

Sets of polynomial equations, decompositions of higher-order tensors and multidimensional harmonic retrieval: connections and algorithms

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Thesis voorgedragen tot het behalen
van de graad van Master of Science
in de ingenieurswetenschappen:
wiskundige ingenieurstechnieken

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Voorafgaande schriftelijke toestemming van de promotor is eveneens vereist voor het aanwenden van de in deze masterproef beschreven (originele) methoden, producten, schakelingen en programma's voor industrieel of commercieel nut en voor de inzending van deze publicatie ter deelname aan wetenschappelijke prijzen of wedstrijden.

Dankwoord

Graag behoud ik deze bladzijde voor om enkele mensen te bedanken.

Mijn grote dank gaat uit naar mijn promotor, prof. Lieven De Lathauwer. Hij heeft me het voorbije jaar laten kennismaken met de wondere wereld van de multilineaire algebra. Groot is mijn bewondering voor zijn inzichten en voor de manier waarop hij me wist te prikkelen tot nieuwe ontdekkingen.

Ook dank ik graag mijn begeleider, Dr. Alwin Stegeman, voor de aanzet tot dit werk en voor zijn waardevolle feedback op deze tekst. Hij hielp me om door de bomen het bos te blijven zien.

Verder dank ik de assessoren van deze thesis voor hun tijd en moeite. Ik maak ook van de gelegenheid gebruik om bij uitbreiding alle docenten die verbonden zijn aan de masteropleiding Wiskundige Ingenieurstechnieken, te bedanken. Hun tijd en moeite hebben de opleiding doen uitgroeien tot een stimulerende leeromgeving.

Aan Robyn, m'n vriendin, bedankt voor de steun en voor het begrip. Het zal ongetwijfeld even duren voor we de tijd die naar dit werk is gegaan, samen hebben ingehaald.

Tot slot is een dankwoord voor mama en papa meer dan op z'n plaats. Omdat ze me er op tijd en stond aan herinnerden een back-up te nemen. Maar veel belangrijker was hun onnavolgbare steun en de kans op hoger onderwijs die ze mij geschonken hebben.

Jeroen Vanderstukken

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Abstract

Sets or systems of multivariate polynomial equations arise frequently as the result of modeling in science and engineering. To solve such a system means finding all common roots of the polynomials. Traditional algebraic geometry-based high-precision computer algebra methods are error-prone when the polynomial coefficients are subject to experimental noise. Macaulay (1902) was among the first to look at the problem from a linear algebra point of view. In his Numerical Polynomial Algebra (NPA), Stetter (2004) linked the problem to eigenvalue computations and brought it to the field of numerical linear algebra. Recently, Batselier and Dreesen (2013) built on NPA in their Polynomial Numerical Linear Algebra (PNLA). Applying an ESPRIT-like reasoning that expresses the shift-invariance property of the multivariate monomials, to a numerical basis for the null space of the system's Macaulay matrix, gives an eigenvalue decomposition (EVD) that reveals the common roots. This thesis brings the problem to the field of multilinear algebra: the algebra of higher-order tensors. In this thesis, a tensor is viewed as a higher-order generalization of a vector and a matrix, *i.e.* an array indexed by three or more indexes. A connection between symmetric higher-order tensors and homogeneous polynomials is long known in algebraic geometry. Yet, we take the well-known connections between univariate polynomial root-finding, linear algebra and HR and translate them into connections between their higher-order generalizations: 0-dimensional sets of polynomial equations, multilinear algebra and multidimensional harmonic retrieval (MHR). We rely on the shift-invariance properties in each mode in MHR to jointly exploit the shift-invariance in each variable present in the null space of the Macaulay matrix. The result is in an easily unique third-order tensor canonical polyadic decomposition (CPD) that reveals the roots of the system. No difference between affine and projective roots exists in multilinear algebra. The CPD is exactly the joint EVD of the multiplication tables in NPA — opposed to only one EVD in PNLA. Taking roots with multiplicities into account, a third-order tensor block term decomposition (BTD) arises as a generalization of the CPD. The BTD is exactly the joint triangularization of the multiplication tables in NPA. It sheds a new light on the border rank, the problem of diverging rank-1 terms and the typical rank of a higher-order tensor. The established connections in this thesis can serve as a firm basis for future tensor computation-based and complex optimization-based multivariate polynomial root-finding algorithms.

Notation

Acronyms

BTD	Block Term Decomposition
CPD	Canonical Polyadic Decomposition
ESPRIT	Estimation of Signal Parameters via Rotational Invariance Techniques
EVD	Eigenvalue Decomposition
GEVD	Generalized Eigenvalue Decomposition
HR	Harmonic Retrieval
INDSCAL	Individual Differences in Scaling
MHR	Multidimensional Harmonic Retrieval
MLSVD	Multilinear Singular Value Decomposition
NLS	Nonlinear Least Squares
NPA	Numerical Polynomial Algebra
PHC	Polynomial Homotopy Continuation
PNLA	Polynomial Numerical Linear Algebra
SD	Simultaneous Diagonalization
SVD	Singular Value Decomposition

List of symbols

\mathbb{F}	field
\mathbb{R}	set of the real numbers
\mathbb{C}	set of the complex numbers
\mathbb{C}^I	set of the complex-valued vectors
$\mathbb{C}^{I_1 \times I_2}$	set of the complex-valued matrices
$\mathbb{C}^{I_1 \times \dots \times I_N}$	set of the complex-valued N th-order tensors
\mathbb{P}^n	n -dimensional projective space over \mathbb{C}
\mathcal{C}^n	ring of n -variate polynomials over \mathbb{C}
\mathcal{C}_d^n	vector space of n -variate polynomials up to degree d
\mathcal{P}^n	ring of homogeneous $(n + 1)$ -variate polynomials over \mathbb{C}
\mathcal{P}_d^n	vector space of homogeneous $(n + 1)$ -variate polynomials up to degree d
$\langle f_1, \dots, f_s \rangle$	polynomial ideal generated by the polynomials f_1, \dots, f_s
$[r]$	residue class of the polynomial r in a quotient ring
$\partial_{\mathbf{j}}[\mathbf{z}](f)$	differential functional of f evaluated in \mathbf{z}
$\text{range}(f)$	range of the mapping f
$\text{span}(\{\mathbf{a}_1, \dots, \mathbf{a}_I\})$	span of the vectors $\mathbf{a}_1, \dots, \mathbf{a}_I$
$\text{col}(\mathbf{A})$	column space of the matrix \mathbf{A}
$\text{row}(\mathbf{A})$	row space of the matrix \mathbf{A}
$\text{null}(\mathbf{A})$	right null space of the matrix \mathbf{A}
$r_{\mathbf{A}}$	rank of the matrix \mathbf{A}
$k_{\mathbf{A}}$	Kruskal rank of the matrix \mathbf{A}
$r_{\mathcal{A}}$	rank of the tensor \mathcal{A}
$\text{rank}_n(\mathcal{A})$	n -rank of the tensor \mathcal{A}
$\text{rank}_{\boxplus}(\mathcal{A})$	multilinear rank of the tensor \mathcal{A}
$\mathbf{a} \otimes \mathbf{b}$	outer product of the vectors \mathbf{a} and \mathbf{b}
$\mathbf{A} \otimes \mathbf{B}$	Kronecker product of the matrices \mathbf{A} and \mathbf{B}
$\mathbf{A} \odot \mathbf{B}$	Khatri-Rao product of the matrices \mathbf{A} and \mathbf{B}
$\mathcal{A} \cdot_n \mathbf{B}$	n -mode product of the tensor \mathcal{A} and the matrix \mathbf{B}
$\langle \mathcal{A}, \mathcal{B} \rangle$	inner product of the tensors \mathcal{A} and \mathcal{B}
$\ \mathcal{A}\ $	Frobenius norm of the tensor \mathcal{A}
$\llbracket \mathbf{U}^{(1)}, \dots, \mathbf{U}^{(N)} \rrbracket$	CPD with factor matrices $\mathbf{U}^{(1)}, \dots, \mathbf{U}^{(N)}$
$\text{diag}(\mathbf{a})$	diagonal matrix with the vector \mathbf{a} on its diagonal
$\text{vec}(\mathbf{A})$	vectorization of the matrix \mathbf{A}
\mathbf{I}_I	identity matrix of size $I \times I$
$\mathcal{C}_k(\mathbf{A})$	k th compound matrix of \mathbf{A}
$\mathbf{M}(d)$	Macaulay matrix of degree d
\mathcal{M}_d	row space of $\mathbf{M}(d)$

Chapter 1

Introduction

This chapter introduces the problem of solving a set of multivariate polynomial equations in Section 1.1. Polynomial equations arise very often as the result of modeling in science and engineering. Section 1.1 contains examples covering existing methods to solve the problem. In Section 1.2, higher-order tensors and their applications are introduced. Section 1.3 states the goal of this thesis and Section 1.4 comments on the structure of the text.

1.1 Sets of Polynomial Equations

1.1.1 Problem Statement

Definition 1.1.1 (system of polynomial equations).

$$\begin{cases} f_1(x_1, x_2, \dots, x_n) = 0 \\ \vdots \\ f_s(x_1, x_2, \dots, x_n) = 0 \end{cases} \quad (1.1)$$

where each f_i , $1 \leq i \leq s$ is a polynomial of degree d_i in the n unknowns $x_j \in \mathbb{C}$, $1 \leq j \leq n$, is a set or a system of s polynomial equations.

The goal of solving (1.1) is to find all common roots $(x_1 \dots x_n)^T \in \mathbb{C}^n$ of the polynomials f_i . This problem is ubiquitous in science and engineering.

1.1.2 Existing Methods

The problem of solving (1.1) has been studied extensively in pure mathematics as well. The many methods for approximating the square root of a real number $a \in \mathbb{R}$, dating back to the ancient Babylonians and Greeks, are in fact algorithms to solve the univariate¹ polynomial equation $x^2 - a^2 = 0$. The Fundamental Theorem of

¹ $n = 1$ in (1.1).

Algebra, which was proven for the first time by the German mathematician Carl F. Gauss (1799) and which states that

Every polynomial equation having complex coefficients and at least degree one, has at least one complex root [46],

is also the solution to a univariate root-finding problem. The field of modern mathematics that is concerned with the study of multivariate polynomials is algebraic geometry. Most of the computational methods to solve (1.1) that have become available in computer algebra, require symbolic manipulations in very high precision. They compute a so-called *Gröbner basis* for the system at hand. One seminal method to compute a Gröbner basis for a given set of polynomials is due to Buchberger (1965) [4].

Example 1.1.1. [41, Example 1.3.1] Consider the system of multivariate polynomial equations

$$\begin{cases} f_1(x_1, x_2) = x_1x_2 - 2x_2 = 0 \\ f_2(x_1, x_2) = 2x_2^2 - x_1^2 = 0 \end{cases}$$

where $s = n = 2$ and $d_1 = d_2 = 2$. Fig. 1.1a shows the zero level curves² of f_1 and f_2 . The system defines a basis³

$$M = \{x_1x_2 - 2x_2, 2x_2^2 - x_1^2\}.$$

The Buchberger algorithm computes an alternative, Gröbner basis for $\text{span}(M)$. The result of the algorithm is dependent on the ordering agreed upon for the monomials. A widely used monomial ordering scheme is the degree negative lexicographic order, which will be properly defined in Chapter 2. For now, it suffices to say that the scheme orders monomials by decreasing degree and decreasing index, such that $1 < x_1 < x_2 < x_1^2 < x_1x_2 < x_2^2 < \dots$. The Gröbner basis found is

$$G = \{-2x_1^2 + x_1^3, x_1x_2 - 2x_2, 2x_2^2 - x_1^2\}.$$

The roots of the original system are then the same as the roots of

$$\begin{cases} g_1(x_1, x_2) = -2x_1^2 + x_1^3 = 0 \\ g_2(x_1, x_2) = x_1x_2 - 2x_2 = 0 \\ g_3(x_1, x_2) = 2x_2^2 - x_1^2 = 0 \end{cases}$$

Evidently, the roots of the latter system are much easier to compute, since one only has to solve the univariate root-finding problem⁴ $g_1(x_1) = 0$ for x_1 , and substitute the obtained values in g_2 and g_3 . Fig. 1.1b illustrates the equivalence with solving the original system. In Chapter 4, we will reconsider the original system.

²The zero level curve of f is the set of points \mathbf{x} where $f(\mathbf{x}) = 0$.

³In Chapter 2, it will become clear that this is a basis for a *polynomial ideal*.

⁴See Example 1.1.2.

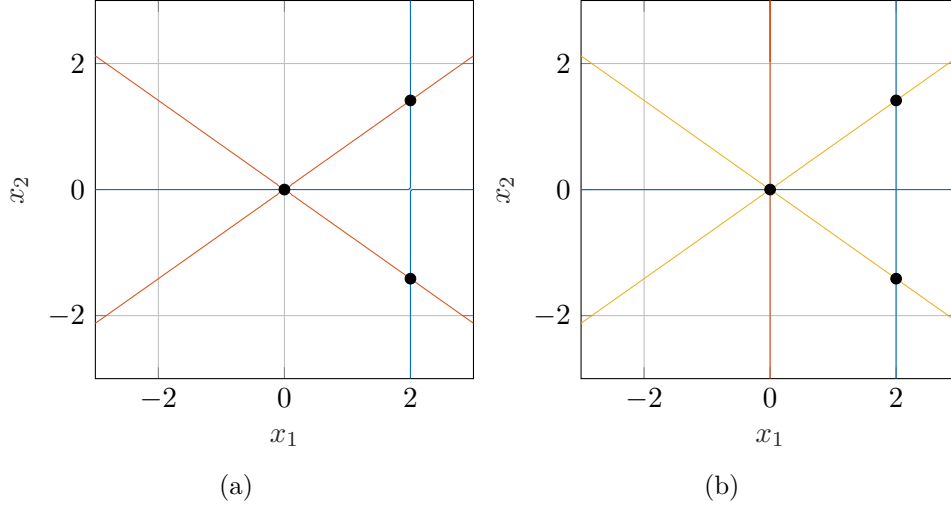


Figure 1.1: (a) The (real part of the) zero level curves of f_1 (—) and f_2 (—) in Example 1.1.1. (b) The same, but of g_1 (—), g_2 (—) and g_3 (—). The solutions are marked with ‘•’.

The Buchberger algorithm is still implemented in computer algebra tools such as Mathematica and Maple. However, not only are the symbolic operations for computing a Gröbner basis involved and subject to numerical infeasibilities and instabilities, the high-precision results in exact arithmetic are also not very meaningful when the coefficients in (1.1) are derived from measured data [22, 23].

Among the first to look at the problem from a linear algebra point of view, were Sylvester (1853) and Macaulay (1902). In the simplest form, $s = n = 1$ in (1.1), and the problem of solving (1.1) becomes a univariate polynomial root-finding problem. Connections between univariate polynomial root-finding, linear algebra and systems theory are well-known [22].

Example 1.1.2. Consider the linear time-invariant (LTI) discrete-time single-output autonomous system, governed by the difference equation

$$y_{k+2} - \frac{5}{6}y_{k+1} + \frac{1}{6}y_k = 0 \quad (1.2)$$

where y_k is the output at instant k . Fig. 1.2a shows the output of system (1.2) for the initial condition $\begin{pmatrix} y_0 & y_1 \end{pmatrix}^T = \begin{pmatrix} 0 & \frac{1}{6} \end{pmatrix}^T$. Taking the Z-transform⁵, we may associate the polynomial equation of degree $d = 2$

$$f(x) = a_d x^2 + a_{d-1}x + a_{d-2} = x^2 + a_1x + a_0 = x^2 - \frac{5}{6}x + \frac{1}{6} = 0 \quad (1.3)$$

with (1.2). Fig. 1.3a shows $f(x)$. In systems theory, the roots of f are called the poles of system (1.2). They determine the dynamical behavior of the system. A

⁵The Z-transform of y_k is $\mathcal{Z}\{y_k\} = \sum_{k=-\infty}^{\infty} y_k x^{-k}$.

well-known result from linear algebra states that the roots of f with $a_d = 1$ in (1.3), i.e. the poles, can be obtained as the eigenvalues of the Frobenius companion matrix [21, 22]

$$\mathbf{A} = \left(\begin{array}{c|c} \mathbf{0}_{d-1 \times 1} & \mathbf{I}_{d-1 \times d-1} \\ \hline -a_0 & \dots & -a_{d-1} \end{array} \right) = \begin{pmatrix} 0 & 1 \\ -\frac{1}{6} & \frac{5}{6} \end{pmatrix}. \quad (1.4)$$

The poles are equal to $x^{(1)} = \frac{1}{2}$ and $x^{(2)} = \frac{1}{3}$ (Fig. 1.2b). The matrix \mathbf{A} in (1.4) is called the system matrix of (1.2) in realization theory.

[34] shows how a technique named ESPRIT in signal processing yields the eigenvalue decomposition (EVD). The two roots of f generate two Vandermonde-structured vectors \mathbf{x} in the null space of the coefficient “matrix” \mathbf{f}^T of (1.3):

$$\mathbf{f}^T \mathbf{x} = \begin{pmatrix} \frac{1}{6} & -\frac{5}{6} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ x \\ x^2 \end{pmatrix} = \mathbf{0}.$$

Write now

$$\mathbf{V} = \begin{pmatrix} \mathbf{x}^{(1)} & \mathbf{x}^{(2)} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ x^{(1)} & x^{(2)} \\ x^{(1)2} & x^{(2)2} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \frac{1}{2} & \frac{1}{3} \\ \frac{1}{4} & \frac{1}{9} \end{pmatrix},$$

then we have that

$$\bar{\mathbf{V}} = \underline{\mathbf{V}} \mathbf{D} \quad (1.5)$$

where $\mathbf{D} = \text{diag}(x^{(1)}, x^{(2)})$ and $\bar{\mathbf{V}}$ and $\underline{\mathbf{V}}$ denote \mathbf{V} with the first and last row removed, respectively. Because the shift-invariance property (1.5) is a property of the entire null space of \mathbf{f}^T , it holds for any basis \mathbf{K} where $\mathbf{V} = \mathbf{K}\mathbf{T}$ and \mathbf{T} is an invertible transformation matrix. (1.5) becomes

$$\bar{\mathbf{K}}\mathbf{T} = \underline{\mathbf{K}}\mathbf{T}\mathbf{D}. \quad (1.6)$$

By computing the so-called column echelon basis⁶ for the null space of \mathbf{f}^T

$$\mathbf{K} = \mathbf{H} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ -\frac{1}{6} & \frac{5}{6} \end{pmatrix}, \quad \text{where} \quad \mathbf{T} = \mathbf{U} = \begin{pmatrix} 1 & 1 \\ \frac{1}{2} & \frac{1}{3} \end{pmatrix}, \quad (1.7)$$

the shift-invariance property (1.6) becomes the EVD of the matrix \mathbf{A} in (1.4):

$$\begin{pmatrix} 0 & 1 \\ -\frac{1}{6} & \frac{5}{6} \end{pmatrix} \mathbf{U} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \mathbf{U} \mathbf{D} \Leftrightarrow \mathbf{A} \mathbf{U} = \mathbf{U} \mathbf{D}.$$

The eigenvalues of \mathbf{A} are indeed $x^{(1)}$ and $x^{(2)}$. Note that the eigenvectors in \mathbf{U} are also Vandermonde-structured vectors that reveal the roots. A similar line of reasoning will form the foundation for the work in this thesis.

⁶We will not elaborate on how to compute \mathbf{H} , as it is hardly ever done in practice.

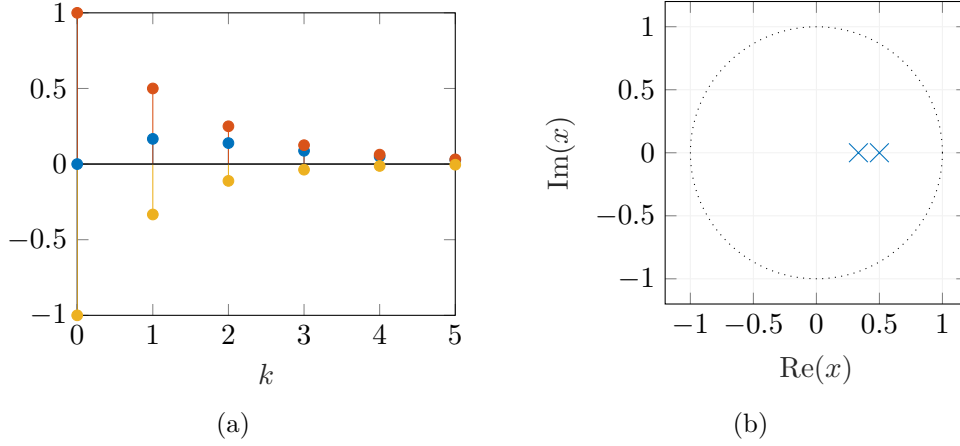


Figure 1.2: (a) Output y_k (—) of the system (1.2), $(\frac{1}{2})^k$ (—) and $-(\frac{1}{3})^k$ (—). (b) Poles of the system in the complex plane.

The output y_k of (1.2) can now be found as

$$y_k = \alpha x^{(1)k} + \beta x^{(2)k} = \alpha \left(\frac{1}{2}\right)^k + \beta \left(\frac{1}{3}\right)^k \quad (1.8)$$

where α and β are determined to match the given initial condition, i.e. $\alpha = 1$ and $\beta = -1$. The contributions of both terms in (1.8) are indeed visible in Fig. 1.2a.

Consider now the case $n = 1$, but $s > 1$. Sylvester showed that the common roots of two univariate polynomials can be found by constructing the *Sylvester matrix*.

Example 1.1.3. [24, Example 2] Consider the system of polynomial equations

$$\begin{cases} f_1(x) = x^3 + 2x^2 - 5x - 6 = 0 \\ f_2(x) = x^2 - x - 2 = 0 \end{cases}$$

where $d_1 = 3$ and $d_2 = 2$. The $(d_1 + d_2) \times (d_1 + d_2)$ Sylvester matrix is obtained by multiplying each f_i with powers of x such that at most a total degree $d_1 + d_2 - 1 = 4$ is reached. This corresponds to shifting the \mathbf{f}_i^T to the right and stacking the shifted coefficient vectors as rows in the Sylvester matrix in (1.9). It should be clear that the common roots of f_1 and f_2 then generate Vandermonde-structured vectors in the null space of the Sylvester matrix:

$$\begin{matrix} f_1(x) \\ x f_1(x) \\ f_2(x) \\ x f_2(x) \\ x^2 f_2(x) \end{matrix} \begin{pmatrix} -6 & -5 & 2 & 1 & 0 \\ 0 & -6 & -5 & 2 & 1 \\ -2 & -1 & 1 & 0 & 0 \\ 0 & -2 & -1 & 1 & 0 \\ 0 & 0 & -2 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ x \\ x^2 \\ x^3 \\ x^4 \end{pmatrix} = \mathbf{0}. \quad (1.9)$$

If there lies (at least) one non-trivial Vandermonde-structured vector in the null space of the Sylvester matrix, the two polynomials have (at least) one common root.

