensor decompositions with structure and/or symmetry CPD, LMLRA, MLSVD, block term decompositions
- \triangleright Global minimization of bivariate polynomials Exact line and plane search for tensor optimization
- \triangleright Cumulants, tensor visualization, estimating a tensor's rank or multilinear rank, . . .

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minimize
$$
\frac{1}{2} ||\mathcal{M}(z + \alpha \Delta z) - \mathcal{T}||_F^2
$$
 (LS)
\nminimize $\frac{1}{\alpha, \gamma} ||\mathcal{M}(\gamma z + \alpha \Delta z) - \mathcal{T}||_F^2$ (SLS)
\nminimize $\frac{1}{\alpha, \beta} ||\mathcal{M}(z + \alpha \Delta z_1 + \beta \Delta z_2) - \mathcal{T}||_F^2$ (PS)
\nminimize $\frac{1}{\alpha, \beta, \gamma} ||\mathcal{M}(\gamma z + \alpha \Delta z_1 + \beta \Delta z_2) - \mathcal{T}||_F^2$ (SPS)

(S) LS-C and (S) PS- $\mathbb R$ are equivalent to solving

$$
\begin{cases}\n p(x, y) = 0 \\
q(x, y) = 0\n\end{cases}
$$
 where $x, y \in \mathbb{R}$

for some polynomials p and q

How? Newton's method, interval methods, semidefinite programming, Gröbner bases, resultants, homotopy continuation, . . .

[Examples](#page-58-0)

compact_surf

 χ

Examples

curve_issac

Examples

deg16_7_curves

 χ

Examples

deg16_7_curves

 χ

Examples

dfold_10_6

Examples

grid_deg_10

Examples

 \boldsymbol{X}

Examples

spiral29_24

Examples

ten_circles

 $\boldsymbol{\mathsf{X}}$

Examples

vert_lines

 χ

[Algorithm performance comparison](#page-68-0)

Performance profile (low degree)

Tensorlab v2.0

www.tensorlab.net

Tensorlab v1.0

www.tensorlab.net

A MATLAB toolbox for tensor computations

- \blacktriangleright Tensor decompositions cpd lmlra btd
- \blacktriangleright Complex optimization minf_lbfgs nls_gndl
- \blacktriangleright Bivariate polynomial systems polymin2 polysol2
- ▶ Visualization, rank estimation, statistics, . . . voxel3 rankest mlrankest cum4
www.tensorlab.net

Major upgrade which brings:

- ▶ Full support for sparse and incomplete tensors
- \blacktriangleright Structured data fusion

Structured: choose from a large library of constraints to impose on factors (nonnegative, orthogonal, Toeplitz, . . .) Data fusion: jointly factorize multiple data sets

[Tensorlab v2.0](#page-71-0)

Example 1: eigenvalue decomposition

The colleague matrix

$$
A = \begin{bmatrix} 0 & 1/2 & & \\ 1 & 0 & 1/2 & \\ & 1/2 & 0 & \ddots \\ & & & \ddots & \ddots \end{bmatrix}
$$

of order n has eigenvalues

$$
\lambda_i = \cos\left(\frac{\pi(2i+1)}{2n}\right)
$$

for $i = 0, \ldots, n-1$

Example 1: eigenvalue decomposition

```
In MATLAB (solve EVD):
```

```
[V,D] = eig(A);
```
With SDF (define and solve EVD):

```
model.variables.v = randn(size(V));model.variables.d = randn(1, length(D));
```

```
model.factors.V = 'v';model.factors.Vinv = \{'v',@struct_invtransp};
model.factors.D = 'd':
```

```
model.factorizations.evd.data = A;
model.factorizations.evd.cpd = {'V', 'Vinv', 'D'};
sol = sdf_nls(model); % sol.factors, sol.variables
```
[Tensorlab v2.0](#page-71-0)

Example 1: eigenvalue decomposition

Example 2: Netflix \$1M challenge

An incomplete 480k users x 18k movies x 2k timestamps tensor containing 100M integer ratings between 1 and 5 stars

Challenge: predict movie ratings with a RMSE which is 10 % better than Netflix's proprietary Cinematch algorithm

Solution with SDF: model ratings as mean $+$ user bias $+$ movie $bias + time bias + low-rank$

$$
r_{u,m,t} = \mu + b_u + b_m + b_t + \sum_k a_{u,k} b_{m,k} c_{t,k}
$$

Bias vectors are in fact structured rank-1 tensors ⇒ model is a structured CPD

Example 2: Netflix \$1M challenge

We have worked hard so that large data sets such as this 2 GB example can be easily factorized with Tensorlab!

Example 3: InsPyro materials data set

An incomplete tensor in which each dimension represents the concentration of a metal in an alloy (e.g., 9 dimensions)

The tensor's entries are the melting temperatures of an alloy comprising of the selected concentrations

Challenge: predict melting temperatures of different alloys

Solution with SDF: use structured CPD where each factor vector $u_r^{(n)}$ is a sum of RBF kernels

$$
u_{b,r}^{(n)} = \sum_{i=1}^{8} a \exp(-(t-b)^2/(2c^2))
$$

where *a b* and *c* are the free parameters in $\bm{u}_r^{(n)}$

[Tensorlab v2.0](#page-71-0)

Example 4: GPS data set

Five coupled data sets: user-location-activity, user-user, location-feature, activity-activity and user-location

Challenge: predict user participation in activities

Solution with SDF: compute coupled tensor factorization

minimize
\n
$$
\mathcal{L}_{U,L,A,F,\lambda,\mu,\nu} \left\{ \frac{\omega_1}{2} \left\| \mathcal{M}^{(1)}(U,L,A) - \mathcal{T}^{(1)} \right\|_{\mathcal{W}^{(1)}}^2 + \frac{\omega_2}{2} \left\| \mathcal{M}^{(2)}(U,U,\lambda) - \mathcal{T}^{(2)} \right\|^2 + \frac{\omega_3}{2} \left\| \mathcal{M}^{(3)}(L,F) - \mathcal{T}^{(3)} \right\|^2 + \frac{\omega_4}{2} \left\| \mathcal{M}^{(4)}(A,A,\mu) - \mathcal{T}^{(4)} \right\|^2 + \frac{\omega_5}{2} \left\| \mathcal{M}^{(5)}(U,L,\nu) - \mathcal{T}^{(5)} \right\|^2 + \frac{\omega_6}{2} \left(\left\| U \right\|^2 + \left\| L \right\|^2 + \left\| A \right\|^2 + \left\| F \right\|^2 + \left\| \lambda \right\|^2 + \left\| \mu \right\|^2 + \left\| \nu \right\|^2 \right)
$$

[Tensorlab v2.0](#page-71-0)

Example 4: 80% missing entries in user-location-activity tensor

[Tensorlab v2.0](#page-71-0)

Example 4: 50 users missing in user-location-activity tensor

Conclusion

- Complex optimization
- Quasi-Newton/NLS vs ALS
- Exact (scaled) line/plane search
- Sets of two bivariate polynomials in real unknowns
- Structured factors: orthogonal, nonnegative, matrix inverse, Toeplitz, Hankel, sums of exponentials, exponentially damped sinusoids, radial basis functions, exponential polynomials, rational functions, . . .
- Coupled decompositions
- www.tensorlab.net