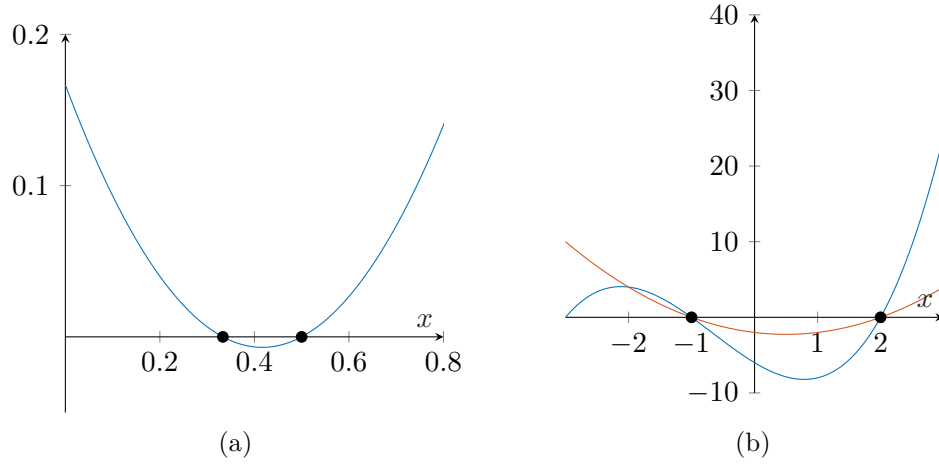


Figure 1.3: (a) The graph of f in (1.3). (b) The graphs of f_1 (—) and f_2 (—) in Example 1.1.3.

Equivalently, the determinant of the Sylvester matrix, which was shown to be equal to the so-called resultant⁷ of f_1 and f_2 , will be zero. By exploiting again the shift-invariance property of the null space of the Sylvester matrix, one could once more find these structured vectors from an EVD. Here, the rank of the Sylvester matrix is 3. There are two linearly independent Vandermonde-structured vectors in the null space of the Sylvester matrix. The common roots are $x^{(1)} = -1$ and $x^{(2)} = 2$ (Fig. 1.3b).

For a “true” system of multivariate polynomial equations, i.e. the case $s > 1$ and $n > 1$, Macaulay showed that the solutions can be found by constructing the *Macaulay matrix* $\mathbf{M}(d)$. $\mathbf{M}(d)$ is dependent on a variable degree d . Example 1.1.4 illustrates that $\mathbf{M}(d)$ is a generalization of the Sylvester matrix to the case $n > 1$.

Example 1.1.4. [21, p. 17] Consider the system of $s = 2$ polynomial equations in $n = 2$ variables

$$\begin{cases} f_1(x_1, x_2) = -x_1^2 + 2x_1x_2 + x_2^2 + 5x_1 - 3x_2 - 4 = 0 \\ f_2(x_1, x_2) = x_1^2 + 2x_1x_2 + x_2^2 - 1 = 0 \end{cases}$$

where $d_1 = d_2 = 2$. Fig. 1.4a shows the zero level curves of f_1 and f_2 . In the generic $s = n$ case, where (1.1) has a zero-dimensional solution set⁸, the number of affine solutions is given by the Bézout number

$$m = \prod_{i=1}^n d_i = 2 \cdot 2 = 4.$$

⁷The resultant of two polynomials f_1 and f_2 is itself a polynomial in the coefficients of f_1 and f_2 that is equal to zero iff the two polynomials have (at least) one common root.

⁸Note that the case $s = 1$ and $n > 1$ generates a higher-dimensional solution set, e.g., the one-dimensional zero level curve of f_1 or f_2 only in Fig. 1.4a. We will not consider this case any further.

Indeed, the $m = 4$ intersections in Fig. 1.4a at $(x_1 \ x_2)^T = (0 \ -1)^T$, $(1 \ 0)^T$, $(3 \ -2)^T$ and $(4 \ -5)^T$ are the sought for solutions.

As a generalization of the Sylvester matrix, the Macaulay matrix $\mathbf{M}(d)$ contains as its rows shifts of each \mathbf{f}_i^T , where the shifts are now the results of multiplying each f_i with monomials of degrees $\leq d - d_i \in \mathbb{N}$ in x_1 and x_2 .

Because $d_1 = d_2 = 2$, we start at $d = 2$. $\mathbf{M}(2)$ contains as its rows shifts that are the results of multiplying each f_i with each $x_j^{2-2} = x_j^0 = 1$, $1 \leq j \leq 2$: $\mathbf{M}(2)$ in (1.10) contains no shifts. It should again be clear that the common roots of f_1 and f_2 generate bivariate Vandermonde-structured vectors in the null space of $\mathbf{M}(2) \in \mathbb{R}^{2 \times 6}$:

$$\begin{array}{c} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{array} \begin{array}{c} 1 \\ \left(\begin{array}{c|cc|ccc} -4 & 5 & -3 & -1 & 2 & 1 \\ -1 & 0 & 0 & 1 & 2 & 1 \end{array} \right) \end{array} \begin{array}{c} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_1x_2 \\ x_2^2 \end{array} = \mathbf{0} \quad (1.10)$$

where we have adopted the degree negative lexicographic order for the monomials. The rank of $\mathbf{M}(2)$ is 2, hence its nullity⁹ is 4. Indeed, the $m = 4$ solutions in Fig. 1.4a give rise to a linearly independent set, for which

$$\begin{array}{c} \left(\begin{array}{c|cc|ccc} -4 & 5 & -3 & -1 & 2 & 1 \\ -1 & 0 & 0 & 1 & 2 & 1 \end{array} \right) \end{array} \begin{array}{c} 1 \\ 0 \\ -1 \\ 0 \\ 0 \\ 1 \end{array} \begin{array}{c} 1 \\ 1 \\ 3 \\ 0 \\ 0 \\ 0 \end{array} \begin{array}{c} 1 \\ 3 \\ -2 \\ 9 \\ -6 \\ 4 \end{array} \begin{array}{c} 1 \\ 4 \\ -5 \\ 16 \\ -20 \\ 25 \end{array} = \mathbf{0},$$

i.e. the linearly independent set is a basis for the null space of $\mathbf{M}(2)$.

At $d = 3$, $\mathbf{M}(3)$ contains four additional rows, as the result of multiplying both f_1 and f_2 with x_1 and x_2 .

$$\begin{array}{c} f_1(x_1, x_2) \\ f_2(x_1, x_2) \\ x_1 f_1(x_1, x_2) \\ x_2 f_1(x_1, x_2) \\ x_1 f_2(x_1, x_2) \\ x_2 f_2(x_1, x_2) \end{array} \begin{array}{c} 1 \\ \left(\begin{array}{c|cc|ccc|ccc|cc} -4 & 5 & -3 & -1 & 2 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & -4 & 0 & 5 & -3 & 0 & -1 & 2 & 1 & 0 \\ 0 & 0 & -4 & 0 & 5 & -3 & 0 & -1 & 2 & 1 \\ 0 & -1 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \end{array} \right) \end{array} \begin{array}{c} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_1x_2 \\ x_2^2 \\ x_1^3 \\ x_1^2x_2 \\ x_1x_2^2 \\ x_2^3 \end{array} = \mathbf{0}. \quad (1.11)$$

⁹The dimension of the right null space.

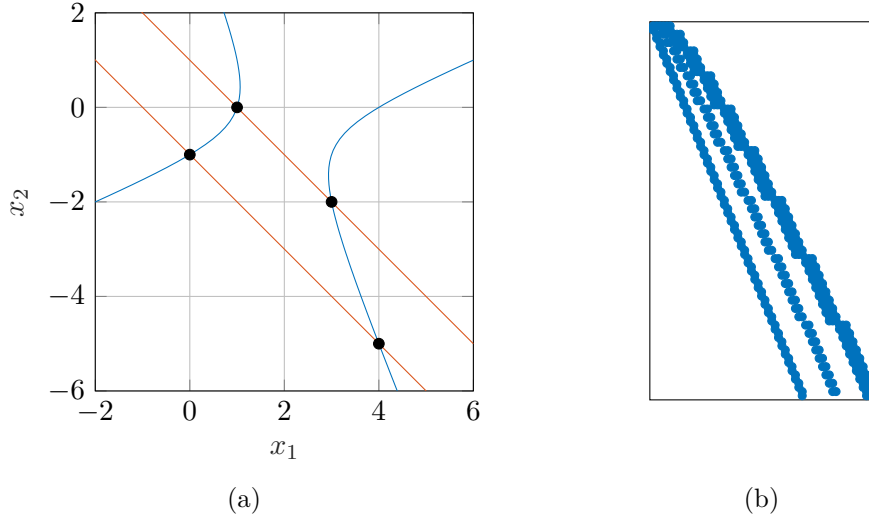


Figure 1.4: (a) The zero level curves of f_1 (—) and f_2 (—) and (b) sparsity plot of the structured Macaulay matrix $\mathbf{M}(10)$ in Example 1.1.4.

Consequently, the dimension of the embedding space of the row space of $\mathbf{M}(3)$ grows to 10, and the Vandermonde-structured vectors reach the additional monomials x_1^3 , $x_1^2x_2$, $x_1x_2^2$ and x_2^3 . It can be verified that the rank of $\mathbf{M}(3)$ has increased to 6 now, but its nullity $10 - 6 = 4$ has remained the same: equal to the number of solutions m .

The number of monomials in n variables grows rapidly with d and the Macaulay matrix $\mathbf{M}(d)$ soon becomes very large. As can already be appreciated from (1.11), $\mathbf{M}(d)$ is a very structured and sparse matrix though. $\mathbf{M}(10) \in \mathbb{R}^{90 \times 66}$ in Fig. 1.4b has a relative number of 7.5% nonzero elements. The number keeps decreasing as d grows.

Lazard (1981), Emiris and Mourrain (1999) and Stetter (2004), a.o., built on the work by Sylvester and Macaulay [22]. Stetter successfully established a link between solving (1.1) and eigenvalue computations in his work Numerical Polynomial Algebra (NPA) [40]. The work was a milestone to take the problem of solving systems of multivariate polynomial equations to the field of numerical linear algebra.

However, NPA still required the computation of a Gröbner basis before proceeding to the numerical eigenvalue computations [23]. This encouraged Batselier and Dreesen (2013) to develop their Polynomial Numerical Linear Algebra (PNLA) framework, which requires no symbolic manipulations of any kind. The Macaulay matrix takes a central position in this framework instead [2, 21]. An eponymous Matlab implementation of all the presented algorithms accompanies PNLA [1]. We will use parts of it for the numerical experiments in Chapter 3 and 4. Example 1.1.5 shows how the linear algebra-based reasoning from Example 1.1.2 can also be applied to solve the system of polynomial equations in Example 1.1.4.

Recently, [41] has derived and implemented a numerical linear algebra two-parameter eigenvalue approach to solve systems of bivariate polynomials. Probably

the most popular numerical method to solve a system of multivariate polynomial equations is numerical polynomial homotopy continuation (PHC) [44]. We will come back to it later.

Example 1.1.5. Consider the system in Example 1.1.4 again. In the generic case, it suffices to construct the Macaulay matrix for degree

$$d = \sum_{i=1}^n d_i - n + 1 = 2 + 2 - 2 + 1 = 3,$$

to find the solutions in the PNLA framework [21]. Write

$$\mathbf{V} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ x_1^{(1)} & x_1^{(2)} & x_1^{(3)} & x_1^{(4)} \\ x_2^{(1)} & x_2^{(2)} & x_2^{(3)} & x_2^{(4)} \\ \hline x_1^{(1)2} & x_1^{(2)2} & x_1^{(3)2} & x_1^{(4)2} \\ x_1^{(1)}x_2^{(1)} & x_1^{(2)}x_2^{(2)} & x_1^{(3)}x_2^{(3)} & x_1^{(4)}x_2^{(4)} \\ x_2^{(1)2} & x_2^{(2)2} & x_2^{(3)2} & x_2^{(4)2} \\ \hline x_1^{(1)3} & x_1^{(2)3} & x_1^{(3)3} & x_1^{(4)3} \\ x_1^{(1)2}x_2^{(1)} & x_1^{(2)2}x_2^{(2)} & x_1^{(3)2}x_2^{(3)} & x_1^{(4)2}x_2^{(4)} \\ x_1^{(1)}x_2^{(1)2} & x_1^{(2)}x_2^{(2)2} & x_1^{(3)}x_2^{(3)2} & x_1^{(4)}x_2^{(4)2} \\ x_2^{(1)3} & x_2^{(2)3} & x_2^{(3)3} & x_2^{(4)3} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 3 & 4 \\ -1 & 0 & -2 & -5 \\ \hline 0 & 1 & 9 & 16 \\ 0 & 0 & -6 & -20 \\ 1 & 0 & 4 & 25 \\ \hline 0 & 1 & 27 & 64 \\ 0 & 0 & -18 & -80 \\ 0 & 0 & 12 & 100 \\ -1 & 0 & -8 & -125 \end{pmatrix}$$

for the “multivariate Vandermonde” basis of the null space of $\mathbf{M}(3)$. By exploiting the multiplicative shift structure of the multivariate Vandermonde basis, it holds that

$$\begin{pmatrix} 1 \\ x_1 \\ x_2 \\ \hline x_1^2 \\ x_1x_2 \\ x_2^2 \\ \hline x_1^3 \\ x_1^2x_2 \\ x_1x_2^2 \\ x_2^3 \end{pmatrix} x_1 = \begin{pmatrix} x_1 \\ x_1^2 \\ x_1x_2 \\ \hline x_1^3 \\ x_1^2x_2 \\ x_1x_2^2 \\ \hline x_1^4 \\ x_1^3x_2 \\ x_1^2x_2^2 \\ x_1x_2^3 \end{pmatrix},$$

where $x = x^{(k)}$, $1 \leq k \leq 4$. The effect of multiplying the left-hand side with x_1 is a particular row selection in the right-hand side of that same left-hand side. Note that the last four monomials in the right-hand side do not occur in \mathbf{V} . Let therefore $\mathbf{S}_0, \mathbf{S}_1 \in \mathbb{R}^{6 \times 10}$ denote the row-selection matrices that select all rows of \mathbf{V} from degree 0 up to $d - 1 = 2$, and the rows onto which they are mapped after multiplication with x_1 ¹⁰, respectively. Then we have that

$$\mathbf{S}_0 \mathbf{V} \mathbf{D}_1 = \mathbf{S}_1 \mathbf{V}$$

¹⁰We could as well have expressed the multiplication of all rows with x_2 .

where $\mathbf{D}_1 = \text{diag}(x_1^{(1)}, \dots, x_1^{(4)})$. In practice, not \mathbf{V} , but a numerical basis \mathbf{K} for the null space of $\mathbf{M}(3)$, where $\mathbf{V} = \mathbf{K}\mathbf{T}$ and \mathbf{T} is an invertible transformation matrix, can be calculated, e.g., using the `null` command in Matlab.

$$\mathbf{S}_0 \mathbf{K} \mathbf{T} \mathbf{D}_1 = \mathbf{S}_1 \mathbf{K} \mathbf{T} \quad (1.12)$$

is a rectangular generalized eigenvalue decomposition (GEVD). It can be converted into a square EVD

$$\mathbf{T} \mathbf{D}_1 \mathbf{T}^{-1} = (\mathbf{S}_0 \mathbf{K})^\dagger \mathbf{S}_1 \mathbf{K}.$$

The eigenvalues correspond to the x_1 components of the solutions. Calculating $\mathbf{V} = \mathbf{K}\mathbf{T}$ shows all solution components. It also becomes clear now why it is not sufficient to construct $\mathbf{M}(2)$: $\mathbf{S}_0, \mathbf{S}_1 \in \mathbb{R}^{3 \times 6}$, and a 3×3 EVD cannot reveal the $m = 4$ solutions.

1.2 Higher-Order Tensors

1.2.1 Multi-Way Arrays

Definition 1.2.1 (tensor). [31, p. 452] A tensor is a multidimensional array.

We could have stopped here — yet, there is much more to tensors than one might expect from reading Definition 1.2.1. More concisely, an N th-order tensor or N -way array is an array indexed by N indices. N is called the number of *dimensions* or *modes*. As such, a tensor naturally generalizes the concept of a one-way vector, which is indexed by one index, and a two-way matrix, which is indexed by two indices. Fig. 1.5 visualizes a third-order tensor, which is indexed by three indices. Opposed to Definition 1.2.1, the thesis will use the term *higher-order* or *multi-way* array, since a vector in \mathbb{F}^I is already multi- I -dimensional. Much like polynomials and polynomial equations, tensors have been studied extensively in numerous fields in mathematics¹¹. Because of the natural link there is between homogeneous polynomials and fully symmetric higher-order tensors, algebraic geometry is one of them¹².

Higher-order tensors arise naturally in many application areas.

- A gray-scale image is a matrix of pixel values. A color image with an R, G, and B-value at every pixel, is a third-order tensor (Fig. 1.5), where the “length” of the third mode is equal to three. A color movie adds a fourth, time dimension and is a fourth-order tensor.
- Many video-streaming services such as Netflix make use of recommender systems. After watching a movie, users can leave a rating, which is then stored

¹¹More formally, an N -th order tensor can be thought of as the member of a tensor space: the outer product of N vector spaces [9]. Write an N th-order tensor as \mathcal{A} , then $\mathcal{A} \in \mathbb{F}^{I_1} \times \mathbb{F}^{I_2} \times \dots \times \mathbb{F}^{I_N}$, where \mathbb{F} is a field and \mathbb{F}^I is a vector space. As such, a higher-order tensor naturally generalizes the view of a vector as an element of a vector space. Mathematicians tend to prefer this coordinate-free definition [33]. This thesis will mainly take the first view, as it is common in science and engineering.

¹²An illustrative example of the isomorphism is given in Appendix B.

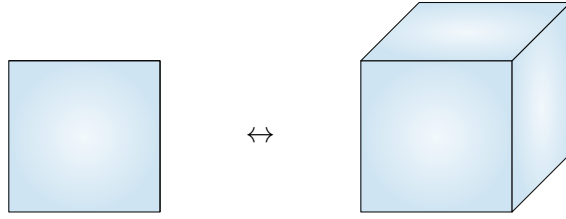


Figure 1.5: Higher-order tensors (right) are natural extensions to matrices (left).

in, *e.g.*, a users \times movies rating matrix. Recommender systems try to predict missing entries in the matrix, to recommend new movies to current and new users. Often, a lot more information is available, such as the time of the day of the rating or the social context of the user. Storing these data requires a higher-order tensor.

- In statistics, the first-order cumulant of a stochastic vector \mathbf{x} is its expected value or mean $\bar{\mathbf{x}} = \mathcal{E}(\mathbf{x})$. The second-order cumulant is its covariance matrix $\mathbf{C}_{\mathbf{x}} = \mathcal{E}(\tilde{\mathbf{x}}\tilde{\mathbf{x}}^T)$, where $\tilde{\mathbf{x}} = \mathbf{x} - \bar{\mathbf{x}}$ denotes the mean-centered vector now. By generalizing these definitions, the third- and fourth-order cumulant $\mathcal{C}_{\mathbf{x}}^{(3)}$ and $\mathcal{C}_{\mathbf{x}}^{(4)}$ are third and fourth-order tensors.
- The previous examples all give natural tensor data. As an example of *tensorization*, [16] converts a 21-channel electroencephalogram (EEG) time series, which is a $21 \times \text{time}$ matrix, to a third-order tensor by means of a wavelet transform. A tensor decomposition may then reveal meaningful factors (components) in the brain activity waves.

Tensor decompositions can be considered natural generalizations of matrix decompositions, such as the ubiquitous singular value decomposition (SVD), depicted in Fig. 1.6. Generalizations for tensors have been studied since the early 1900s. The first applications in factor analysis date from the 1960s. Perhaps surprisingly, the benefits of using tensor decompositions as a tool for factor analysis, were first discovered in non-traditional scientific areas, such as psychometrics and chemometrics. The Tucker decomposition was introduced in psychometrics [43], which is the quantitative study of psychological experimental data. The canonical polyadic decomposition (CPD) stems from the linguistics society and was independently rediscovered in psychometrics [28]. Fig. 1.6 shows the CPD as an example of a tensor decomposition. De Lathauwer, De Moor and Vandewalle (2000) showed that the multilinear singular value decomposition (MLSVD), a constrained Tucker model, is a convincing generalization of the SVD [13]. Chapter 2 will introduce the CPD. Appendix B elaborates on the MLSVD. In the 1990s, signal processing followed as an application area for tensor decompositions. Applications here include blind source separation [9], biomedical data analysis of brain activity [16] and radar and communication applications, such as harmonic retrieval (HR) [36, 37] and the multi-modulus algorithm presented in [17]. Chapter 2 will introduce HR. Sorber *et al.* (2013) developed Tensorlab, a

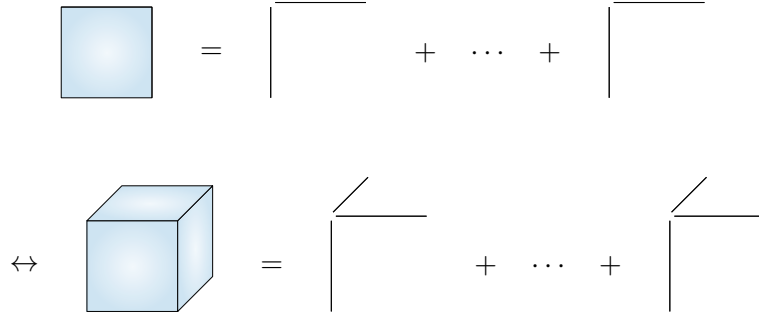


Figure 1.6: Higher-order tensor decompositions (bottom) are natural extensions to matrix decompositions (top).

Matlab toolbox for computing tensor decompositions and for complex optimization [45]. We will use it in Chapter 3 and 4.

Tensor methods suffer from the *curse of dimensionality*: storing all entries of higher-order tensors and performing computations on them can be impracticable. Ever-improving computer hardware and computer software and the interest of the computer science and machine learning community in tensor methods, some ten years ago, contributed to overcome this issue [5]. Regarding the future, [5] states that the use of multisensor technology and the resulting big data sets have highlighted the limitations of matrix models and the need for data analysis tools that can account for the intrinsic higher-dimensional patterns in the data. As the previous examples illustrate, it's just a matter of “putting on the right glasses” then, to see the higher-dimensional patterns arise. The work in this thesis, to go from the reasoning outlined in Example 1.1.5 and the “flat” Macaulay matrix to higher-order tensor decompositions, fits this adagio.

It should be noted at this point that, although higher-order tensors are natural generalizations of matrices, multilinear (tensor) algebra exhibits striking differences with linear (matrix) algebra. Basic results for an $I_1 \times I_2$ matrix \mathbf{A} , that (i) $\text{rowrank}(\mathbf{A}) = \text{colrank}(\mathbf{A}) \triangleq \text{rank}(\mathbf{A})$, (ii) $\text{rank}(\mathbf{A}) \leq \min(I, J)$ and (iii) generically, $\text{rank}(\mathbf{A}) = \min(I, J)$, do not hold for tensors. In fact, it will become clear in Chapter 2 that there are multiple ways to define tensor rank, each giving a different result.

1.2.2 A Real-Life Application

To demonstrate how “putting on the right glasses” can reveal the presence of tensors in many scientific application areas, this section contains a real-life application from signal processing.

Magnetic Resonance Spectroscopy (MRS) is a nuclear magnetic resonance (NMR) technique that can observe changes in biochemical brain activity. Biochemical changes can, *e.g.*, indicate the presence of a brain tumor. The technique excites the magnetic nuclei of the biochemicals in the human brain by applying a magnetic field. The

resulting resonance signal $\{x_n\}_{n=0}^{N-1}$ is modeled as a sum of complex exponentials

$$x_n = \sum_{r=1}^R c_r z_r^n = \sum_{r=1}^R a_r e^{i\phi_r} e^{(\alpha_r + 2\pi i\nu_r)n\Delta t} \quad (1.13)$$

where $c_r = a_r e^{i\phi_r} \in \mathbb{C}, 1 \leq r \leq R$, are the complex amplitudes and $z_r = e^{(\alpha_r + 2\pi i\nu_r)\Delta t} \in \mathbb{C}, 1 \leq r \leq R$, are the *poles*. Only $\alpha_r < 0$ is physically meaningful for MRS, so the complex exponentials are exponentially damped sinusoids. Note that the signal (1.13) is ubiquitous in signal processing, *e.g.*, as the output of the discrete-time system (1.2).

A common method to extract the poles is the Hankel Singular Value Decomposition (HSVD). Construct the Hankel matrix

$$\mathbf{H} = \begin{pmatrix} x_0 & x_1 & \dots & x_{L-1} \\ x_1 & x_2 & \dots & x_L \\ \vdots & \vdots & & \vdots \\ x_{K-1} & x_K & \dots & x_{N-1} \end{pmatrix} \quad (1.14)$$

where $K + L = N + 1$ and $K, L \geq R$. Given model (1.13), we have that \mathbf{H} allows the decomposition

$$\mathbf{H} = \begin{pmatrix} 1 & & 1 \\ z_1 & \dots & z_R \\ \vdots & & \vdots \\ z_1^{K-1} & & z_R^{K-1} \end{pmatrix} \text{diag}(c_1, \dots, c_R) \begin{pmatrix} 1 & & 1 \\ z_1 & \dots & z_R \\ \vdots & & \vdots \\ z_1^{L-1} & & z_R^{L-1} \end{pmatrix}^H \triangleq \mathbf{Z}^{(K)} \mathbf{C} \mathbf{Z}^{(L)H}. \quad (1.15)$$

Because of the harmonic structure contained in $\mathbf{Z}^{(K)}$, (1.13) is called a *harmonic retrieval* (HR) problem with *generators* z_r . Since the Vandermonde matrices¹³ generated by distinct poles in (1.15) have full rank, the rank of \mathbf{H} is exactly equal to R . Using the “economic size” SVD¹⁴ $\mathbf{H} = \mathbf{U}_R \mathbf{S}_R \mathbf{V}_R^H$, we have that there exists an invertible matrix $\mathbf{T} \in \mathbb{R}^{R \times R}$ such that

$$\mathbf{Z}^{(K)} = \mathbf{U}_R \mathbf{T}.$$

Like in Example 1.1.2, one can come to an EVD by exploiting the multiplicative shift structure of $\mathbf{Z}^{(K)}$. Write

$$\bar{\mathbf{Z}}^{(K)} = \mathbf{Z}^{(K)} \mathbf{D}$$

where $\mathbf{D} = \text{diag}(z_1, \dots, z_R)$ and $\bar{\mathbf{Z}}^{(K)}$. We then have that

$$\bar{\mathbf{U}}_R \mathbf{T} = \underline{\mathbf{U}}_R \mathbf{T} \mathbf{D} \Leftrightarrow (\underline{\mathbf{U}}_R)^\dagger \bar{\mathbf{U}}_R \mathbf{T} = \mathbf{T} \mathbf{D}, \quad (1.16)$$

¹³For a concise definition, see Definition 2.3.1.

¹⁴If $R = \text{rank}(\mathbf{H})$, using conventional Matlab notation for indexing, $\mathbf{H} = \mathbf{U}(:, 1 : R) \mathbf{S}(1 : R, 1 : R) \mathbf{V}(:, 1 : R)^H$ is the “economic size” SVD — see Theorem A.2.1.

which is an EVD. There is, however, no reason why we could not extend (1.14) to a third-order tensor

$$\mathcal{H}(:, :, 1) = \begin{pmatrix} x_0 & x_1 & \dots & x_{L-1} \\ x_1 & x_2 & \dots & x_L \\ \vdots & \vdots & & \vdots \\ x_{K-2} & x_{K-1} & \dots & x_{N-2} \end{pmatrix}, \quad \mathcal{H}(:, :, 2) = \begin{pmatrix} x_1 & x_2 & \dots & x_L \\ x_2 & x_3 & \dots & x_{L+1} \\ \vdots & \vdots & & \vdots \\ x_{K-1} & x_K & \dots & x_{N-1} \end{pmatrix} \quad (1.17)$$

in obvious Matlab notation, and with harmonic structure in the third mode too. The technique goes by the name *hankelization*, and is another example of *tensorization*. In Chapter 2, we will see that (1.17) allows a natural CPD (Fig 1.6) that is easily unique. This real-life application already hints at the close connection between the CPD and an EVD.

1.3 Goal

The goal of this thesis is two-fold.

First, it is our aim to unravel some fundamental connections between the set of polynomial equations (1.1) and higher-order tensor decompositions, such as the CPD. We will apply these connections to gain insight into the properties of the first and of the latter.

Second, building on the insights, we will propose a natural multilinear algebra-based approach to find the solutions of a(n over-constrained) set of polynomial equations. We will implement and illustrate some algorithms in Matlab. Eventually, *multilinear algebra* should increase the robustness of the obtained solutions, when compared with the original algorithm in the PNLA framework.

1.4 Contents

The rest of the text is structured as follows. Chapter 2 contains the preliminaries on polynomial equations, higher-order tensors and multidimensional harmonic retrieval. Toward the end, one particular higher-order tensor decomposition, namely the CPD, is explained in more detail. Chapter 3 and 4 then properly establish the connections between the different topics introduced in Chapter 2. We suggest the reader to welcome the algorithms and numerical experiments at the end of every chapter for digestibility. Chapter 4 puts the connections and algorithms from Chapter 3 in a more general context, when the sets of polynomial equations under study have roots with multiplicities. Along the way, correctness, some numerical issues and a comparison of the proposed algorithms with existing methods will be addressed.

Chapter 2

Polynomial Equations, Higher-Order Tensors and Multidimensional Harmonic Retrieval

This chapter contains the preliminaries for this thesis. First, the problem of solving a set of polynomial equations will be formally defined in Section 2.1. The Macaulay matrix and its properties will be visited. Section 2.2 contains a brief introduction to multilinear algebra: the algebra of higher-order tensors. For a good understanding, we encourage the reader to review linear algebra basics in Appendix A and the multilinear algebra tools in Appendix B. Lastly, Section 2.3 defines the (multidimensional) harmonic retrieval problem.

2.1 Polynomial Equations

2.1.1 Definitions

Monomials and Polynomials

The basic building blocks in the system of polynomial equations (1.1) are *monomials* and *polynomials*.

Definition 2.1.1 (monomial). [40, p. 4] A monomial in the n variables $x_1, x_2, \dots, x_n \in \mathbb{C}$ is a power product of the form

$$\mathbf{x}^\alpha \triangleq \prod_{j=1}^n x_j^{\alpha_j}$$

where $\mathbf{x} = (x_1 \ x_2 \ \dots \ x_n)^T \in \mathbb{C}^n$ and $\alpha = (\alpha_1 \ \alpha_2 \ \dots \ \alpha_n)^T \in \mathbb{N}^n$ is the monomial exponent vector.

2. POLYNOMIAL EQUATIONS, HIGHER-ORDER TENSORS AND MULTIDIMENSIONAL HARMONIC RETRIEVAL

The *degree* of a monomial is defined as the sum of all powers contained in the exponent vector α :

$$\deg(\mathbf{x}^\alpha) \triangleq \|\alpha\|_1 = \sum_{j=1}^n \alpha_j.$$

Several schemes for ordering monomials by their monomial exponent vector, exist. In this text, the *degree negative lexicographic order* will consistently be used.

Definition 2.1.2 (degree negative lexicographic order). [24, p. 3] Let $\alpha, \beta \in \mathbb{N}^n$ be monomial exponent vectors, then the monomials $\mathbf{x}^\alpha < \mathbf{x}^\beta$ are ordered by the degree negative lexicographic order if one of the following two conditions is satisfied.

- (i) $\deg(\mathbf{x}^\alpha) < \deg(\mathbf{x}^\beta)$,
- (ii) $\deg(\mathbf{x}^\alpha) = \deg(\mathbf{x}^\beta)$ and the leftmost nonzero entry of $\beta - \alpha$ is negative.

Definition 2.1.2 is most easily understood by means of an example.

Example 2.1.1. The monomials in 2 variables up to degree 3 are ordered by the degree negative lexicographic order as

$$1 < x_1 < x_2 < x_1^2 < x_1x_2 < x_2^2 < x_1^3 < x_1^2x_2 < x_1x_2^2 < x_2^3.$$

In particular, considering two monomials $\mathbf{x}^\alpha < \mathbf{x}^\beta$, we have that (i) $x_2 < x_1^2$ because $\deg(\mathbf{x}^\alpha) = 1 < 2 = \deg(\mathbf{x}^\beta)$ and (ii) $x_1^2 < x_1x_2$, because $\deg(\mathbf{x}^\alpha) = \deg(\mathbf{x}^\beta) = 2$ and $\beta - \alpha = \begin{pmatrix} -1 & 1 \end{pmatrix}^T$, the first entry of which is negative.

Definition 2.1.3 (polynomial). A complex (multivariate) polynomial f in the n variables $x_1, x_2, \dots, x_n \in \mathbb{C}$ is a linear combination with complex coefficients of monomials in the n variables:

$$f(x_1, x_2, \dots, x_n) = \sum_{l=1}^p a_l \mathbf{x}_l^{\alpha_l} \tag{2.1}$$

where $\mathbf{a} = \begin{pmatrix} a_1 & a_2 & \dots & a_p \end{pmatrix}^T \in \mathbb{C}^p$ is the coefficient vector.

The *degree* of the polynomial f is defined as the degree of the monomial with the highest degree in f :

$$\deg(f) \triangleq \max_{\{l \mid a_l \neq 0\}} \deg(\mathbf{x}_l^{\alpha_l}).$$

Polynomial Ring

The *ring* of all multivariate polynomials in n variables is denoted by \mathcal{C}^n . A ring is essentially a set in which an addition, for which every element has its inverse, and a multiplication are defined.

Example 2.1.2. *The set of integers \mathbb{Z} , equipped with the usual addition and multiplication, is a ring. Indeed, for any $z_1, z_2 \in \mathbb{Z} : z_1 + z_2 \in \mathbb{Z}$ and $\exists z'_1 = -z_1 \in \mathbb{Z} : z_1 + z'_1 = 0$ — but not for all $z_1 : \exists z''_1 \in \mathbb{Z} : z_1 \cdot z''_1 = 1$.*

\mathcal{C}_d^n is the subset of \mathcal{C}^n that contains all polynomials up to degree d :

$$\mathcal{C}_d^n = \{f \in \mathcal{C}^n \mid 0 \leq \deg(f) \leq d\}.$$

\mathcal{C}_d^n is a *vector space*. A vector space is a set that is closed under vector addition and scalar multiplication. By fixing a well-ordered monomial basis for \mathcal{C}_d^n , it follows from (2.1) that \mathcal{C}_d^n is indeed isomorphic to its coefficient vector space.

Corollary 2.1.1. *The dimension $q(d)$ of \mathcal{C}_d^n is given by*

$$q(d) \triangleq \dim \mathcal{C}_d^n = \binom{n+d}{n}.$$

Definition 2.1.4 (homogeneous polynomial). *A homogeneous polynomial is a polynomial whose monomials all have the same degree.*

Definition 2.1.5. [23, p. 263] *Let $f \in \mathcal{C}_d^n$ be a polynomial of degree d , then its homogenization $f^h \in \mathcal{C}_d^{n+1}$ is the polynomial obtained by multiplying each monomial $\mathbf{x}_l^{\alpha_l}$ in f with a power β_l of x_0 , such that $\deg(x_0^{\beta_l} \mathbf{x}_l^{\alpha_l}) = d, 1 \leq l \leq p$.*

The ring (vector space) of all resulting homogeneous polynomials in $n+1$ variables (up to degree d) is denoted by \mathcal{P}^n (\mathcal{P}_d^n). Obviously, $\mathcal{P}_d^n \subset \mathcal{C}_d^{n+1}$. Definition 2.1.5 in fact implies that \mathcal{P}_d^n is isomorphic with $\mathcal{C}_d^n \subset \mathcal{C}_d^{n+1}$.

Example 2.1.3. *Consider the polynomial $f(x_1, x_2) = x_1x_2 - 2x_2$. It holds true that $f \in \mathcal{C}_2^2$ and $\deg(f) = \deg(x_1x_2) = 2$. Its homogenization $f^h(x_0, x_1, x_2) = x_1x_2 - 2x_2x_0 \in \mathcal{P}_2^2$, but also $f^h \in \mathcal{C}_2^3$.*

A System of Polynomial Equations

Definition 2.1.6 (system of polynomial equations). *Let $f_i \in \mathcal{C}_{d_i}^n, 1 \leq i \leq s$, be s polynomials of degree d_i in n variables x_1, x_2, \dots, x_n , then*

$$\begin{cases} f_1(x_1, x_2, \dots, x_n) = 0 \\ \vdots \\ f_s(x_1, x_2, \dots, x_n) = 0 \end{cases} \quad (2.2)$$

defines a set or a system of s multivariate polynomial equations.

The *degree* of (2.2) is defined as $d_0 \triangleq \max_{1 \leq i \leq s} d_i$. We will write \mathbf{f}_i instead of \mathbf{a}_i to emphasize its role as the coefficient vector of f_i in (2.2). The points $\mathbf{x} \in \mathbb{C}^n$ that satisfy (2.2) are called the *roots* of (2.2); the set of all roots is called the *solution*

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set. In this thesis, we will make the important assumption that the solution set is *0-dimensional*¹, meaning that the number of solutions is *finite*. One can show that this is the case as long as $s = n > 1$ and the f_i have a constant greatest common divisor².

The *homogenization* of (2.2) is the system (2.2) where each f_i is replaced by its homogenization f_i^h . The solution set of the homogenization of (2.2) can be described once the *projective space* \mathbb{P}^n has been introduced.

Definition 2.1.7 (projective space). [23, p. 262] *The n -dimensional projective space \mathbb{P}^n is the set of equivalence classes \sim on $\mathbb{C}^{n+1} \setminus \{\mathbf{0}\}$, defined by*

$$\begin{aligned} \begin{pmatrix} x'_0 & x'_1 & \dots & x'_n \end{pmatrix}^T &\sim \begin{pmatrix} x_0 & x_1 & \dots & x_n \end{pmatrix}^T \\ \Leftrightarrow \exists \lambda \in \mathbb{C} : \begin{pmatrix} x'_0 & x'_1 & \dots & x'_n \end{pmatrix}^T &= \lambda \begin{pmatrix} x_0 & x_1 & \dots & x_n \end{pmatrix}^T. \end{aligned}$$

The *affine space*³ \mathbb{C}^n appears as a subspace of the projective space, namely where $x_0 = 1$. The affine counterpart of a given projective point $p = \begin{pmatrix} x_0 & x_1 & \dots & x_n \end{pmatrix}^T$ is then $\begin{pmatrix} 1 & \frac{x_1}{x_0} & \dots & \frac{x_n}{x_0} \end{pmatrix}^T$. This does not work for projective points with $x_0 = 0$: they are called *points at infinity*.

Theorem 2.1.1 (Bézout's theorem). [24, p. 6] *Let $f_i^h \in \mathcal{P}_{d_i}^n$, $1 \leq i \leq n$, be n homogeneous polynomials of degree d_i in $n + 1$ variables x_0, \dots, x_n . Under the assumption that the solution set of (2.2) is 0-dimensional, the number of solutions m in the projective space, including multiplicities, is given by the Bézout number*

$$m = \prod_{i=1}^n d_i.$$

Polynomial Ideals

To ease notation and to develop insight, this section introduces concepts in \mathcal{C}^n . With a little thought, all results pass to \mathcal{P}^n . Definition 2.1.3 defines a polynomial as a linear combination of p monomials. A linear combination of s polynomials f_i with complex coefficients $c_i \in \mathbb{C}$ is also a polynomial. An extension is given by a *polynomial combination*.

¹The solution set is called a *variety* in algebraic geometry. Its dimension equals the degree of the so-called *Hilbert polynomial*.

²A polynomial multiplication is defined in \mathcal{C}^n . f_1 and f_2 have a constant greatest common divisor when they have no non-constant multiplicative factors in common.

³The affine space is sometimes denoted by \mathbb{A}^n in the literature.

Definition 2.1.8 (polynomial combination). [41, p. 87] Let $\mathcal{F} = \{f_i\}_{i=1}^s$ be a set of s polynomials f_i , then any polynomial that can be written as

$$g = \sum_{i=1}^s c_i f_i$$

where $c_i \in \mathbb{C}^n$, $1 \leq i \leq s$, is a polynomial combination of the elements of \mathcal{F} .

The subset of the ring \mathbb{C}^n that is reached by polynomial combinations of the elements of \mathcal{F} is an *ideal*.

Definition 2.1.9 (polynomial ideal). [41, p. 87] A polynomial ideal in \mathbb{C}^n is a subset of \mathbb{C}^n that is closed under polynomial combination. Let $\mathcal{F} = \{f_i\}_{i=1}^s$ be a set of s polynomials f_i , then the polynomial ideal that contains all polynomial combinations of the elements of \mathcal{F} is said to be generated by \mathcal{F} and is denoted by $\langle \mathcal{F} \rangle = \langle f_1, f_2, \dots, f_s \rangle$.

Example 2.1.4. To keep the ideal concept tactile, consider again the set of integers in Example 2.1.2. The subset $\{z \in \mathbb{Z} \mid z \bmod 2 = 0\}$ is the ideal $\langle 2 \rangle$ in \mathbb{Z} .

Let $\mathcal{Z} = \{\mathbf{z}_k\}_{k=1}^m$ be a fixed set of m points in \mathbb{C}^n , then the set $\mathcal{I}_{\mathcal{Z}}$ of polynomials in \mathbb{C}^n that attain zero in \mathcal{Z} is an ideal. Indeed, every polynomial combination of the polynomials in $\mathcal{I}_{\mathcal{Z}}$ is again zero in \mathcal{Z} . \mathcal{Z} is called the *zero set of the ideal*⁴. Write $\mathcal{I}_{\mathcal{Z}} = \mathcal{I} = \langle \mathcal{F} \rangle$, where \mathcal{F} contains *generators* f_i for \mathcal{I} and is called a *basis*. The basis is not unique. From Definition 2.1.6, \mathcal{Z} equals the solution set of the system of polynomials defined by \mathcal{F} .

If g is a polynomial that satisfies $\exists \mathbf{z} \in \mathcal{Z} : g(\mathbf{z}) = a \neq 0$, then it is impossible to have $g \in \mathcal{I}$. Instead, we have that

$$g = \sum_{i=1}^s c_i f_i + r \quad (2.3)$$

and $r(\mathbf{z}) = a$. More generally, if (2.3) holds, $g(\mathbf{z}_k) = r(\mathbf{z}_k)$, $1 \leq k \leq m$.

Definition 2.1.10 (residue class). [41, p. 89] Let g and r be two polynomials in \mathbb{C}^n , then g and r are equivalent (with respect to the ideal \mathcal{I}) if their difference is in \mathcal{I} , i.e.

$$g \sim r \Leftrightarrow g - r \in \mathcal{I}.$$

The residue class of $g \bmod \mathcal{I}$ is the set

$$[g] \triangleq \{r \in \mathbb{C}^n \mid g - r \in \mathcal{I}\}.$$

In particular, $[0] = \mathcal{I}$. If $g \in \mathcal{I}$, from (2.3), it follows that $g(\mathbf{z}_k) = r(\mathbf{z}_k) = 0$, $1 \leq k \leq m$. One can show that, if all roots of (2.2) defined by the elements of \mathcal{F} are simple, the inverse is true, i.e. $g(\mathbf{z}_k) = 0$, $1 \leq k \leq m \Rightarrow g \in \mathcal{I}$.

⁴The zero set is, again, called a *variety* in algebraic geometry.

Definition 2.1.11 (quotient ring). *The quotient ring $\mathcal{C}^n/\mathcal{I}$ of the polynomial ideal $\mathcal{I} \subset \mathcal{C}^n$ is the set of all residue classes $[r], r \in \mathcal{C}^n$.*

As any residue class is completely defined by the values its members take on the zero set of the ideal,

$$\dim \mathcal{C}^n/\mathcal{I} = m.$$

If not all roots are simple, *i.e.* if there are points in the solution set \mathcal{Z} that occur with multiplicities greater than 1, things become more subtle.

Definition 2.1.12 (differential functional). [41, p. 90] *Let $\mathbf{z} \in \mathbb{C}^n$ and $f \in \mathcal{C}^n$, then the differential functional $\partial_{\mathbf{j}}[\mathbf{z}]$ is defined by*

$$\partial_{\mathbf{j}}[\mathbf{z}](f) \triangleq \frac{1}{j_1!j_2!\dots j_n!} \left(\frac{\partial^{\sum_{l=1}^n j_l}}{\partial x_1^{j_1} \partial x_2^{j_2} \dots \partial x_n^{j_n}} f \right) (\mathbf{z})$$

where $\mathbf{j} = (j_1 \ j_2 \ \dots \ j_n)^T \in \mathbb{N}^n$.

Let m_0 denote the number of disjoint roots. If $m_0 < m$, the dimension of $\mathcal{C}^n/\mathcal{I}$ is still m , but one can show that a residue class $[r]$ is only completely defined now by the m_0 values $\{r(\mathbf{z}_k)\}_{k=1}^{m_0} = \{\partial_{\mathbf{0}}[\mathbf{z}_k](r)\}_{k=1}^{m_0}$ and $m - m_0$ values $\partial_{\mathbf{j}}[\mathbf{z}_{k'}](r)$ where $\mathbf{j} \neq \mathbf{0}$ and $\mathbf{z}_{k'} \in \mathcal{Z}$ are the roots with multiplicities greater than 1⁵.

2.1.2 The Macaulay Matrix

Definition 2.1.13. [23, p. 263] *Let $f_i \in \mathcal{C}_{d_i}^n$, $1 \leq i \leq s$, be s polynomials of degree d_i in n variables x_1, x_2, \dots, x_n , then the Macaulay matrix $\mathbf{M}(d)$ of degree d contains as its rows the coefficients of*

$$\mathbf{M}(d) = \begin{pmatrix} f_1 \\ x_1 f_1 \\ \vdots \\ x_n^{d-d_1} f_1 \\ f_2 \\ x_1 f_2 \\ \vdots \\ x_n^{d-d_s} f_s \end{pmatrix}$$

where each polynomial $f_i, 1 \leq i \leq s$, is multiplied with all possible monomials \mathbf{x}^α , $0 \leq |\alpha| \leq d - d_i \in \mathbb{N}$.

The construction of the Macaulay matrix is most easily understood by means of an example.

⁵These differential functionals constitute a basis for the so-called *dual space* of the ideal \mathcal{I} .

Example 2.1.5. [2, Example 5.1] Consider the system of $s = 2$ polynomial equations in $n = 2$ variables

$$\begin{cases} f_1(x_1, x_2) = x_1x_2 - 2x_2 = 0, \\ f_2(x_1, x_2) = x_2 - 3 = 0 \end{cases}$$

where $d_1 = 2$ and $d_2 = 1$. $d_0 = 2$, so we start constructing the Macaulay matrix at $d = 2$. The Macaulay matrix $\mathbf{M}(2)$ of degree 2 contains as its rows the coefficient vector of f_1 and, since $d_2 = 1 < 2$, the coefficient vector of f_2 multiplied with the monomials of degree 1: x_1 and x_2 .

$$\mathbf{M}(2) = \begin{matrix} & 1 & x_1 & x_2 & x_1^2 & x_1x_2 & x_2^2 \\ \begin{matrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \\ x_1f_2(x_1, x_2) \\ x_2f_2(x_1, x_2) \end{matrix} & \begin{pmatrix} 0 & 0 & -2 \\ -3 & 0 & 1 \\ 0 & -3 & 0 \\ 0 & 0 & -3 \end{pmatrix} & \begin{vmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \end{matrix}.$$

Similar to what Example 1.1.4 has shown, the Macaulay matrix $\mathbf{M}(3)$ of degree 3 contains additional rows that are the coefficient vectors of x_1f_1 , x_2f_1 , $x_1^2f_2$, $x_1x_2f_2$ and $x_2^2f_2$.

Homogenization gives rise to the same $\mathbf{M}(d)$. As Example 2.1.6 illustrates, the homogeneous interpretation is in fact a mere relabeling of the rows and columns of $\mathbf{M}(d)$ [2, p. 59].

Example 2.1.6. Consider the homogenization of the system in Example 2.1.5. The Macaulay matrix $\mathbf{M}(2)$ of degree 2 is the same as $\mathbf{M}(2)$ in Example 2.1.5.

$$\mathbf{M}(2) = \begin{matrix} & x_0^2 & x_0x_1 & x_0x_2 & x_1^2 & x_1x_2 & x_2^2 \\ \begin{matrix} f_1^h(x_0, x_1, x_2) \\ x_0f_2^h(x_0, x_1, x_2) \\ x_1f_1^h(x_0, x_1, x_2) \\ x_2f_1^h(x_0, x_1, x_2) \end{matrix} & \begin{pmatrix} 0 & 0 & -2 \\ -3 & 0 & 1 \\ 0 & -3 & 0 \\ 0 & 0 & -3 \end{pmatrix} & \begin{vmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \end{matrix}$$

From section 2.1.1, it should be clear that the construction of $\mathbf{M}(d)$ ensures that its row space \mathcal{M}_d is the set of polynomial combinations

$$\mathcal{M}_d = \left\{ \sum_{i=1}^s c_i f_i \mid c_i \in \mathcal{C}_{d-d_i}^n \right\}.$$

Let now $\langle f_1, f_2, \dots, f_s \rangle_d \triangleq \mathcal{I} \cap \mathcal{C}_d^n$. As Example 2.1.7 illustrates, $\mathcal{M}_d \neq \langle f_1, f_2, \dots, f_s \rangle_d$. The homogeneous interpretation of \mathcal{M}_d ,

$$\mathcal{M}_d = \left\{ \sum_{i=1}^s c_i f_i^h \mid c_i \in \mathcal{P}_{d-d_i}^n \right\},$$

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ensures that $\mathcal{M}_d = \langle f_1^h, f_2^h, \dots, f_s^h \rangle_d$ holds.

Example 2.1.7. Consider the Macaulay matrix in Example 2.1.5. $x_1^2 \in \mathcal{C}_2^2$ and, from $\mathbf{M}(3)$ in reduced row echelon form, $x_1^2 \in \mathcal{M}_3$, so x_1^2 is a polynomial of degree 2 that can be written as a polynomial combination of f_1 and f_2 , i.e. $x_1^2 \in \langle f_1, f_2 \rangle_2$. But from $\mathbf{M}(2)$, $x_1^2 \notin \mathcal{M}_2$. Consider now the Macaulay matrix in Example 2.1.6. $x_1^2 \in \mathcal{P}_2^2$ and $x_1^2 \notin \mathcal{M}_2$, but due to the homogeneous interpretation, this time $x_1^2 \notin \mathcal{M}_d$ when $d \geq 2$.

Now flip the columns of $\mathbf{M}(d)$ from left to right and bring the result into reduced row echelon form. The monomials that correspond to the linearly dependent columns of the result are called the *standard monomials* or the *normal set* in, a.o., [2, p. 97]. They “span” the orthogonal complement of \mathcal{M}_d . At a sufficiently large $d \geq d^*$, the null space of $\mathbf{M}(d)$ is isomorphic with $\mathcal{P}_d^n / \langle f_1^h, f_2^h, \dots, f_s^h \rangle$, its dimension

$$r(d) \triangleq \dim \mathcal{P}_d^n / \langle f_1^h, f_2^h, \dots, f_s^h \rangle = m^6,$$

and the null space of $\mathbf{M}(d)$ contains all the necessary information to determine whether (2.2) has any common roots.

Definition 2.1.14 (degree of regularity). [23, p. 275] The degree of regularity is the minimal degree d^* such that, for all $d \geq d^*$, $\mathbf{M}(d)$ always allows one to determine whether the associated polynomial system has a nontrivial common root.

Let $f_i^h \in \mathcal{P}_{d_i}^n$, $1 \leq i \leq s$, be s homogeneous polynomials of degree d_i in $n + 1$ variables x_0, \dots, x_n . From his study of resultants, Macaulay has derived an upper bound for the square, homogeneous case, i.e. $s = n + 1$ [7, p. 104]:

$$d^* \leq \sum_{i=1}^s (d_i - 1) + 1 = \sum_{i=1}^{n+1} d_i - n. \quad (2.4)$$

Note that, for the case $n = 1$, the Sylvester matrix in Example 1.1.3 is indeed constructed for $d = d_1 + d_2 - 1$. For the case where one starts from a square, affine system, i.e. $s = n$, and one is interested in solutions in the projective space, one can take $d_{n+1} = 0$ in the right-hand side in (2.4)⁷.

Multiplication Tables

Let $\mathbf{A}_h \in \mathbb{C}^{m \times m}$ be the matrix representation of a multiplication with the residue class $[h]$ in the m -dimensional quotient ring $\mathcal{C}^n / \mathcal{I}$ w.r.t. some basis, e.g., the normal set — say $\{[t_k]\}_{k=1}^m$:

$$\phi_h : \mathcal{C}^n / \mathcal{I} \rightarrow \mathcal{C}^n / \mathcal{I} : \begin{pmatrix} [t_1] \\ \vdots \\ [t_m] \end{pmatrix} \mapsto \begin{pmatrix} [h \cdot t_1] \\ \vdots \\ [h \cdot t_m] \end{pmatrix} \triangleq \mathbf{A}_h \begin{pmatrix} [t_1] \\ \vdots \\ [t_m] \end{pmatrix}.$$

⁶ $r(d)$ is in fact the Hilbert polynomial, which has degree 0 under the assumption of a 0-dimensional solution set.

⁷This amounts to dropping the so-called *u-resultant* [30].

Because \mathcal{C}^n is a commutative ring, the set of multiplication tables $\{\mathbf{A}_{x_j}\}_{j=1}^n$, where $h = x_j, 1 \leq j \leq n$, is a *commuting family*.

Theorem 2.1.2 (Central Theorem of NPA). [40, Theorem 2.27] *Let the system $\mathcal{F} = \{f_i\}_{i=1}^s$ of s polynomial equations in n variables x_1, x_2, \dots, x_n possess $m_0 \leq m$ disjoint roots. Consider the commuting family of multiplication tables $\{\mathbf{A}_{x_j}\}_{j=1}^n$ for the quotient ring $\mathcal{C}^n/\mathcal{I} = \mathcal{C}^n/\langle \mathcal{F} \rangle$ w.r.t. an arbitrary basis $\{[t_k]\}_{k=1}^m$. For each root $\mathbf{x}^{(k)}$ with multiplicity $\mu_k, 1 \leq k \leq m_0$, the \mathbf{A}_{x_j} have the μ_k -fold eigenvalue $x_j^{(k)}$ and the associated joint eigenvector*

$$\begin{pmatrix} [t_1(\mathbf{x}^{(k)})] & \dots & [t_m(\mathbf{x}^{(k)})] \end{pmatrix}^T \in \text{span}(\mathbf{X}_k).$$

Furthermore, $\text{span}(\mathbf{X}_k)$ is an associated joint invariant subspace of dimension μ_k , such that

$$\mathbf{A}_{x_j} \begin{pmatrix} \mathbf{X}_1 & \dots & \mathbf{X}_{m_0} \end{pmatrix} = \begin{pmatrix} \mathbf{X}_1 & \dots & \mathbf{X}_{m_0} \end{pmatrix} \begin{pmatrix} \mathbf{T}_{x_{j,1}} & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \mathbf{T}_{x_{j,m_0}} \end{pmatrix} \quad (2.5)$$

with upper-triangular $\mathbf{T}_{x_{j,k}} \in \mathbb{C}^{\mu_k \times \mu_k}$ with diagonal elements $x_j^{(k)}$.

If $m_0 = m$, i.e. if all roots are simple, then Theorem 2.1.2 implies that (2.5) is an EVD and that the family $\{\mathbf{A}_{x_j}\}_{j=1}^n$ is jointly diagonalizable.

Example 2.1.8. Consider the polynomial equation in $n = 1$ variable x in Example 1.1.2 again. Flipping the columns of \mathbf{f}^T from left to right and bringing the result into reduced row echelon form results in the normal set $\{1, x\}$. The Frobenius companion matrix \mathbf{A} in (1.4) describes the result of the multiplication of $\{1, x\}$ with $h = x$ in terms of $\{1, x\}$:

$$\mathbf{A} = \mathbf{A}_x = \begin{pmatrix} 0 & 1 \\ -a_0 & -a_1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\frac{1}{6} & \frac{5}{6} \end{pmatrix}.$$

The 1-fold eigenvalues of \mathbf{A} are $x^{(1)} = \frac{1}{2}$ and $x^{(2)} = \frac{1}{3}$: the roots of f .

If $h \in \mathcal{I}$, then $[h \cdot r] = [h] \cdot [r] = [0] \cdot [r] = [0]$, and $\mathbf{A}_h = \mathbf{0}$. An intuitive explanation for Theorem 2.1.2 now proceeds as in Example 2.1.9.

Example 2.1.9. Consider the set of $s = 2$ polynomial equations in $n = 2$ variables with $m = 4$ simple roots in Example 1.1.4.

$$f_2(x_1, x_2) = x_1^2 + 2x_1x_2 + x_2^2 - 1 \in \mathcal{I},$$

so $\mathbf{0} = \mathbf{A}_{f_2} \in \mathbb{C}^{4 \times 4}$. Express \mathbf{A}_{f_2} in terms of the commuting family $\{\mathbf{A}_{x_j}\}_{j=1}^2$:

$$\mathbf{A}_{f_2} = \mathbf{A}_{x_1}^2 + 2\mathbf{A}_{x_1}\mathbf{A}_{x_2} + \mathbf{A}_{x_2}^2 - \mathbf{I}_2$$

where \mathbf{I}_2 is the identity matrix of order 2. Let

$$\mathbf{X} \triangleq \begin{pmatrix} \mathbf{X}_1 & \dots & \mathbf{X}_4 \end{pmatrix} \in \mathbb{C}^{4 \times 4}$$

in Theorem 2.1.2. Like the Cayley-Hamilton theorem, Theorem 2.1.2 assures that indeed

$$\mathbf{A}_{f_2} = \mathbf{X} \begin{pmatrix} x_1^{(1)2} + 2x_1^{(1)}x_2^{(1)} + x_1^{(1)2} - 1 & & & \mathbf{0} \\ & \ddots & & \\ & & x_1^{(4)2} + 2x_1^{(4)}x_2^{(4)} + x_1^{(4)2} - 1 & \\ \mathbf{0} & & & \end{pmatrix} \mathbf{X}^{-1} = \mathbf{0}.$$

Theorem 2.1.2 will prove useful to found the remainder of this thesis.

2.2 Multilinear Algebra

2.2.1 Higher-Order Tensors

Vectors and matrices are the key building blocks of linear algebra. A *vector* $\mathbf{a} \in \mathbb{F}^{I_1}$ (denoted by a boldface lower case letter) is an element of an I_1 -dimensional vector space over the field \mathbb{F} . The field \mathbb{F} could be \mathbb{R} , the set of the real numbers, or \mathbb{C} , the set of the complex numbers. Unless stated otherwise, we will take $\mathbb{F} = \mathbb{C}$ in the remainder of this thesis. A vector can be seen as a 1-dimensional array of I_1 entries: $(\mathbf{a})_{i_1} = \mathbf{a}(i_1) = a_{i_1} \in \mathbb{C}$, $1 \leq i_1 \leq I_1$ (Fig. 2.1a). An $I_1 \times I_2$ *matrix* $\mathbf{A} \in \mathbb{C}^{I_1 \times I_2}$ (denoted by a boldface upper case letter) is then a 2-dimensional array, consisting of entries $(\mathbf{A})_{i_1, i_2} = \mathbf{A}(i_1, i_2) = a_{i_1, i_2}$ (Fig. 2.1b). Appendix A reviews basic notions from matrix algebra, such as the singular value decomposition (SVD).

In multilinear algebra, an N th-order *tensor* $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ (denoted by a calligraphic letter) is a natural higher-order generalization of a vector and a matrix. Higher-order tensors are thus arrays, indexed by three or more indexes: the (i_1, i_2, \dots, i_N) th entry of \mathcal{A} is denoted by $(\mathcal{A})_{i_1, i_2, \dots, i_N} = \mathcal{A}(i_1, i_2, \dots, i_N) = a_{i_1, i_2, \dots, i_N} \in \mathbb{C}$, $1 \leq i_n \leq I_n$, $1 \leq n \leq N$ (Fig. 2.1c). N is the *order* of the tensor: the number of dimensions (*modes*). Capitals I_n will consistently be used for the dimensions, *i.e.* the upper bound on the set of mode- n indexes. Appendix B walks the unpracticed reader through basic multilinear algebra tools.

Appendix B discusses the *multilinear singular value decomposition* (MLSVD) as a convincing generalization of the matrix SVD in Appendix A. We will discuss the *canonical polyadic decomposition* (CPD) and a *block term decomposition* (BTD) here. Before doing so, we need the following two definitions.

Definition 2.2.1 (n -rank). The n -rank $R_n = \text{rank}_n(\mathcal{A})$ of a tensor \mathcal{A} is the dimension of the mode- n fiber space⁸ of \mathcal{A} .

⁸A mode- n fiber $\mathbf{a}_{i_1, i_2, \dots, i_{n-1}, i_{n+1}, \dots, i_N} = (\mathcal{A})_{i_1, i_2, \dots, i_{n-1}, :, i_{n+1}, \dots, i_N}$ is a vector obtained when fixing all but the n th index of \mathcal{A} — see Appendix B.

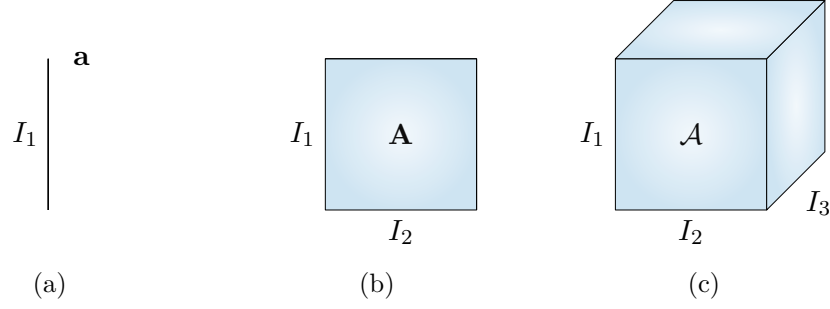


Figure 2.1: (a) A vector $\mathbf{a} \in \mathbb{C}^{I_1}$, (b) a matrix $\mathbf{A} \in \mathbb{C}^{I_1 \times I_2}$ and (c) a third-order tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$.

Definition 2.2.2 (multilinear rank). The tuple $\text{rank}_{\boxplus}(\mathcal{A}) = (R_1, R_2, \dots, R_N)$ is called the multilinear rank⁹ of the tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$.

2.2.2 The Canonical Polyadic Decomposition

Definition 2.2.3 (rank-1 tensor). A rank-1 tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ is the outer product of N nonzero vectors $\mathbf{u}^{(n)} \in \mathbb{C}^{I_n}, 1 \leq n \leq N$

$$\mathcal{A} = \mathbf{u}^{(1)} \otimes \mathbf{u}^{(2)} \otimes \dots \otimes \mathbf{u}^{(N)}.$$

Definition 2.2.4 (polyadic decomposition). A polyadic decomposition (PD) of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ expresses \mathcal{A} as a sum of rank-1 terms:

$$\mathcal{A} = \sum_{r=1}^R \mathbf{u}_r^{(1)} \otimes \mathbf{u}_r^{(2)} \otimes \dots \otimes \mathbf{u}_r^{(N)} \triangleq \llbracket \mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \dots, \mathbf{U}^{(N)} \rrbracket \quad (2.6)$$

in which $\mathbf{U}^{(n)} = \begin{pmatrix} \mathbf{u}_1^{(n)} & \dots & \mathbf{u}_R^{(n)} \end{pmatrix} \in \mathbb{C}^{I_n \times R}$ is called the n th factor matrix.

Example 2.2.1. Consider the third-order tensor $\mathcal{A} \in \mathbb{C}^{3 \times 3 \times 3}$ defined by

$$\begin{cases} a_{1,1,1} = a_{2,2,1} = a_{2,2,2} = a_{3,3,2} = 1 \\ a_{1,1,3} = -a_{3,3,3} = 2 \end{cases}$$

and $a_{i_1, i_2, i_3} = 0$ elsewhere. It is easy to verify that \mathcal{A} can be written as

$$\mathcal{A} = \llbracket \mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \mathbf{U}^{(3)} \rrbracket$$

where

$$\mathbf{U}^{(1)} = \mathbf{I}_3, \quad \mathbf{U}^{(2)} = \mathbf{I}_3, \quad \mathbf{U}^{(3)} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 2 & 0 & -2 \end{pmatrix}.$$

Definition 2.2.5 (tensor rank). The rank¹⁰ $r_{\mathcal{A}}$ of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ is the

⁹Definition 2.2.2 is a proper generalization of view (i) on the matrix rank in Appendix A.

¹⁰Definition 2.2.5 is a proper generalization of view (ii) on the matrix rank in Appendix A.

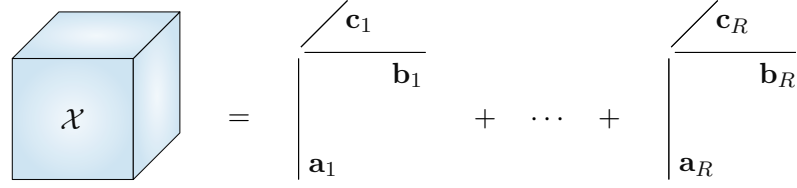


Figure 2.2: Visualization of the CPD.

minimal number of rank-1 terms that yield \mathcal{A} in a linear combination.

First introduced in [28], the canonical PD is a polyadic decomposition (2.6) where $R = r_{\mathcal{A}}$.

Definition 2.2.6 (CPD). A canonical polyadic decomposition (CPD) of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ expresses \mathcal{A} as a minimal sum of rank-1 terms.

To ease notation and to develop insight, we will stick to the third-order case from here, and write the CPD of a tensor $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ as

$$\mathcal{X} = \llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket = \sum_{r=1}^R \mathbf{a}_r \otimes \mathbf{b}_r \otimes \mathbf{c}_r. \quad (2.7)$$

Fig. 2.2 visualizes the CPD of a third-order tensor. We will denote the matrix slice $\mathbf{X}_k \triangleq \mathcal{X}(:, :, k)$ and $\mathbf{D}_k(\mathbf{C}) \triangleq \text{diag}(\mathbf{C}(k, :))$, such that (2.7) can be written as $\mathbf{X}_k = \mathbf{A} \mathbf{D}_k(\mathbf{C}) \mathbf{B}^T$, $1 \leq k \leq K$. (2.7) can also be written as

$$\mathbf{X}_{[1,2;3]} = \sum_{r=1}^R (\mathbf{a}_r \otimes \mathbf{b}_r) \mathbf{c}_r^T = \begin{pmatrix} \mathbf{a}_1 \otimes \mathbf{b}_1 & \dots & \mathbf{a}_R \otimes \mathbf{b}_R \end{pmatrix} \mathbf{C}^T = (\mathbf{A} \odot \mathbf{B}) \mathbf{C}^T$$

and, analogously, $\mathbf{X}_{[2,3;1]} = (\mathbf{B} \odot \mathbf{C}) \mathbf{A}^T$ and $\mathbf{X}_{[1,3;2]} = (\mathbf{A} \odot \mathbf{C}) \mathbf{B}^T$. Individual Differences in Scaling (INDSCAL) is a particular CPD of a third-order tensor that is symmetric in two modes, *i.e.* $\mathbf{A} = \mathbf{B}$ in (2.7).

Determining the *exact* rank of a tensor is NP-hard [26]. In many applications, however, one may rather be interested in a limited number of interpretable components that capture the meaningful information in a data tensor \mathcal{X} and leave out the noise. For an overview and a comparison of algorithms to compute the CPD, or a low-rank approximation¹¹, see [35].

A word on the *uniqueness* of (2.7) is in place. Whereas the SVD (A.2) and the MLSVD (B.2) thank their uniqueness to additional constraints, the CPD is easily unique, making it a crucial tool for signal processing applications. Let us first make mention of the fact that the CPD is *always subject* to trivial permutation and scaling indeterminacies, *i.e.* the order of the terms and the (counter)scaling of the vectors in (2.7) is arbitrary. Apart from those indeterminacies, Theorem 2.2.1 contains a uniqueness condition that will prove useful in Chapter 3.

¹¹A best low-rank approximation of a higher-order tensor may not exist — see Example 2.2.2.

Theorem 2.2.1. [36, p. 530] Let $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ admit a PD $\mathcal{X} = \llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket$, where $\mathbf{A} \in \mathbb{C}^{I \times R}$ and $\mathbf{B} \in \mathbb{C}^{J \times R}$ have full column rank, then $r_{\mathcal{X}} = R$ and the CPD of \mathbf{X} is unique iff $k_{\mathbf{C}}^{12} \geq 2$.

For a discussion of other CPD uniqueness conditions, see Appendix C¹³.

Two striking differences between tensor rank and matrix rank are worth mentioning:

(i) The set

$$\begin{aligned} S_R(I, J, K) &= \{\mathcal{X} \in \mathbb{C}^{I \times J \times K} \mid r_{\mathcal{X}} \leq R\} \\ &= \{\mathcal{X} \in \mathbb{C}^{I \times J \times K} \mid \exists \mathbf{A} \in \mathbb{C}^{I \times R}, \mathbf{B} \in \mathbb{C}^{J \times R}, \mathbf{C} \in \mathbb{C}^{K \times R} : \mathcal{X} = \llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket\} \end{aligned}$$

may not be closed for $R \geq 2$ [15]. This means that the best rank- R approximation $\hat{\mathcal{X}}$ of a higher-order tensor $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$

$$\hat{\mathcal{X}} = \arg \min_{\mathcal{L} \in S_R} \|\mathcal{X} - \mathcal{L}\|^2$$

may not exist. The computation of such a rank- R approximation yields a rank- R sequence \mathcal{X}_n that converges to a boundary point $\hat{\mathcal{X}}$ of $S_R(I, J, K)$, but with $r_{\hat{\mathcal{X}}} > R$: \mathcal{X} has *border rank* R ¹⁴. During computation, convergence is slow, the columns of \mathbf{A} , \mathbf{B} and \mathbf{C} become linearly dependent and their norms grow without bound: one example of a phenomenon known as *diverging rank-1 terms*.

Example 2.2.2. [15, Proposition 4.6] Consider the third-order tensor

$$\mathcal{X} = \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{v} + \mathbf{u} \otimes \mathbf{v} \otimes \mathbf{u} + \mathbf{v} \otimes \mathbf{u} \otimes \mathbf{u}$$

with \mathbf{u} and \mathbf{v} linearly independent. $r_{\mathcal{X}} = 3$, but \mathcal{X} has border rank 2: as $n \rightarrow \infty$, it can be approximated arbitrarily well by a sequence of rank-2 tensors

$$\begin{aligned} \mathcal{X}_n &= n \left(\mathbf{u} + \frac{1}{n} \mathbf{v} \right) \otimes \left(\mathbf{u} + \frac{1}{n} \mathbf{v} \right) \otimes \left(\mathbf{u} + \frac{1}{n} \mathbf{v} \right) - n \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u} \\ &= \mathcal{X} + \frac{1}{n} \left(\mathbf{v} \otimes \mathbf{v} \otimes \mathbf{u} + \mathbf{v} \otimes \mathbf{u} \otimes \mathbf{v} + \mathbf{u} \otimes \mathbf{v} \otimes \mathbf{v} + \frac{1}{n} \mathbf{v} \otimes \mathbf{v} \otimes \mathbf{v} \right). \end{aligned}$$

[39] further proves that it is possible to decompose \mathcal{X} into a third-order generalization of the Jordan canonical form (Definition A.3.2) in the matrix case — as long as there are no groups of more than 4 diverging rank-1 terms.

¹²The Kruskal rank $k_{\mathbf{C}}$ is the largest number k such that any subset of k columns of \mathbf{C} is linearly independent — see Definition C.1.3.

¹³As parts of Chapter 3 will refer to some of these conditions, insight may prove useful.

¹⁴Provided that R is the minimal value for which this phenomenon occurs.

Theorem 2.2.2. [15, Lemma 4.7] For a group of $R = 2$ diverging rank-1 terms, \mathcal{X} can be written as

$$\mathcal{X} = \mathcal{G} \cdot_1 \mathbf{U}^{(1)} \cdot_1 \mathbf{U}^{(2)} \cdot_1 \mathbf{U}^{(3)}$$

where $r_{\mathbf{U}^{(1)}} = r_{\mathbf{U}^{(2)}} = r_{\mathbf{U}^{(3)}} = 2$ and where $\mathcal{G} \in \mathbb{C}^{2 \times 2 \times 2}$ is given by

$$\mathbf{G}_{[1;3,2]} = \left(\begin{array}{cc|cc} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{array} \right). \quad (2.8)$$

Moreover, we have that $r_{\mathcal{G}} = r_{\mathcal{X}} = 3$.

- (ii) The rank of a tensor depends on \mathbb{F} . Consider $\mathcal{X} \in \mathbb{R}^{2 \times 2 \times 2}$ with entries sampled at random from a continuous probability distribution. If \mathbf{A}, \mathbf{B} and \mathbf{C} are constrained to be real, then $r_{\mathcal{X}} = 2$ or $r_{\mathcal{X}} = 3$ with probability < 1 — whereas if \mathbf{A}, \mathbf{B} and \mathbf{C} can be complex, $r_{\mathcal{X}} = 2$, with probability 1 [31, 3]. When the rank can take more than one value, these values are called *typical ranks*. When there is only one typical rank, it is called the *generic rank*.

2.2.3 Block Term Decomposition

Definition 2.2.7 (block term decomposition). A block term decomposition (BTD) of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ expresses \mathcal{A} as a sum of low multilinear rank terms:

$$\mathcal{A} = \sum_{r=1}^R \mathcal{G}_r \cdot_1 \mathbf{U}_r^{(1)} \cdot_2 \mathbf{U}_r^{(2)} \cdot_3 \dots \cdot_N \mathbf{U}_r^{(N)} \quad (2.9)$$

in which $\mathcal{G}_r \in \mathbb{C}^{J_{r,1} \times J_{r,2} \times \dots \times J_{r,N}}$ is called the core tensor and $\mathbf{U}_r^{(n)} = \begin{pmatrix} \mathbf{u}_{r,1}^{(n)} & \dots & \mathbf{u}_{r,J_{r,n}}^{(n)} \end{pmatrix} \in \mathbb{C}^{I_n \times J_{r,n}}$ is called the n th factor matrix in the r th term.

Fig. 2.3 visualizes the BTD of a third-order tensor. (2.9) is subject to indeterminacies that are more involved than scaling and permutation¹⁵. The BTD can be unique, but under more restrictive conditions than the CPD. For a discussion of its uniqueness properties, see [11]. Note that if $J_{r,n} = 1, 1 \leq r \leq R, 1 \leq n \leq N$, (2.9) reduces to a CPD¹⁶. For algorithms to compute the BTD, see [35].

2.3 Multidimensional Harmonic Retrieval

2.3.1 Harmonic Retrieval

Definition 2.3.1 (Vandermonde matrix). [36, p. 531] The matrix $\mathbf{A} \in \mathbb{C}^{I \times R}$ is called Vandermonde if

$$\mathbf{A} = \begin{pmatrix} \mathbf{a}_1 & \dots & \mathbf{a}_R \end{pmatrix}, \quad \mathbf{a}_r = \begin{pmatrix} 1 & z_r & z_r^2 & \dots & z_r^{I-1} \end{pmatrix}^T, \quad 1 \leq r \leq R,$$

where the scalars $z_r \in \mathbb{C}$ are called the generators of \mathbf{A} .

¹⁵The same argument as for the matrix case in Appendix A starts to apply here: the factor matrices are only determined up to a linear transformation.

¹⁶Likewise, the MLSVD (B.2) is a BTD with $R = 1$.

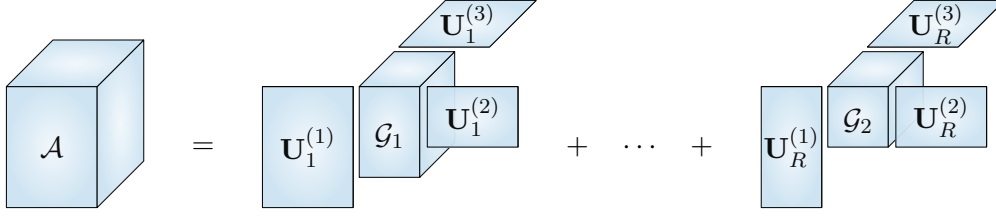


Figure 2.3: Visualization of the BT-D.

Example 2.3.1. Consider again the Vandermonde-structured basis for the null space of the coefficient matrix in Example 1.1.2. It is a Vandermonde matrix where $I = d + 1 = 3$, $R = 2$ and the generators $z_r, 1 \leq r \leq 2$, correspond to the solutions $x^{(k)}, 1 \leq k \leq 2$.

Consider the factorization

$$\mathbf{X} = \mathbf{A}\mathbf{C}^T = \sum_{i=1}^R \mathbf{a}_r \otimes \mathbf{c}_r \quad (2.10)$$

where $\mathbf{X} \in \mathbb{C}^{I \times M}$ contains I observed (row) vectors, $\mathbf{C} \in \mathbb{C}^{M \times R}$ is an unknown mixing matrix and $\mathbf{A} \in \mathbb{C}^{I \times R}$ is a Vandermonde matrix that contains the sources generated by the generators $z_r, 1 \leq r \leq R$. Factorization (2.10) is called a (1D) *harmonic retrieval* (HR) problem. It is obviously subject to the same kind of permutation (and scaling, if $\mathbf{a}_r(1) \neq 1$) ambiguities as the CPD.

Due to their multiplicative shift structure, Vandermonde matrices have several important properties [36, p. 531].

- (i) *Shift-invariance.* Let $\overline{\mathbf{A}}$ and $\underline{\mathbf{A}}$ denote the matrix \mathbf{A} with its first and last row removed, respectively.

$$\begin{aligned} \begin{pmatrix} \overline{\mathbf{A}} \\ \underline{\mathbf{A}} \end{pmatrix} &= \begin{pmatrix} \mathbf{a}_1 & \cdots & \mathbf{a}_R \\ \mathbf{a}_1 z_1 & \cdots & \mathbf{a}_R z_R \end{pmatrix} = \begin{pmatrix} \underline{\mathbf{A}} \\ \underline{\mathbf{A}} \mathbf{D}_2(\mathbf{A}) \end{pmatrix} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_R \end{pmatrix} \odot \underline{\mathbf{A}} \\ &\triangleq \mathbf{A}^{(2)} \odot \underline{\mathbf{A}}. \end{aligned}$$

The r th column of $\mathbf{A}^{(2)} \odot \underline{\mathbf{A}}$ is the Kronecker product of two vectors. Each such column corresponds to a vectorized $(2 \times (I - 1))$ rank-1 Hankel matrix¹⁷.

$$\begin{aligned} \left(\mathbf{A}^{(2)} \odot \underline{\mathbf{A}} \right)_r &= \begin{pmatrix} 1 \\ z_r \end{pmatrix} \otimes \begin{pmatrix} 1 \\ z_r \\ z_r^2 \\ \vdots \\ z_r^{I-2} \end{pmatrix} = \text{vec} \left(\begin{pmatrix} 1 \\ z_r \end{pmatrix} \otimes \begin{pmatrix} 1 \\ z_r \\ z_r^2 \\ \vdots \\ z_r^{I-2} \end{pmatrix} \right) \\ &= \text{vec} \left(\begin{pmatrix} 1 & z_r & \cdots & z_r^{I-2} \\ z_r & z_r^2 & \cdots & z_r^{I-1} \end{pmatrix} \right). \quad (2.11) \end{aligned}$$

¹⁷See Example ??.

(ii) *Spatial smoothing*. More generally, using $z_r^{K+L-2} = z_r^{K-1} z_r^{L-1}$, we have that

$$\begin{aligned} \left(\mathbf{A}^{(K)} \odot \mathbf{A}^{(L)} \right)_r &= \begin{pmatrix} 1 \\ z_r \\ z_r^2 \\ \vdots \\ z_r^{K-1} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ z_r \\ z_r^2 \\ \vdots \\ z_r^{L-1} \end{pmatrix} = \text{vec} \left(\begin{pmatrix} 1 \\ z_r \\ z_r^2 \\ \vdots \\ z_r^{K-1} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ z_r \\ z_r^2 \\ \vdots \\ z_r^{L-1} \end{pmatrix} \right) \\ &= \text{vec} \left(\begin{pmatrix} 1 & z_r & \dots & z_r^{L-1} \\ z_r & z_r^2 & \dots & z_r^L \\ \vdots & \vdots & & \vdots \\ z_r^{K-1} & z_r^K & \dots & z_r^{K+L-2} \end{pmatrix} \right). \end{aligned} \quad (2.12)$$

(2.12) is a generalization of (2.11) with an arbitrary $K \geq 2$.

Using the shift-invariance property of \mathbf{A} , a variant of factorization (2.10)

$$\begin{pmatrix} \underline{\mathbf{X}} \\ \overline{\mathbf{X}} \end{pmatrix} = \begin{pmatrix} \underline{\mathbf{A}} \\ \overline{\mathbf{A}} \end{pmatrix} \mathbf{C}^T = \left(\mathbf{A}^{(2)} \odot \underline{\mathbf{A}} \right) \mathbf{C}^T \triangleq \mathbf{Y}_{[1,2;3]} \quad (2.13)$$

gives the matricization of the constrained CPD of a tensor $\mathcal{Y} \in \mathbb{C}^{2 \times (I-1) \times M}$. (2.13) is the spatially smoothed variant (2.12) of (2.10) with $K = 2$ and $L = I - 1$, *i.e.* simply the case (2.11). Spatial smoothing allows us to go from the second-order matrix model (2.10) to the (matricized) third-order tensor model (2.13).

2.3.2 Multidimensional Harmonic Retrieval

The N -dimensional (*multidimensional*) *harmonic retrieval* (MHR) problem can be formulated as the constrained CPD of a tensor $\mathcal{X} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N \times M}$,

$$\mathcal{X} = \sum_{r=1}^R \mathbf{a}_r^{(1)} \otimes \mathbf{a}_r^{(2)} \otimes \dots \otimes \mathbf{a}_r^{(N)} \otimes \mathbf{c}_r \quad (2.14)$$

where

$$\mathbf{A}^{(n)} = \begin{pmatrix} \mathbf{a}_1^{(n)} & \dots & \mathbf{a}_R^{(n)} \end{pmatrix}, \quad \mathbf{a}_r^{(n)} = \begin{pmatrix} 1 & z_{r,n} & z_{r,n}^2 & \dots & z_{r,n}^{I_n-1} \end{pmatrix}^T, \quad 1 \leq r \leq R,$$

and $\mathbf{C} \in \mathbb{C}^{R \times M}$. Like in the third-order case, the CPD (2.14) can be written as the matricization

$$\mathbf{X} \triangleq \mathbf{X}_{[1,2,\dots,N;N+1]} = \left(\mathbf{A}^{(1)} \odot \dots \odot \mathbf{A}^{(N)} \right) \mathbf{C}^T \in \mathbb{C}^{(\prod_{n=1}^N I_n) \times M}, \quad (2.15)$$

which is a generalization of (2.10). Because all factor matrices $\mathbf{A}^{(n)}$ are Vandermonde, we can apply spatial smoothing in each mode. Like spatial smoothing turns the 2nd-order matrix model (2.10) into the $(2+1)$ th-order CPD model (2.13), it will turn,

by exploiting the shift-invariance property contained in the Vandermonde matrix $\mathbf{A}^{(n)}$, the $(N+1)$ th-order CPD model (2.15) into an $(N+2)$ th-order CPD model (2.16). Let the tensor $\mathcal{Y}^{(n)} \in \mathbb{C}^{2 \times (\times_{p=1}^{n-1} I_p) \times (I_n-1) \times (\times_{p=n+1}^N I_p) \times M}$ implement spatial smoothing in the n th mode. Then $\mathcal{Y}^{(n)}$ has the matricization

$$\mathbf{Y}^{(n)} = \left(\mathbf{A}^{(2,n)} \odot \mathbf{B}^{(n)} \right) \mathbf{C}^T,$$

where now

$$\mathbf{A}^{(2,n)} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ z_{1,n} & z_{2,n} & \dots & z_{R,n} \end{pmatrix}, \quad \mathbf{B}^{(n)} = \left(\odot_{p=1}^{n-1} \mathbf{A}^{(n)} \right) \odot \underline{\mathbf{A}}^{(n)} \odot \left(\odot_{p=n+1}^N \mathbf{A}^{(n)} \right).$$

Let $\bar{\mathbf{S}}^{(n)}$ and $\underline{\mathbf{S}}^{(n)}$ denote the row-selection matrices that delete all rows of \mathbf{X} in (2.15) associated with the upper and bottom row of $\mathbf{A}^{(n)}$, respectively. Then we have that

$$\mathbf{Y}^{(n)} = \begin{pmatrix} \underline{\mathbf{S}}^{(n)} \mathbf{X} \\ \bar{\mathbf{S}}^{(n)} \mathbf{X} \end{pmatrix} = \left(\mathbf{A}^{(2,n)} \odot \mathbf{B}^{(n)} \right) \mathbf{C}^T, \quad (2.16)$$

which is a clear generalization of (2.13).

Definition 2.3.2 (coupled polyadic decomposition). An R -term coupled PD of a collection of tensors $\{\mathcal{Y}^{(n)} \in \mathbb{C}^{I_n \times J_n \times M}\}_{n=1}^N$ expresses each tensor as

$$\mathcal{Y}^{(n)} = \sum_{r=1}^R \mathbf{a}_r^{(n)} \otimes \mathbf{b}_r^{(n)} \otimes \mathbf{c}_r \quad (2.17)$$

in which $\mathbf{A}^{(n)} = \begin{pmatrix} \mathbf{a}_1^{(n)} & \dots & \mathbf{a}_R^{(n)} \end{pmatrix} \in \mathbb{R}^{I_n \times R}$ and $\mathbf{B}^{(n)} = \begin{pmatrix} \mathbf{b}_1^{(n)} & \dots & \mathbf{b}_R^{(n)} \end{pmatrix} \in \mathbb{R}^{J_n \times R}$ and $\mathbf{C} \in \mathbb{C}^{R \times M}$ is a shared factor matrix for each $\mathcal{Y}^{(n)}$.

Definition 2.3.3 (coupled rank). The coupled rank of a collection of tensors $\{\mathcal{Y}^{(n)}\}_{n=1}^N$ is the minimal number of coupled rank-1 terms that yield all $\mathcal{Y}^{(n)}$ together in a linear combination.

A coupled CPD is then a coupled PD (2.17) where R is equal to the coupled rank of the collection $\{\mathcal{Y}^{(n)}\}_{n=1}^N$.

When considered together, the $\{\mathbf{Y}^{(n)}\}_{n=1}^N$ from (2.16) represent a *coupled* CPD (2.17). The coupled CPD is a natural framework for MHR that allows us to jointly exploit the shift-invariance property contained in all Vandermonde matrices $\{\mathbf{A}^{(n)}\}_{n=1}^N$ [36, p. 534]. By exploiting the structure contained in all modes, [36] has been able to derive the most relaxed uniqueness conditions for MHR to date. The coupled CPD (2.17) is clearly subject to the same trivial indeterminacies as the CPD (Definition C.1.1), where the permutation and (counter)scaling are coupled, so “uniqueness” is again to be read as “essential uniqueness”. In Theorem 2.3.1, let $r_{\text{MHR}}(\mathcal{X})$ be defined as the coupled rank of $\{\mathcal{Y}^{(n)}\}_{n=1}^N$.

Theorem 2.3.1 (sufficient generic MHR uniqueness condition). *[36, p. 534] Let $\mathcal{X} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N \times M}$ admit a PD where the factor matrices $\{\mathbf{A}^{(n)}\}_{n=1}^N$ are Vandermonde. If*

$$R \leq M \quad \text{and} \quad R \leq \prod_{n=1}^N I_n - N - 1,$$

then generically, $r_{\text{MHR}}(\mathcal{X}) = R$ and the factorization (2.14) is unique.

A proof can be found in [36]. Tensorlab [45] provides the structured data fusion framework for the computation of coupled decompositions. Also ESPRIT-like methods exist to compute the coupled CPD [37, Algorithm 1].

Chapter 3

Connections between Sets of Polynomial Equations and the Canonical Polyadic Decomposition

The next two chapters properly establish connections between the topics introduced in Chapter 2. Their organization is shown in Fig. 3.1. To develop insight, the text will adopt a bottom-up approach, rather than the top-down approach implied by Fig. 3.1. First, this chapter will study a set of polynomial equations that has only (i) simple roots and its connection with the CPD. Section 3.1 will start from the MHR problem to derive a connection between the null space of the Macaulay matrix of a generic set of polynomial equations, *i.e.* a set that has only (i) simple and (ii) affine roots, and the computation of the CPD of a third-order tensor by means of a generalized eigenvalue decomposition (GEVD). Section 3.2 will drop (ii) and ascends to a more general connection between the third-order tensor CPD and a higher-order INDSCAL model. Finally, Section 3.3 will propose a multilinear algebra-based algorithm to find the roots of a generic set of polynomial equations.

3.1 Affine Case

Let f_1, f_2, \dots, f_s be a system of s polynomial equations in n variables x_1, x_2, \dots, x_n introduced in Chapter 2. If we assume a 0-dimensional solution set, Theorem 2.1.1 gives the number of solutions in the projective space \mathbb{P}^n , counting multiplicities:

$$m = \prod_{i=1}^s d_i.$$

If there are roots with multiplicities greater than 1, we say that the number of disjoint roots $m_0 < m$. If all roots are simple, $m_0 = m$. This section covers the generic, *i.e.* (i) *simple* and (ii) *affine* case. Section 3.1.1 will establish the connection between

3. CONNECTIONS BETWEEN SETS OF POLYNOMIAL EQUATIONS AND THE CANONICAL POLYADIC DECOMPOSITION

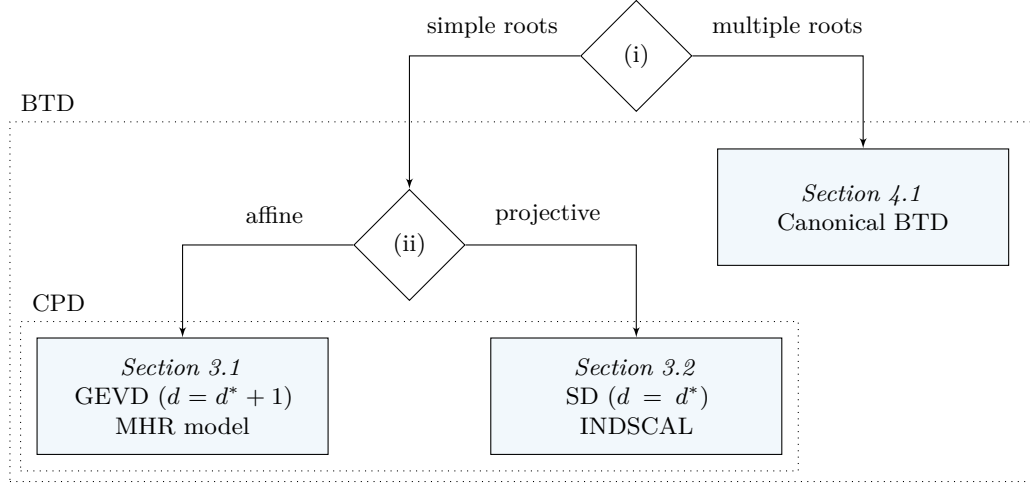


Figure 3.1: Organization of Chapter 3 and 4.

the null space of the Macaulay matrix of a system of polynomial equations and the MHR problem. Section 3.1.2 will rewrite the resulting “MHR model” as the CPD of one third-order tensor, which can be computed by means of a GEVD.

3.1.1 The Decomposition of the Null Space of the Macaulay Matrix as a MHR problem

Example 1.1.5 shows that the null space of the Macaulay matrix $\mathbf{M}(d)$ of degree d contains m *multivariate* Vandermonde vectors — provided that $d \geq d^*$, with d^* the degree of regularity. Let

$$\mathbf{V} = (\mathbf{v}_1 \ \dots \ \mathbf{v}_m) \in \mathbb{C}^{q(d) \times m} \quad (3.1)$$

be such a full, multivariate Vandermonde basis for $\text{null}(\mathbf{M}(d))$, where the dependence on d is implicit. If d is clear from the context or unimportant for the reasoning, we leave it out from here.

$$\begin{aligned} \mathbf{v}_k = (\mathbf{V})_k &= \left(1 \ x_{1,k} \ x_{2,k} \ \dots \ x_{1,k}^2 \ x_{1,k}x_{2,k} \ \dots \ x_{n-1,k}x_{n,k}^{d-1} \ x_{n,k}^d \right)^T \\ &\triangleq \left(1 \ x_1^{(k)} \ x_2^{(k)} \ \dots \ x_1^{(k)2} \ x_1^{(k)}x_2^{(k)} \ \dots \ x_{n-1}^{(k)}x_n^{(k)d-1} \ x_n^{(k)d} \right)^T \in \mathbb{C}^{q(d)}, \quad 1 \leq k \leq m, \end{aligned}$$

is then a multivariate Vandermonde vector, with its entries ordered by the degree negative lexicographic order. \mathbf{V} and \mathbf{v}_k will frequently be used in this chapter. On the other hand, let

$$\mathbf{V}^{(j)} = (\mathbf{v}_1^{(j)} \ \dots \ \mathbf{v}_m^{(j)}) \in \mathbb{C}^{(d+1) \times m}, \quad 1 \leq j \leq n, \quad (3.2)$$

be a *genuine* Vandermonde matrix (Definition 2.3.1), where

$$\mathbf{v}_k^{(j)} = (\mathbf{V}^{(j)})_k = \left(1 \ x_j^{(k)} \ x_j^{(k)2} \ \dots \ x_j^{(k)d} \right)^T \in \mathbb{C}^{d+1}, \quad 1 \leq k \leq m.$$

(3.1) and (3.2) are related by

$$\mathbf{V} = \mathbf{S}_{(d+1)^n \rightarrow q(d)} \left(\mathbf{V}^{(1)} \odot \dots \odot \mathbf{V}^{(n)} \right) \in \mathbb{C}^{q(d) \times m} \quad (3.3)$$

where $\mathbf{S}_{(d+1)^n \rightarrow q(d)} \in \mathbb{C}^{q(d) \times (d+1)^n}$ denotes the row selection and ordering matrix that (i) selects all rows of the Khatri–Rao product $\in \mathbb{C}^{(d+1)^n \times m}$ that correspond to the $q(d)$ monomials from degree 0 up to degree d and (ii) permutes these rows to be ordered by the degree negative lexicographic order, as to match the rows in the left-hand side.

Let $\mathbf{K} \in \mathbb{C}^{q(d) \times m}$ be a numerical basis for $\text{null}(\mathbf{M}(d))$, *e.g.*, calculated using the `null` command in Matlab. \mathbf{K} is related to \mathbf{V} by

$$\mathbf{K} = \mathbf{V} \mathbf{C}^T \quad (3.4)$$

where \mathbf{C}^T is an invertible transformation matrix. Also $\mathbf{C} = \mathbf{C}(d)$ is dependent on d . Indeed, the top rows of $\mathbf{V}(d)$ are equal to the rows of $\mathbf{V}(d-1)$, but this is not the case for $\mathbf{K}(d)$ and $\mathbf{K}(d-1)$. Combining (3.3) and (3.4), we have that

$$\mathbf{K} = \mathbf{S}_{(d+1)^n \rightarrow q(d)} \left(\mathbf{V}^{(1)} \odot \dots \odot \mathbf{V}^{(n)} \right) \mathbf{C}^T \in \mathbb{C}^{q(d) \times m}. \quad (3.5)$$

(3.5) is the MHR model (2.15), where $M = R = m$. (3.5) reveals that $\text{null}(\mathbf{M}(d))$ has the structure of the CPD

$$\sum_{k=1}^m \mathbf{v}_k^{(1)} \otimes \mathbf{v}_k^{(2)} \otimes \dots \otimes \mathbf{v}_k^{(n)} \otimes \mathbf{c}_k \in \mathbb{C}^{(d+1) \times (d+1) \times \dots \times (d+1) \times m}. \quad (3.6)$$

Note that (3.6) contains again more monomials than the $q(d)$ monomials from degree 0 up to degree d in $\text{null}(\mathbf{M}(d))$. By exploiting the shift-invariance property contained in the genuine Vandermonde matrix $\mathbf{V}^{(j)}$,

$$\mathbf{Y}^{(j)} = \left(\mathbf{V}^{(2,j)} \odot \mathbf{B}(d-1) \right) \mathbf{C}^T \in \mathbb{C}^{(2 \cdot q(d-1)) \times m} \quad (3.7)$$

implements a spatial smoothing of (3.5) in the j th mode, where

$$\mathbf{V}^{(2,j)} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ x_j^{(1)} & x_j^{(2)} & \dots & x_j^{(m)} \end{pmatrix} \in \mathbb{C}^{2 \times m}$$

and

$$\mathbf{B}(d-1) = \mathbf{S}_{q(d) \rightarrow q(d-1)} \mathbf{V}(d) = \begin{pmatrix} \mathbf{I}_{q(d-1)} & \mathbf{0}_{q(d-1) \times (n-1+d)} \end{pmatrix} \mathbf{V}(d) = \mathbf{V}(d-1) \in \mathbb{C}^{q(d-1) \times m}$$

contains the rows of $\mathbf{V}(d)$ that correspond to the $q(d-1)$ monomials from degree 0 up to degree $d-1$ ordered by the degree negative lexicographic order.

Let $\bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)}$ and $\underline{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)}$ denote the row selection matrices that delete all rows of \mathbf{K} in (3.5) associated with the upper and bottom row of $\mathbf{V}^{(j)}$, respectively. Combining (3.5) and (3.7), we have that for $1 \leq j \leq n$:

$$\mathbf{Y}^{(j)} = \begin{pmatrix} \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)} \mathbf{K} \\ \underline{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)} \mathbf{K} \end{pmatrix} = \left(\mathbf{V}^{(2,j)} \odot \mathbf{B}(d-1) \right) \mathbf{C}^T \in \mathbb{C}^{(2 \cdot q(d-1)) \times m}, \quad (3.8)$$

3. CONNECTIONS BETWEEN SETS OF POLYNOMIAL EQUATIONS AND THE CANONICAL POLYADIC DECOMPOSITION



Figure 3.2: (a) The monomials in $n = 2$ variables x_1 and x_2 of degree $d \leq 3$ in $\mathbf{V}(3)$. The colored monomials are contained in $\mathbf{B}^{(j)}(2) \equiv \mathbf{B}(2) = \mathbf{V}(2)$, $1 \leq j \leq 2$. (b) The entries in \mathbf{X} in the MHR model (2.16), where $N = 2$ and $I_1 = I_2 = 4$. The blue and red entries are contained in $\mathbf{B}^{(1)}$ and $\mathbf{B}^{(2)} \neq \mathbf{B}^{(1)}$, respectively.

which is very similar to the MHR model (2.16). There is one important difference with (2.16) though: we have used $\mathbf{B}^{(j)}(d-1) \equiv \mathbf{B}(d-1) = \mathbf{V}(d-1)$, $1 \leq j \leq n$, in (3.8). To ensure that the rows onto which the rows of $\mathbf{B}(d-1)$ are mapped after multiplication with x_j , still occur in \mathbf{K} , we need to remove *all* rows of degree d — rather than the rows in which x_j has degree d (Fig. 3.2). As a consequence, the $\{\mathbf{Y}^{(j)}\}_{j=1}^n$ in (3.8) have their first $q(d-1)$ rows in common.

Example 3.1.1. Consider the system of $s = 2$ polynomial equations in $n = 2$ variables with $m = 4$ simple and affine roots in Example 1.1.5 again. At $d = 3$, the multivariate Vandermonde basis for $\text{null}(\mathbf{M}(3))$ is

$$\mathbf{V}(3) = \begin{pmatrix} 1 & 1 & 1 & 1 \\ x_1^{(1)} & x_1^{(2)} & x_1^{(3)} & x_1^{(4)} \\ x_2^{(1)} & x_2^{(2)} & x_2^{(3)} & x_2^{(4)} \\ x_1^{(1)2} & x_1^{(2)2} & x_1^{(3)2} & x_1^{(4)2} \\ x_1^{(1)}x_2^{(1)} & x_1^{(2)}x_2^{(2)} & x_1^{(3)}x_2^{(3)} & x_1^{(4)}x_2^{(4)} \\ x_2^{(1)2} & x_2^{(2)2} & x_2^{(3)2} & x_2^{(4)2} \\ x_1^{(1)3} & x_1^{(2)3} & x_1^{(3)3} & x_1^{(4)3} \\ x_1^{(1)2}x_2^{(1)} & x_1^{(2)2}x_2^{(2)} & x_1^{(3)2}x_2^{(3)} & x_1^{(4)2}x_2^{(4)} \\ x_1^{(1)}x_2^{(1)2} & x_1^{(2)}x_2^{(2)2} & x_1^{(3)}x_2^{(3)2} & x_1^{(4)}x_2^{(4)2} \\ x_1^{(1)3} & x_1^{(2)3} & x_1^{(3)3} & x_1^{(4)3} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 3 & 4 \\ -1 & 0 & -2 & -5 \\ 0 & 1 & 9 & 16 \\ 0 & 0 & -6 & -20 \\ 1 & 0 & 4 & 25 \\ 0 & 1 & 27 & 64 \\ 0 & 0 & -18 & -80 \\ 0 & 0 & 12 & 100 \\ -1 & 0 & -8 & -125 \end{pmatrix}. \quad (3.9)$$

Let $\mathbf{K} = \mathbf{V}\mathbf{C}^T$ be a numerical basis for $\text{null}(\mathbf{M}(3))$. Since

$$\mathbf{V}^{(2,1)} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ x_1^{(1)} & x_1^{(2)} & x_1^{(3)} & x_1^{(4)} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 3 & 4 \end{pmatrix}$$

and, using conventional Matlab notation for indexing,

$$\mathbf{B}^{(1)}(2) \equiv \mathbf{B}(2) = \mathbf{V}(2) = \begin{pmatrix} \mathbf{v}_1(2) & \mathbf{v}_2(2) & \mathbf{v}_3(2) & \mathbf{v}_4(2) \end{pmatrix} = \mathbf{V}(3)(1:6,:),$$

(Fig. 3.2a), we have that

$$\begin{aligned}
 (\mathbf{V}^{(2,1)} \odot \mathbf{B}(2)) \mathbf{C}^T &= \left(\frac{1 \cdot \mathbf{v}_1(2) \quad 1 \cdot \mathbf{v}_2(2) \quad 1 \cdot \mathbf{v}_3(2) \quad 1 \cdot \mathbf{v}_4(2)}{0 \cdot \mathbf{v}_1(2) \quad 1 \cdot \mathbf{v}_2(2) \quad 3 \cdot \mathbf{v}_3(2) \quad 4 \cdot \mathbf{v}_4(2)} \right) \mathbf{C}^T \\
 &= \left(\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 0 & 1 & 3 & 4 \\ -1 & 0 & -2 & -5 \\ 0 & 1 & 9 & 16 \\ 0 & 0 & -6 & -20 \\ 1 & 0 & 4 & 25 \\ 0 & 1 & 3 & 4 \\ 0 & 1 & 9 & 16 \\ 0 & 0 & -6 & -20 \\ 0 & 1 & 27 & 64 \\ 0 & 0 & -18 & -80 \\ 0 & 0 & 12 & 100 \end{array} \right) \mathbf{C}^T = \left(\frac{\underline{\mathbf{S}}_{\mathbf{B}(2)}^{(1)} \mathbf{K}}{\bar{\mathbf{S}}_{\mathbf{B}(2)}^{(1)} \mathbf{K}} \right) = \mathbf{Y}^{(1)}. \quad (3.10)
 \end{aligned}$$

Comparing (3.9) with (3.10), it is clear that

$$\underline{\mathbf{S}}_{\mathbf{B}(2)}^{(1)} = \begin{pmatrix} \mathbf{I}_{q(2)} & \mathbf{0}_{q(2) \times \binom{4}{3}} \end{pmatrix} = \begin{pmatrix} \mathbf{I}_6 & \mathbf{0}_{6 \times 4} \end{pmatrix}$$

and

$$\bar{\mathbf{S}}_{\mathbf{B}(2)}^{(1)} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

delete all rows associated with the bottom and upper row of $\mathbf{V}^{(1)}$, respectively. In fact, we have already encountered $\underline{\mathbf{S}}_{\mathbf{B}(2)}^{(1)}$ and $\bar{\mathbf{S}}_{\mathbf{B}(2)}^{(1)}$ in the GEVD that expresses the multiplication with x_1 in the PNLA framework in Example 1.1.5:

$$\mathbf{S}_0 \mathbf{K} \mathbf{T} \mathbf{D}_1 = \mathbf{S}_1 \mathbf{K} \mathbf{T} \Leftrightarrow \mathbf{S}_0 \mathbf{V} \mathbf{D}_2 (\mathbf{V}^{(2,1)})^T \mathbf{T}^{-1} = \mathbf{S}_1 \mathbf{K}$$

is equal to the lower part in (3.10), where

$$\mathbf{S}_0 \mathbf{V} = \underline{\mathbf{S}}_{\mathbf{B}(2)}^{(1)} \mathbf{V} = \mathbf{B}(2) \quad \mathbf{S}_1 \mathbf{K} = \bar{\mathbf{S}}_{\mathbf{B}(2)}^{(1)} \mathbf{K}, \quad \text{and} \quad \mathbf{T} = (\mathbf{C}^T)^{-1}.$$

We can construct $\mathbf{Y}^{(2)}$ in a completely analogous way, with $\mathbf{B}^{(2)}(2) \equiv \mathbf{B}(2)$ and, therefore, $\underline{\mathbf{S}}_{\mathbf{B}(2)}^{(2)} = \underline{\mathbf{S}}_{\mathbf{B}(2)}^{(1)}$, such that $\mathbf{Y}^{(2)}$ would have the same first $q(2) = 6$ rows as $\mathbf{Y}^{(1)}$.

3.1.2 The Decomposition of the Null Space of the Macaulay Matrix as a GEVD

When considered together, the $\{\mathbf{Y}^{(j)}\}_{j=1}^n$ in (3.8) represent a coupled CPD, like (2.17). Because the $\mathbf{Y}^{(j)}$ do not only have their third factor matrix \mathbf{C} , but also their second factor matrix $\mathbf{B}(d-1)$ and their first $q(d-1)$ rows in common, we can combine (3.8) for $1 \leq j \leq n$ into a third-order tensor \mathcal{Y} and remove the redundant rows as follows:

$$\begin{aligned} \mathbf{Y}_{[1,2;3]} &= \begin{pmatrix} \underline{\mathbf{S}}_{\mathbf{B}(d-1)}^{(1)} \mathbf{K} \\ \overline{\mathbf{S}}_{\mathbf{B}(d-1)}^{(1)} \mathbf{K} \\ \vdots \\ \overline{\mathbf{S}}_{\mathbf{B}(d-1)}^{(n)} \mathbf{K} \end{pmatrix} = \left(\begin{pmatrix} 1 & 1 & \dots & 1 \\ x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(m)} \\ \vdots & \vdots & & \vdots \\ x_n^{(1)} & x_n^{(2)} & \dots & x_n^{(m)} \end{pmatrix} \odot \mathbf{B}(d-1) \right) \mathbf{C}^T \\ &= (\mathbf{V}(1:n+1, :) \odot \mathbf{B}(d-1)) \mathbf{C}^T = (\mathbf{V}(1) \odot \mathbf{V}(d-1)) \mathbf{C}^T \in \mathbb{C}^{((n+1) \cdot q(d-1)) \times m}. \end{aligned} \quad (3.11)$$

Examples in Chapter 1 and Theorem 2.2.1 allow us to interpret (3.11). We encourage the reader to take a moment to read through these examples again.

- By exploiting the multiplicative shift structure of the multivariate Vandermonde vectors in the null space of the Macaulay matrix, an ESPRIT-like method converts (1.6) in Example 1.1.2 and (1.12) in Example 1.1.5 into a rectangular GEVD or a “square” EVD.
- (1.16) and (1.17) demonstrate that the matrices involved in the left- and right-hand side of such a multiplicative shift property can equivalently be seen as the first two slices of a third-order tensor.
- Theorem 2.2.1 then guarantees the uniqueness of the CPD of such a third-order tensor. Its validation in Appendix C is constructive: outlined, an ESPRIT-like line of reasoning shows how, indeed, an EVD involving the two frontal slices of the third-order tensor is able to recover the factor matrices up to trivial eigenvector ordering and scaling indeterminacies.

To summarize, the aforementioned examples implicitly compute the CPD of a 2-slice third-order tensor as the EVD of 1 matrix. Likewise, the CPD of the $(n+1)$ -slice third-order tensor \mathcal{Y} in (3.11) can be interpreted as the *joint* EVD of n matrices. Corollary 3.1.1 shows that there is in fact a close connection between decomposition (3.11) and the *joint diagonalization* of the n multiplication tables in Theorem 2.1.2 in the generic, *i.e.* the simple and affine, case¹.

¹If $m_0 < m$, Theorem 2.1.2 implies that the \mathbf{A}_{x_j} are not jointly diagonalizable — see Corollary 4.1.1. If there are roots at infinity, the definition of the multiplication tables needs to be slightly changed.

Corollary 3.1.1. *Let the system $\mathcal{F} = \{f_i\}_{i=1}^n$ of n polynomials in n variables x_1, x_2, \dots, x_n have m roots and let $\mathbf{H}(d)$ be the column echelon basis of $\text{null}(\mathbf{M}(d))$. If*

- (i) *the roots are simple,*
- (ii) *there are only affine roots and*
- (iii) *$d = d^* + 1$,*

then the slices $\{\mathcal{H}(j, :, :)\}_{j=1}^n$ of the third-order tensor

$$\mathbf{H}_{[1,2,3]} = \begin{pmatrix} \bar{\mathbf{S}}_{\hat{\mathbf{B}}(d-1)}^{(1)} \mathbf{H}(d) \\ \vdots \\ \bar{\mathbf{S}}_{\hat{\mathbf{B}}(d-1)}^{(n)} \mathbf{H}(d) \end{pmatrix} \in \mathbb{C}^{(n \cdot m) \times m}$$

where $\bar{\mathbf{S}}_{\hat{\mathbf{B}}(d-1)}^{(j)}$ denotes the row selection matrix that selects the rows of $\mathbf{H}(d)$ onto which the m standard monomials are mapped after multiplication with x_j , are equal to the multiplication tables $\{\mathbf{A}_{x_j}\}_{j=1}^n$ w.r.t. the normal set basis for the quotient ring $\mathbb{C}^n / \langle \mathcal{F} \rangle$.

Proof. Since the construction of (3.11) does not rely on the specific choice $\mathbf{K} = \mathbf{V}\mathbf{C}^T$ that was made for the basis of $\text{null}(\mathbf{M}(d))$, the CPD (3.11) holds for $\mathbf{K} = \mathbf{H}$ as well, and

$$\mathcal{H}(j, :, :) = \hat{\mathbf{B}}(d-1) \mathbf{D}_j(\mathbf{V}(2 : n+1, :)) \mathbf{C}^T.$$

$\hat{\mathbf{B}}(d-1) \in \mathbb{C}^{m \times m}$ contains the rows of $\mathbf{B}(d-1) \in \mathbb{C}^{q(d-1) \times m}$ that correspond to the m standard monomials. By definition, at least one standard monomial has exactly degree d^* , so $d = d^* + 1$ is needed for $\mathbf{B}(d-1)$ to contain the m rows that correspond to the standard monomials. Let \mathbf{H} be related to \mathbf{V} by $\mathbf{V} = \mathbf{H}\mathbf{U}$, where $\mathbf{U} = \begin{pmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_m \end{pmatrix} \in \mathbb{C}^{m \times m}$ is an invertible transformation matrix, such that $\mathbf{C}^T = \mathbf{U}^{-1}$. In [24, Proposition 1], it is shown that \mathbf{u}_k contains the m standard monomials evaluated at the solution $\begin{pmatrix} 1 & x_1^{(k)} & \dots & x_n^{(k)} \end{pmatrix}^T$ ². From this, it follows that $\hat{\mathbf{B}}(d-1) = \mathbf{U}$, and that

$$\mathcal{H}(j, :, :) = \mathbf{U} \text{diag}(x_j^{(1)}, \dots, x_j^{(m)}) \mathbf{U}^{-1} = \mathbf{A}_{x_j}, \quad 1 \leq j \leq n,$$

where the last equality is implied by Theorem 2.1.2 for simple and affine roots. \square

Example 3.1.2. *Consider the polynomial equation in $n = 1$ variable x in Example 1.1.2 again. $\mathbf{Y}_{[1,2,3]}$ in (3.11) can be constructed from $\mathbf{H}(2)$ in (1.7) for this univariate*

²See Example 1.1.2 for a glimpse of this result.

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Figure 3.3: The colored monomials in Fig. 3.2a, after multiplication with (a) x_1 and (b) x_2 . The PNLA framework uses *either* (a) or (b), whereas (3.11) uses *both* (a) and (b).

polynomial as well:

$$\mathbf{Y}_{[1,2;3]} = \left(-\frac{\begin{pmatrix} \mathbf{I}_2 & \mathbf{0}_{2 \times 1} \\ \mathbf{0}_{2 \times 1} & \mathbf{I}_2 \end{pmatrix} \mathbf{H}}{\begin{pmatrix} \mathbf{H} \\ \overline{\mathbf{H}} \end{pmatrix}} \right) = \left(\frac{\mathbf{H}}{\overline{\mathbf{H}}} \right) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ -\frac{1}{6} & \frac{5}{6} \end{pmatrix}.$$

It is easy to verify that \mathcal{Y} can be written as

$$\mathcal{Y} = \llbracket \mathbf{A}, \mathbf{A}, \mathbf{C} \rrbracket$$

where

$$\mathbf{A} = \begin{pmatrix} 1 & 1 \\ \frac{1}{2} & \frac{1}{3} \end{pmatrix} \quad \text{and} \quad \mathbf{C} = \mathbf{U}^{-T} = \begin{pmatrix} -2 & 3 \\ 6 & -6 \end{pmatrix}$$

follow from a GEVD of the matrix pencil $(\mathcal{Y}(1, :, :), \mathcal{Y}(2, :, :)) = (\underline{\mathbf{H}}, \overline{\mathbf{H}}) = (\mathbf{I}_2, \mathbf{A}_x)$, which is precisely the EVD of \mathbf{A}_x in Example 2.1.8.

Recall that the PNLA framework selects the rows of \mathbf{K} (or, if you want: the rows of \mathbf{H}) before and after multiplication with *either one* of the x_j to come to *one* GEVD, *e.g.*, $x_j = x_1$ in Example 1.1.5. Fig. 3.4 jointly exploits the multiplicative shift structure contained in *all* n modes of (3.6) in Fig. 3.3³. Fig. 3.5 visualizes the eventual CPD (3.11).

Uniqueness at $d = d^* + 1$

It is now straightforward to establish the uniqueness of decomposition (3.11) at $d = d^* + 1$.

Theorem 3.1.1 (sufficient uniqueness condition for (3.11)). *Let $\mathcal{Y} \in \mathbb{C}^{(n+1) \times q(d-1) \times m}$ admit a PD of the form (3.11), then decomposition (3.11) is a CPD and the CPD is unique if $d \geq d^* + 1$.*

³In practice, the PNLA framework suggests to use a linear combination of multiplications with x_j , $1 \leq j \leq n$, but Section 3.3 will show that it is preferable to take *all* slices in Fig. 3.4 into account, when the polynomial coefficients are only known with limited precision.

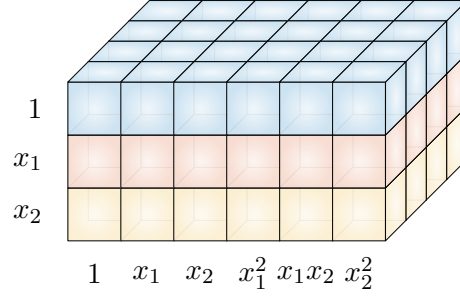


Figure 3.4: The third-order tensor $\mathcal{Y} \in \mathbb{C}^{(n+1) \times q(d-1) \times m}$ in (3.11) with $n = 2$, $d = 3$ and $m = 4$ takes all slices with the rows corresponding to the monomials in Fig. 3.2a, 3.3a and 3.3b into account. The third dimension corresponds to the different roots $\mathbf{x}^{(k)}$, $1 \leq k \leq m$.

$$\begin{array}{c} n+1 \\ \text{ } \\ m \end{array} \begin{array}{c} \text{ } \\ \mathcal{Y} \\ \text{ } \end{array} \begin{array}{c} \text{ } \\ q(d-1) \\ \text{ } \end{array} = \left[\begin{array}{c} \mathbf{c}_1 \\ \left(\begin{array}{c} 1 \\ x_1^{(1)} \\ x_2^{(1)} \end{array} \right) \mathbf{b}_1(d-1) \end{array} \right] + \dots + \left[\begin{array}{c} \mathbf{c}_m \\ \left(\begin{array}{c} 1 \\ x_1^{(m)} \\ x_2^{(m)} \end{array} \right) \mathbf{b}_m(d-1) \end{array} \right]$$

Figure 3.5: Visualization of (3.11) for the third-order tensor in Fig. 3.4.

Proof. It suffices to show that all conditions in Theorem 2.2.1 are satisfied if $d \geq d^* + 1$.

- If all roots are simple, then no columns in $\mathbf{V}(1)$ are collinear, and $k_{\mathbf{V}(1)} \geq 2$.
- If all roots are simple and $d \geq d^*$, then \mathbf{K} is related to \mathbf{V} by $\mathbf{K} = \mathbf{V}\mathbf{C}^T$ where $\mathbf{C} \in \mathbb{C}^{m \times m}$ is an invertible matrix and thus has full column rank m .
- The m standard monomials correspond to the linearly independent rows of \mathbf{V} . By definition, at least one standard monomial has exactly degree d^* , and $d \geq d^* + 1$ is needed for $\dim \text{row}(\mathbf{B}(d-1)) = \dim \text{row}(\mathbf{V}(d^*)) = m$, such that also $\mathbf{B}(d-1) \in \mathbb{C}^{q(d-1) \times m}$ has full column rank m .

□

Because Theorem 3.1.1 guarantees that the conditions in Theorem 2.2.1 are satisfied, the computation of the CPD reduces to a GEVD.

Theorem 3.1.1 does not yield less restrictive conditions than the conditions in the PNLA framework yet: its proof relies on $k_{\mathbf{V}(1)} \geq 2$, which is already satisfied for a 2-slice third-order tensor if $n = 1$. Indeed, it suffices to construct $\mathbf{M}(d)$ at $d = d^* + 1$ in the PNLA framework in Example 1.1.5.

3.2 Projective Case

This section drops the constraint of only (ii) affine roots (Fig. 3.1). Section 3.2.1 will re-interpret the third-order tensor CPD (3.11) in the *homogeneous* case. Section 3.1.2 will establish a connection between this homogeneous interpretation and a higher-order INDSCAL model.

3.2.1 The Decomposition of the Null Space of the Macaulay Matrix as a SD

The MHR problem and the derived CPD (3.11) require that (ii) $x_0 = 1$, such that only affine solutions can be found⁴. The natural link between higher-order tensors and homogeneous polynomials suggests a better, homogeneous interpretation of (3.11):

$$\begin{aligned} \mathbf{Y}_{[1,2;3]}^h &= \begin{pmatrix} \overline{\mathbf{S}}_{\mathbf{B}^h(d-1)}^{(0)} \mathbf{K} \\ \overline{\mathbf{S}}_{\mathbf{B}^h(d-1)}^{(1)} \mathbf{K} \\ \vdots \\ \overline{\mathbf{S}}_{\mathbf{B}^h(d-1)}^{(n)} \mathbf{K} \end{pmatrix} = \left(\begin{pmatrix} x_0^{(1)} & x_0^{(2)} & \dots & x_0^{(m)} \\ x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(m)} \\ \vdots & \vdots & & \vdots \\ x_n^{(1)} & x_n^{(2)} & \dots & x_n^{(m)} \end{pmatrix} \odot \mathbf{B}^h(d-1) \right) \mathbf{C}^T \\ &\triangleq \left(\mathbf{A} \odot \mathbf{B}^h(d-1) \right) \mathbf{C}^T \in \mathbb{C}^{((n+1) \cdot q(d-1)) \times m} \quad (3.12) \end{aligned}$$

in which

$$\mathbf{B}^h(d) = \mathbf{V}^h(d) = \begin{pmatrix} \mathbf{v}_1^h(d) & \dots & \mathbf{v}_m^h(d) \end{pmatrix} \in \mathbb{C}^{q(d) \times m}$$

and

$$\begin{aligned} \mathbf{v}_k^h(d) &= \left(\mathbf{V}^h(d) \right)_k \\ &= \left(x_0^{(k)d} \quad x_0^{(k)d-1} x_1^{(k)} \quad x_0^{(k)d-1} x_2^{(k)} \quad \dots \quad x_0^{(k)d-2} x_1^{(k)2} \quad x_0^{(k)d-2} x_1^{(k)} x_2^{(k)} \quad \dots \quad x_n^{(k)d} \right)^T \\ &\in \mathbb{C}^{q(d)}, \quad 1 \leq k \leq m. \end{aligned}$$

If the homogeneous interpretation is clear from the context or if it is unimportant in the reasoning, we leave the superscript h out from here. The trivial scaling indeterminacies of the CPD are now to be interpreted as the scaling ambiguities in the coordinates of a solution point $\begin{pmatrix} x_0^{(k)} & x_1^{(k)} & \dots & x_n^{(k)} \end{pmatrix}^T$ in the projective space \mathbb{P}^n .

Uniqueness at $d = d^*$

Theorem 3.1.1 already establishes the uniqueness of (3.12) if $d \geq d^* + 1$. Theorem 3.2.1 is a new uniqueness condition for (3.12) if $d \geq d^*$.

⁴Note that Theorem 3.1.1 itself does not rely on the assumption that $x_0 = 1$. It remains valid here. Rather the GEVD might fail if $x_0 = 0$ — see the validation of Theorem C.1.2.

Theorem 3.2.1 (sufficient uniqueness condition for (3.12)). *Let $\mathcal{Y} \in \mathbb{C}^{(n+1) \times q(d-1) \times m}$ admit a PD of the form (3.12), then decomposition (3.12) is a CPD and the CPD is unique if $d \geq d^*$ and condition (U2) in Definition C.1.5 holds for \mathbf{A} and $\mathbf{B}(d-1)$.*

Proof. If the roots are simple and $d \geq d^*$, $\mathbf{C} \in \mathbb{C}^{m \times m}$ has full column rank. The proof then readily follows from Theorem C.1.3. \square

Evidently, Theorem 3.2.1 holds in the affine case as well, after rescaling $x_0 = 1$, and is then more relaxed than Theorem 3.1.1. As opposed to the sufficient condition used in the proof of Theorem 3.1.1, $\mathbf{B}(d-1)$ is not (required to have) full column rank here anymore.

Example 3.2.1. *Consider the system of $s = 2$ polynomial equations in $n = 2$ variables with $m = 4$ simple and affine roots in Example 1.1.5 again. At $d = d^* + 1 = 3$, the CPD of $\mathcal{Y} \in \mathbb{C}^{3 \times 6 \times 4}$ (Fig. 3.4) is unique, because*

$$\mathbf{B}(2) = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 3 & 4 \\ -1 & 0 & -2 & -5 \\ 0 & 1 & 9 & 16 \\ 0 & 0 & -6 & -20 \\ 1 & 0 & 4 & 25 \end{pmatrix} \in \mathbb{C}^{6 \times 4}$$

has full column rank. At $d = d^ = 2$, the CPD of $\mathcal{Y} \in \mathbb{C}^{3 \times 3 \times 4}$ is also unique: \mathcal{Y} has a factor matrix $\mathbf{B}(1) = \mathbf{B}(2)(1 : 3, :) = \mathbf{A} \in \mathbb{C}^{3 \times 4}$, which cannot have full column rank, but it can be verified that $\mathcal{C}_2(\mathbf{A}) \odot \mathcal{C}_2(\mathbf{A}) \in \mathbb{C}^{9 \times 6}$ has full column rank.*

Theorem 3.2.2 establishes the *generic* uniqueness of (3.12) if $d \geq d^*$. A generic uniqueness condition makes sense, as the assumption of a 0-dimensional solution set, Theorem 2.1.1 and the assumption of only (i) simple roots were in fact already generic. First, similar to Definition C.1.2, Definition 3.2.1 draws from [20] to explain when decomposition (3.12) is called *generically* unique.

Definition 3.2.1 (generic uniqueness of (3.12)). *Let $\mathbf{z} \in \Omega \subset \mathbb{C}^{m \cdot (n+1)}$ contain the roots of a system of n homogeneous polynomials in $n+1$ variables and let $\mu_{m(n+1)}$ be a measure that is absolutely continuous with respect to the Lebesgue measure on $\mathbb{C}^{m \cdot (n+1)}$. We say that the CPD (3.12) is generically unique if*

$$\mu_{m(n+1)}\{\mathbf{z} \in \Omega \mid \text{the CPD of the tensor } \mathcal{Y} = [\mathbf{A}(\mathbf{z}), \mathbf{B}(d-1)(\mathbf{z}), \mathbf{C}(\mathbf{z})] \text{ in (3.12) is not unique}\} = 0.$$

Clearly, $\mathbf{z} = \text{vec}(\mathbf{A})$. We do not make any assumptions on how \mathbf{C} depends on \mathbf{z} . The use of Ω rather than $\mathbb{C}^{m \cdot (n+1)}$ follows from the observation that not every choice of m points in \mathbb{C}^{n+1} forms the solution set of a system of n polynomial equations of degree d_0 if $d_0 < m$ [27].

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Theorem 3.2.2 (necessary and sufficient generic uniqueness condition for (3.12)).
 Let $\mathcal{Y} \in \mathbb{C}^{(n+1) \times q(d-1) \times m}$ admit a PD of the form (3.12), then, generically, decomposition (3.12) is a CPD and the CPD is unique iff

$$d \geq d^* \quad \text{and} \quad m \leq \binom{n+d}{n} - n - 1. \quad (3.13)$$

Proof. We show that (3.13) is necessary and generically sufficient for CPD uniqueness.

- (\Rightarrow). The m standard monomials correspond to the linearly independent rows of \mathbf{V} . By definition, at least one standard monomial has exactly degree d^* . So if $d < d^*$, $\dim \text{row}(\mathbf{A} \odot \mathbf{B}(d-1)) = \dim \text{row}(\mathbf{V}(d)) < m$, while Theorem C.1.1 states that full column rank m of $\mathbf{A} \odot \mathbf{B}(d-1)$ is necessary for uniqueness.
- (\Leftarrow). To show the sufficiency of (3.13), we resort to an algebraic geometry-based tool for checking generic uniqueness of a structured matrix factorization of the form $\mathbf{Y}(\mathbf{z}) = \mathbf{M}(\mathbf{z})\mathbf{C}(\mathbf{z})^T$, where the entries of $\mathbf{M}(\mathbf{z})$ can be parametrized by rational functions of \mathbf{z} [20, Theorem 1] — see also [36].

In (3.12), $\mathbf{z} = (x_0^{(1)} \dots x_n^{(m)})^T$ and $\mathbf{M}(\mathbf{z}) = \mathbf{A} \odot \mathbf{B}(d-1) \in \mathbb{C}^{((n+1) \cdot q(d-1)) \times m}$ with entries $\prod_{j=0}^n x_j^{(k)\alpha_j}$ that are monomials and thus rational functions of \mathbf{z} . [20, Theorem 1] states that the structured matrix factorization is generically unique if the number of rank-1 terms m is bounded by $m \leq \hat{N} - \hat{l}$.

- \hat{N} is a lower bound on the dimension of the vector space spanned by arbitrary column vectors of $\mathbf{M}(\mathbf{z})$, *i.e.* vectors of the form $\mathbf{a} \otimes \mathbf{b}(d-1)$. The distinct entries in $\mathbf{a} \otimes \mathbf{b}(d-1)$ are the same as the distinct entries in $\underbrace{\mathbf{a} \otimes \dots \otimes \mathbf{a}}_{d \text{ times}}$, which in turn are the entries in $\mathbf{v}(d)$, so $\hat{N} \leq q(d)$. We will show that $\hat{N} = q(d)$. Let

$$x_0^{(k)} = 1 \quad \text{and} \quad x_j^{(k)} = e^{2\pi \cdot i \cdot \frac{k-1}{q(d)} \cdot (\sum_{l=0}^{j-1} d^l)}, \quad 1 \leq k \leq q(d). \quad (3.14)$$

$\underbrace{\mathbf{A} \odot \dots \odot \mathbf{A}}_{d \text{ times}} \in \mathbb{C}^{(n+1)^d \times q(d)}$ and $\mathbf{A} \odot \mathbf{B}(d-1) \in \mathbb{C}^{((n+1) \cdot q(d-1)) \times q(d)}$ then contain $q(d)$ distinct rows of a Vandermonde matrix with $q(d)$ different generators $x_1^{(k)}, 1 \leq k \leq q(d)$, in (3.14), which are shown to span the entire $q(d)$ -dimensional space [29, Proposition 4]. Hence, $\hat{N} = q(d)$.

- \hat{l} is an upper bound on the number of parameters needed to parametrize a vector $\mathbf{a}_k \otimes \mathbf{b}_k(d-1)$, so $\hat{l} = n+1$ is equal to the number of components $\{x_j^{(k)}\}_{j=0}^n$.

Together, (3.12) is generically unique if $d \geq d^*$ and $m \leq q(d) - n - 1$.

□

It is readily verified that the second condition in (3.13) is easily satisfied at $d = d^* = \sum_{i=1}^n d_i - n$, given that $m = \prod_{i=1}^n d_i$ ⁵. Because Theorem 3.2.2 guarantees that the condition in Theorem 3.2.1 is generically satisfied, the CPD (3.12) can be computed by means of the rank-1 detection procedure in [10, p. 651], which boils down to a simultaneous diagonalization (SD)⁶.

[20, Theorem 1] is a generic version of Theorem C.1.3 for structured matrix factorizations — instead of for the CPD. The theorem applies here, because (3.12) exploits the multiplicative shift structure contained in *all* modes of (3.6). The same argument actually proves Theorem 2.3.1 for MHR, such that the bound for R there and the bound for m here are very alike. Only $\prod_{j=1}^n I_j = (d+1)^n$ is replaced by $q(d)$ here: $q(d)$ is exactly the number of rows that is selected by $\mathbf{S}_{(d+1)^n \rightarrow q(d)} \in \mathbb{C}^{q(d) \times (d+1)^n}$ in (3.5) and the number of rows that is left when going from Fig. 3.2b to Fig. 3.2a. In Theorem 2.3.1, $\hat{l} = n \neq n+1$, but the -1 there stems from the fact that the $\mathbf{a}_r^{(n)}$ are not invariant under scaling [20]. We could have used Theorem 2.3.1 to already prove (3.13) for (3.11), but the proof here shows that there is no reason to treat the affine case, where the factor matrices are not invariant under scaling, any differently than the projective case in a multilinear algebra framework.

The PNLA framework suggests some artificial solutions to cope with roots at infinity: either the affine roots are separated from the roots at infinity in $\mathbf{K}(d)$ at a degree $d \gg d^*$, or projective shift relations are introduced to make the EVD work [24].

3.2.2 The Decomposition of the Null Space of the Macaulay Matrix as a Higher-Order INDSCAL model

Example 3.2.1, in which $d^* = 2$, writes

$$\mathbf{Y}_{[1,2;3]} = (\mathbf{A} \odot \mathbf{B}(d^* - 1)) \mathbf{C}^T = (\mathbf{A} \odot \mathbf{B}(1)) \mathbf{C}^T = (\mathbf{A} \odot \mathbf{A}) \mathbf{C}^T,$$

which is a third-order tensor decomposition with symmetry in its first two modes, known as INDSCAL. If $d^* > 2$,

$$\mathbf{S}_{q(d^*) \rightarrow (n+1)d^*} \mathbf{K}(d^*) = \left(\underset{l=1}{\overset{d^*}{\odot}} \mathbf{A} \right) \mathbf{C}^T \in \mathbb{C}^{((n+1) \cdot (n+1) \cdot \dots \cdot (n+1)) \times m} \quad (3.15)$$

is needed for all monomials of degree d^* to appear. $\mathbf{S}_{q(d) \rightarrow (n+1)d} \in \mathbb{C}^{(n+1)^d \times q(d)}$ denotes the row repetition and ordering matrix that repeats the rows in $\mathbf{K}(d)$ to match the Khatri–Rao products in the right-hand side — $\mathbf{S}_{q(d) \rightarrow (n+1)d}$ only repeats rows that are already present in $\mathbf{Y}_{[1,2;3]}(d)$ in (3.12). (3.15) reveals that $\text{null}(\mathbf{M}(d))$ has the structure of a CPD

$$\sum_{k=1}^m \underbrace{\mathbf{a}_k \otimes \mathbf{a}_k \otimes \dots \otimes \mathbf{a}_k}_{d \text{ times}} \otimes \mathbf{c}_k \quad (3.16)$$

⁵See Section 3.3.

⁶See also Section F.1 in Appendix F.

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with symmetry in its first d modes: (3.16) is a higher-order INDSCAL model. Whereas the CPD (3.6) contains $(d+1)^n$ distinct monomials up to degree d^n , (3.16) contains exactly the $q(d)$ distinct monomials up to degree d in $\text{null}(\mathbf{M}(d))$.

(3.16) also highlights the isomorphism between homogeneous polynomials and fully symmetric higher-order tensors. Indeed, like in Example B.1.5, the rank-1 tensors $\mathbf{a}_k \otimes \mathbf{a}_k \otimes \dots \otimes \mathbf{a}_k$ can be thought of as the representation of a multilinear form $\in \mathcal{P}_d^n$ that can be written as the d th power of a linear form⁷. Put in other words: the higher-order INDSCAL model (3.16) tells us that solving a set of s homogeneous polynomials in $n+1$ variables boils down to looking for another set of m homogeneous polynomials in $n+1$ variables.

Computing (3.15) with a symmetry constraint for the first d modes exploits the same structure as (3.12). The proof of Theorem 3.2.2 relies solely on this structure. Therefore, the same results apply here, *i.e.* (i) $d = d^*$ is necessary for uniqueness and (ii) the decomposition is generically unique if (3.13) holds. However, (3.15) misses a clear link with the joint diagonalization of the multiplication tables and the GEVD in Section 3.1.1.

3.3 Algorithms

The goal of this section is to put the theoretic insights in the previous sections to the fore to arrive at a new multivariate polynomial root-finding algorithm.

3.3.1 A Multivariate Polynomial Root-Finding Algorithm

$\mathcal{Y} \in \mathbb{C}^{(n+1) \times q(d-1) \times m}$ in Fig. 3.4 is constructed in *exactly the same way* in (3.11) and (3.12) from $\mathbf{K}(d)$. (3.11) and (3.12) express that \mathcal{Y} admits a CPD

$$\mathcal{Y} = \llbracket \mathbf{A}, \mathbf{B}(d-1), \mathbf{C} \rrbracket$$

that reveals the m disjoint and *simple* roots of the associated set of polynomial equations

$$\mathbf{X} \triangleq \begin{pmatrix} \mathbf{x}^{(1)} & \dots & \mathbf{x}^{(m)} \end{pmatrix} = \mathbf{V}(1) = \mathbf{A} \in \mathbb{C}^{(n+1) \times m}$$

in its first factor matrix \mathbf{A} (Fig. 3.5). Whereas (3.11) “imposes” that $\mathbf{x}^{(k)} = \begin{pmatrix} 1 & x_1^{(k)} & \dots & x_n^{(k)} \end{pmatrix}$, (3.12) represents a more general, homogeneous interpretation in which $\mathbf{x}^{(k)} = \begin{pmatrix} x_0^{(k)} & x_1^{(k)} & \dots & x_n^{(k)} \end{pmatrix}$. The polynomial root-finding procedure in Algorithm 3.1 summarizes the findings.

⁷The image of the mapping

$$\nu_{n+1,d} : \mathbb{C}^{n+1} \rightarrow \mathcal{P}_d^n : \mathbf{a} \mapsto (\mathbf{a}^T \mathbf{x})^d \cong \mathbf{a} \otimes \mathbf{a} \otimes \dots \otimes \mathbf{a}$$

to the set of homogeneous polynomials that can be written as the d th power of a linear form, is called the *Veronese variety* in algebraic geometry [6]. Restricting $\nu_{n+1,d}$ to a set of m vectors $\Omega \subset \mathbb{C}^{n+1}$ that together form the solution set of a set of polynomial equations yields a proper *subvariety*. That subvariety is precisely the zero set \mathcal{Z} of the ideal in Definition 2.1.9.

Algorithm 3.1 CPD for Multivariate Polynomial Root-Finding

Input: A system $f_i \in \mathcal{C}_{d_i}^n, 1 \leq i \leq s = n$, in the $n + 1$ projective unknowns $x_j \in \mathbb{C}, 0 \leq j \leq n$, with $m_0 = m$ simple roots.

Output: $\{\mathbf{x}^{(k)}\}_{k=1}^m$

- 1: Take $d \geq d_0 = \max_{1 \leq i \leq n} d_i$.
- 2: Construct the Macaulay matrix $\mathbf{M}(d)$.
- 3: $\mathbf{K} \leftarrow \text{null}(\mathbf{M}(d))$.
- 4: **for** $0 \leq j \leq n$ **do**
- 5: $\mathcal{Y}(j+1, :, :) \leftarrow \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)} \mathbf{K}$.
- 6: Compute the SVD $\mathbf{Y}_{[2;1,3]} = \mathbf{U}^{(2)} \mathbf{S}^{(2)} \mathbf{U}^{(1,3)H}$.
- 7: $\hat{\mathcal{Y}} \leftarrow \mathcal{Y} \cdot_2 \hat{\mathbf{U}}^{(2)H}$.
- 8: Compute the CPD $\hat{\mathcal{Y}} = \llbracket \mathbf{A}, \hat{\mathbf{B}}(d-1), \mathbf{C} \rrbracket$.
- 9: $\mathbf{X} \leftarrow \sim \mathbf{A}$
- 10: **return** \mathbf{X}

Although the sequence of steps in Algorithm 3.1 should appear self-evident, the comments below are in order.

Step 1. It is clear that $d \geq d_0$ is necessary to construct $\mathbf{M}(d)$ according to Definition 2.1.13. Theorem 3.2.2 shows that if one takes $d \geq d^*$, Algorithm 3.1 will reveal the roots of a generic system⁸. Theorem 3.1.1 guarantees that if $d \geq d^* + 1$, the roots can always be determined.

Step 2-3. Recall from Fig. 1.4b that $\mathbf{M}(d)$ can easily become large and sparse. It is possible to construct $\mathbf{M}(d)$ explicitly and to calculate \mathbf{K} using either *dense* linear algebra tools, *e.g.*, the SVD-based `null` command in Matlab, or a *sparse* QR algorithm [8].

Alternatively, it is possible to not construct $\mathbf{M}(d)$ explicitly. [2, Algorithm 4.2] is a recursive orthogonalization scheme that exploits the sparsity properties of $\mathbf{M}(d)$ to update $\mathbf{K}(\delta), d_0 \leq \delta \leq d$. The expected gain of the recursive orthogonalization scheme is $\approx d^3/n^3$, but the bottleneck remains the memory that is needed to store the matrices involved. One could also try to fit (3.12) directly to \mathbf{Y} in $\mathbf{M}(d)\mathbf{Y} = \mathbf{0}$ using optimization-based algorithms in Tensorlab [45]⁹.

Step 6-7. First, the number of rows of $\mathbf{B}(d-1) \in \mathbb{C}^{q(d-1) \times m}$ grows as $q(d-1) \approx \frac{1}{n!}(d-1)^n \gg m$, but $r_{\mathbf{B}(d-1)} \leq m$ ¹⁰. Second, the higher-degree entries $x_j^{(k)d-1}$ in the factor matrix $\mathbf{B}(d-1) = \mathbf{V}(d-1)$ can become very large for roots with $|x_j^{(k)}| \gg 1$. To address computational cost and numerical instabilities in Step 8, we may consider a compressed variant of (3.12):

$$\hat{\mathcal{Y}} \triangleq \mathcal{Y} \cdot_2 \hat{\mathbf{U}}^{(2)H} = \llbracket \mathbf{A}, \hat{\mathbf{U}}^{(2)H} \mathbf{B}(d-1), \mathbf{C} \rrbracket \triangleq \llbracket \mathbf{A}, \hat{\mathbf{B}}(d-1), \mathbf{C} \rrbracket$$

⁸See also Section 3.3.2.

⁹Research in so-called *Kronecker Product Equations* to this end is ongoing.

¹⁰ $\mathbf{B}(d-1)$ contains $\leq m$ rows that correspond to the linearly independent monomials.

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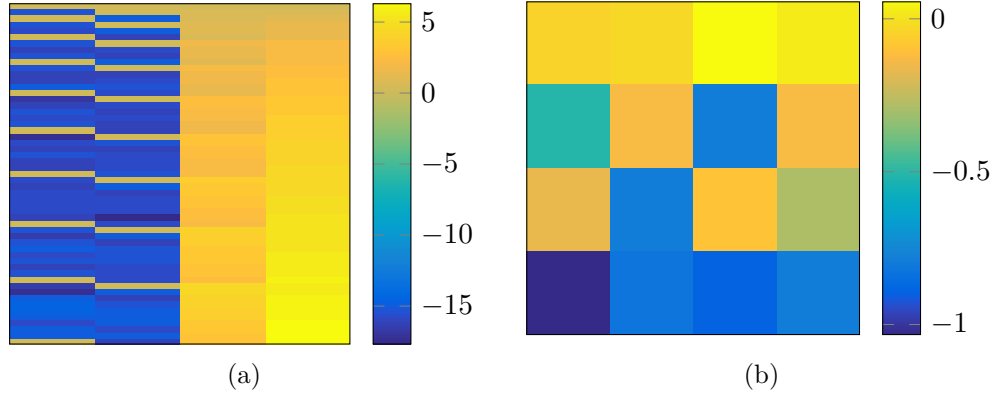


Figure 3.6: Absolute value of the entries of (a) $\mathbf{B}(10-1) \in \mathbb{C}^{55 \times 4}$ before SVD compression and (b) $\hat{\mathbf{B}}(10-1) \in \mathbb{C}^{4 \times 4}$ after SVD compression on a \log_{10} -scale for the system in Example 3.1.1.

in which $\hat{\mathbf{U}}^{(2)} \in \mathbb{C}^{q(d-1) \times m}$ is the matrix of left singular vectors in the “economic size” SVD of the mode-2 matricization of \mathcal{Y} (Theorem A.2.1)¹¹. Appendix G proves that the uniqueness conditions for the CPD of \mathcal{Y} pass to the CPD of $\hat{\mathcal{Y}}$. Fig. 3.6 illustrates the effect of this SVD compression step.

Step 8. The computation of the CPD of $\hat{\mathcal{Y}}$ is at the core of Algorithm 3.1. Many algorithms, *e.g.*, optimization-based nonlinear least squares (NLS) type algorithms, exist to compute a CPD [35]. If one takes $d \geq d^* + 1$, the CPD can be computed by means of a GEVD. In the remainder of this chapter, `poly_cpd` is a Matlab implementation of Algorithm 3.1 with the choice for the many CPD algorithms available in Tensorlab [45].

If one takes $d \geq d^*$, the CPD can be computed by means of the SD in Algorithm F.1 [10, Algorithm 2.1]: the problem is translated to finding the CPD of *another* rank- m $m \times m \times m$ third-order tensor¹², which can in turn be computed in Tensorlab. `poly_sd` is a Matlab implementation of Algorithm 3.1 that computes the CPD of $\hat{\mathcal{Y}}$ by means of an adaptation of the SD method in [10]^{13 14}.

Step 9. To find solutions at infinity, we propose to normalize each $\mathbf{x}^{(k)}$, $1 \leq k \leq m$, to its affine counterpart ($x_0^{(k)} = 1$) if $x_0^{(k)} \geq \tau \|\mathbf{x}^{(k)}\|$ given some predefined tolerance τ , or such that the largest $x_j^{(k)}$ becomes 1 otherwise.

¹¹ $\hat{\mathcal{Y}}$ can then be viewed as a preliminary \mathcal{S} in Theorem B.2.1.

¹²In fact, if $d < d^*$, *i.e.* if $r_{\mathbf{K}(d)} = \nu < m$, the SD boils down to finding an m -term CPD of a $\nu \times \nu \times \nu$ third-order tensor with $\nu < m$ — see Section 3.3.2.

¹³The construction of \mathcal{P} in Step 2 in Algorithm F.1 [10, Algorithm 2.1] requires inner products

$$\left(\bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j_1)} \mathbf{K} \right)^H \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j_2)} \mathbf{K} \in \mathbb{C}^{m \times m}.$$

`poly_sd` takes the orthonormality of the columns in the numerical basis \mathbf{K} into account to compute the inner products. Note that the SD makes Steps 6-7 obsolete.

¹⁴[37, Algorithm 1] is also an adaptation of the SD method [10, Algorithm 2.1] to compute the coupled CPD in MHR.

d_0	2			3			4		
n	d^*	m	M	d^*	m	M	d^*	m	M
2	2	4	3	4	9	12	6	16	25
3	3	8	16	6	27	80	9	64	216
4	4	16	65	8	81	480	12	256	1815

Table 3.1: $d^* = \sum_{i=1}^n d_i - n = n \cdot (d_0 - 1)$, $m = \prod_{i=1}^n d_i = d_0^n$ and $M = \binom{n+d^*}{n} - n - 1$ for systems of polynomial equations in n affine variables with $d_i = d_0, 1 \leq i \leq n$: systems where $m > M$ and systems in Fig. 3.7.

Step 10. If $d = d^* < d^* + 1$, the result in Theorem 3.2.1 provides a way to verify whether the CPD obtained in Step 8, and therefore the factor matrix $\mathbf{X} \sim \mathbf{A}$ in Step 9, is unique.

3.3.2 Numerical Experiments

The use of the Matlab programs `poly_cpd` and `poly_sd` is highlighted in Appendix H. Below, we give the results of some interesting experiments that show the potential of the multilinear approach.

Uniqueness

Theorem 3.2.2 states that the CPD in Algorithm 3.1 is generically unique iff one takes $d \geq d^*$ and if

$$m \leq M(d) \triangleq \binom{n+d}{n} - n - 1.$$

Table 3.1 shows the degree of regularity d^* and the Bézout number m for systems of n multivariate ($n > 1$) nonlinear ($d_0 > 1$) polynomial equations (2.2) in n affine variables for various combinations of n and $d_i = d_0, 1 \leq i \leq n$. The table also shows $M(d^*)$. The table indicates that the extra condition $m \leq M(d)$ is very relaxed at the minimum necessary degree $d = d^*$: it is only not satisfied if $n = d_0 = 2$, and the gap between m and $M(d^*)$ only grows with n and d_0 .

Our numerical experiments confirm these findings. By way of example, Fig. 3.7 shows histograms over 200 Monte Carlo simulations of the relative forward error

$$\epsilon_{\hat{\mathbf{X}}} \triangleq \frac{\|\hat{\mathbf{X}} - \mathbf{X}\|}{\|\mathbf{X}\|} \quad (3.17)$$

of the solution $\hat{\mathbf{X}}$ of 200 systems in the second column in Table 3.1 obtained with (the adaptation of) the SD method: `poly_sd`. The systems are *generic* in the sense that their coefficient vectors $\mathbf{f}_i^T \in \mathbb{R}^{q(d_0)}$ have nonzero entries for all monomials of degree $\leq d_0$, drawn at random from a Gaussian distribution with mean 0 and

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standard deviation 1. The reference solution \mathbf{X} in (3.17) was obtained with the general purpose homotopy continuation-based solver from PHCPACK [44].

In Fig. 3.7, every $d_0 \leq d \leq d^* + 1$ is considered. We observe that

- indeed, $d \geq d^*$ is necessary and generically sufficient to retrieve the correct roots up to machine precision in every trial;
- it is remarkable that even if $d < d^*$, *i.e.* if $r_{\mathbf{K}(d)} = \nu < m$, the m -term CPD of the $\nu \times \nu \times \nu$ third-order tensor in `poly_sd`¹⁵ is mostly able to retrieve the roots with a reasonable accuracy. *E.g.*, $\epsilon_{\mathbf{X}} < 10^{-7}$ in the left-hand pane in Fig. 3.7a. It could be meaningful to stick with this precision, *e.g.*, when the polynomial coefficients are derived from measured data¹⁶.

`poly_cpd` (GEVD) retrieves all roots correctly if $d \geq d^* + 1$. If $d \leq d^*$, the GEVD cannot be used. If $d < d^*$, the forward error from *directly* trying to compute the CPD in Step 8 in Algorithm 3.1 using a NLS type algorithm is $\mathcal{O}(1)$. Similarly, if $d \leq d^*$, a the square EVD cannot be used in the PNLA framework.

An Over-Constrained Set of Polynomial Equations

As explained before, a GEVD could already be obtained from *only two* (horizontal) slices in \mathcal{Y} in Fig. 3.4, taking the multiplicative shift structure in *only one* variable into account, (cf. PNLA). From a numerical point of view, it is preferable to take *all* $n + 1$ slices in \mathcal{Y} into account, when the polynomial coefficients are only known with limited precision [10].

Formalizing, Stetter introduces the notion of an *empirical polynomial* (\bar{f}, \mathbf{e}) with (i) a *specified polynomial* with coefficient vector $\bar{\mathbf{a}} \in \mathbb{R}^p$:

$$\bar{f}(\mathbf{x}) = \sum_{l=1}^p \bar{a}_l \mathbf{x}_l^{\alpha_l}$$

and (ii) a vector of *tolerances* $\mathbf{e} \in \mathbb{R}^{+p}$ that forces us to interpret the specified coefficients \bar{a}_l as mere instances of a *neighbourhood* $\mathcal{N}(a_l, e_l)$ [40, Definition 3.4].

[21] looks at an *over-constrained system* that consists of N noisy specifications of the same underlying square ($s = n$) system of empirical polynomial equations, *e.g.*, as the result of N same experiments in the presence of noise. The new system has more equations ($s = Nn$) than unknowns (n) and typically no solution. The high-precision algorithms from computer algebra cannot cope with it. Nonetheless, finding an approximation of the roots of the underlying system can be of interest in, *e.g.*, molecular chemistry, kinematics and computer vision. With a small change, Algorithm 3.1 can be used. First, note that if $s = Nn > n$, $m = \prod_{i=1}^m d_i$ and $d^* = \sum_{i=1}^n d_i - n$ are as easily obtained from the unchanged d_i of the underlying system. Solely Step 3 might pose problems, since the null space of the Macaulay matrix of the over-constrained set might be empty now. Instead, we could fill \mathbf{K}

¹⁵Because $\nu < m$, the SD is computed using a NLS type algorithm rather than using a GEVD.

¹⁶See also the next section.

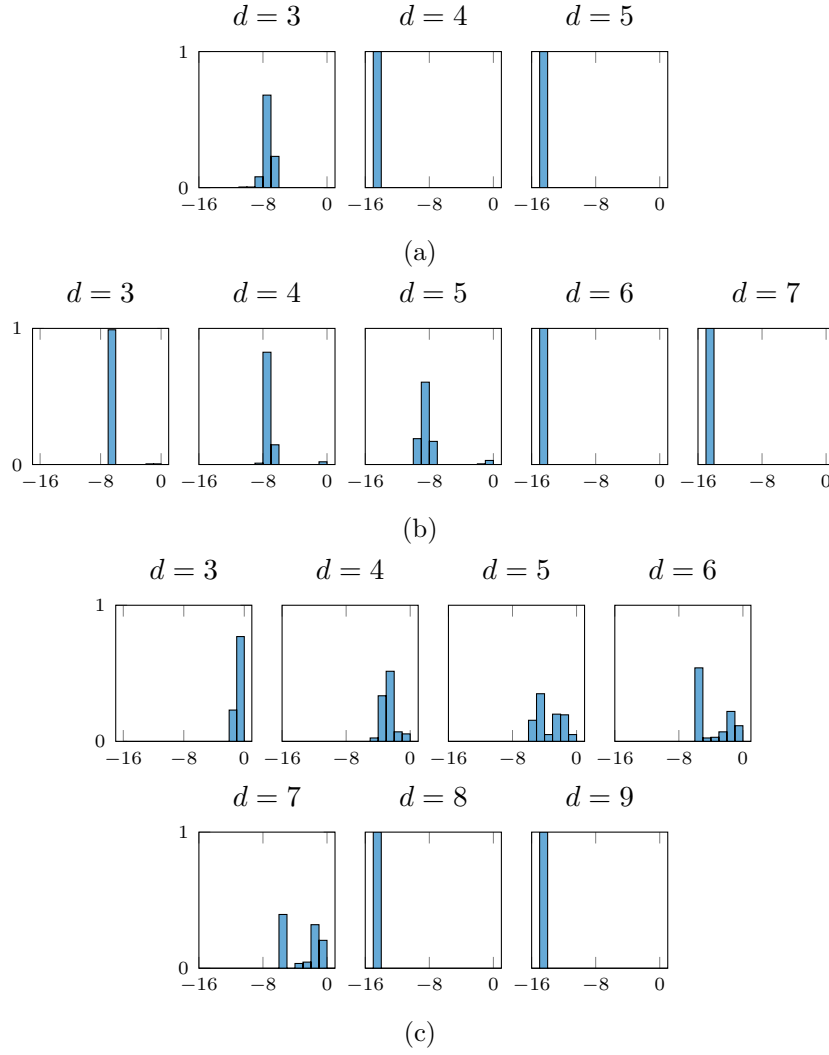


Figure 3.7: Histogram over 200 trials of the relative forward error $\log_{10}(\epsilon_{\mathbf{X}})$ on the roots of a generic set of polynomial equations with random, real coefficients obtained with `poly_sd`. $d_0 = d_i = 3, 1 \leq i \leq n$, and (a) $n = 2$ and $d^* = 4$; (b) $n = 3$ and $d^* = 6$; (c) $n = 4$ and $d^* = 8$.

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with the right singular vectors corresponding to the m smallest singular values of $\mathbf{M}(d)$ and proceed as normally. The PNLA package [21, Algorithm 6] proposes the same adjustment for over-constrained systems.

In an experiment, consider the underlying system

$$\begin{cases} f_1(x_1, x_2) = x_1^3 + x_2^3 - 9x_1^2x_2 + 20x_1x_2^2 - 3x_1 - 20 = 0 \\ f_2(x_1, x_2) = x_1^2 + 4x_2^2 - x_1x_2 - 80 = 0 \end{cases} \quad (3.18)$$

where $s = n = 2$ and $m = 6$ from [21, Example 8.3] in which both polynomials are assumed empirical. Gaussian noise \mathbf{e}_i^T with mean 0 is added to the $n = 2$ coefficient vectors \mathbf{f}_i^T of the square system (3.18), such that

$$10 \log_{10} \left(\frac{\|\mathbf{f}_i\|^2}{\|\mathbf{e}_i\|^2} \right)$$

is equal to a preset signal-to-noise ratio (SNR). This is repeated N times then, and the Nn $\bar{\mathbf{f}}_{i,j}^T = \mathbf{f}_i^T + \mathbf{e}_{i,j}^T, 1 \leq j \leq N$, are collected in an over-constrained system.

Fig. 3.8 shows the relative error $\epsilon_{\hat{\mathbf{X}}}$ of the approximation $\hat{\mathbf{X}}$ from the over-constrained variant of (3.18). The median error over 200 independent trials for each SNR and each $N \in \{1, 2, 5, 10\}$ is shown. `poly_sd` ($d = d^*$) and `poly_cpd` ($d = d^* + 1$) use a GEVD to find their CPD. Because PHCPACK doesn't provide a solver for over-constrained systems, its reported error reflects the error from a square noisy system. The figure indicates that

- (i) if $N = 1$, all algorithms “see” the square noisy system as if it represented another, exact system. They return the same roots and show the same asymptotic performance as the SNR increases¹⁷;
- (ii) as N increases, the over-constrained sets contain more information, and the gap between the standard asymptotic performance of PHCPACK and the other algorithms grows;
- (iii) at low SNR, it is preferable to jointly exploit the multiplicative shift structure contained in all variables in the multilinear framework over using the matrix model that expresses one (linear combination of) multiplication(s) in PNLA¹⁸;
- (iv) like in Fig. 3.7, `poly_sd` benefits from translating the problem to a SD. With a good initialization for `poly_cpd` and NLS, we obtain the same results as with `poly_sd`.

¹⁷The standard asymptotic performance depends on the condition of the roots. We have found that in Fig. 3.8, it is representative for a large number of relatively well-conditioned polynomial root-finding problems with $n = 2$ and $n = 3$.

¹⁸`poly_cpd` (GEVD) really computes the GEVD of \mathcal{S} in the MLSVD (Theorem B.2.1) and shows improved results over the matrix model in PNLA by doing this *multilinear* decomposition first.

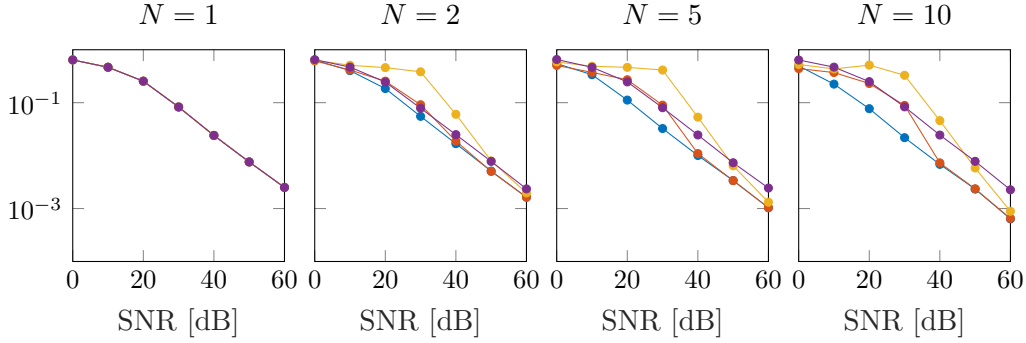


Figure 3.8: Median relative forward error $\epsilon_{\hat{\mathbf{x}}}$ on the roots of the over-constrained set of noisy polynomial equations (3.18) over 200 trials as a function of the signal-to-noise ratio: `poly_sd` (—), `poly_cpd` (—), the PNLA package (—) and PHCPACK (—).

A word on the computational cost of the methods in Fig. 3.8 is in order. Even though tensor methods typically suffer from the curse of dimensionality, our curse of dimensionality resides in $q(d)$: the number of columns of $\mathbf{M}(d)$. As n and d grow, $\mathbf{M}(d)$ becomes prohibitively large to manipulate. Indeed, we have found that the bottleneck in Algorithm 3.1 is not the CPD in Step 8, but it is inherited from the PNLA framework in Step 2-3. Hence, Algorithm 3.1 also inherits, *e.g.*, the observation in [41, Fig. 6.4]: the PNLA package needs roughly 10 times as much time as PHCPACK to solve a generic set with $n = 2$ and $d_i = d_0 = 10, 1 \leq i \leq 2$, on a 16 GB RAM Intel Core i7-5500U CPU server.

Constraints

Oftentimes, one has *prior knowledge* on (some of) the roots of a set of polynomial equations. If desired, *e.g.*, to improve the accuracy or interpretability of the roots at low SNR, prior knowledge can be incorporated into (3.12) by way of imposing constraints on the CPD. Optimization-based algorithms as NLS can handle constraints.

As one basic example, consider the univariate polynomial equation

$$f(x) = x^4 + 0.6628x^3 - 1.3587x^2 - 1.4491x - 0.3673 = 0 \quad (3.19)$$

of degree $d = 4$ with $m = d = 4$ *real* roots $x^{(1)} = -0.8624$, $x^{(2)} = -0.5810$, $x^{(3)} = -0.5506$ and $x^{(4)} = 1.3312$. We add Gaussian noise $\mathbf{e} \in \mathbb{R}^5$ with mean 0 and a preset SNR to $\mathbf{f} \in \mathbb{R}^5$. Fig. 3.9 shows the median error on the roots of (3.19) over 200 independent trials calculated by `poly_cpd`. The CPD in Step 8 is computed using NLS: first, \mathbf{A} , $\hat{\mathbf{B}}(d-1)$ and \mathbf{C} are constrained to be real-valued — second, they can be complex-valued, as always. Imposing the first constraint on the CPD already improves the estimation accuracy of the roots at low SNR. Tensorlab provides the structured data fusion framework to impose more complicated constraints than shown here. `poly_cpd` without constraints does *not* show improved results over

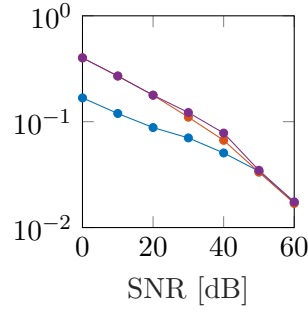


Figure 3.9: Median relative forward error on the real roots of (3.19) over 200 trials as a function of the signal-to-noise ratio: constrained `poly_cpd` (—), `poly_cpd` (—) and PHCPACK (—).

PHCPACK, in view of the fact that there is *no joint* multiplicative shift structure to exploit in $n = 1$ variable.

3.4 Conclusion

In his seminal Numerical Polynomial Algebra, Stetter has formulated the implication of the Central Theorem of NPA, that

The numerical solution of 0-dimensional systems of polynomial equations is a task of numerical linear algebra [40, p. 52].

This chapter has attempted to show that *multilinear* algebra is a very natural framework for formulating a multivariate polynomial root-finding problem and for finding its roots. The framework is a flexible framework: various higher-order tensor decompositions, exploiting various properties of the null space of the Macaulay matrix, are possible. The CPD in (3.12) is arguably the central decomposition in this chapter, as (i) it improves upon a “flat” matrix model by jointly exploiting the multiplicative shift structure contained in all variables, (ii) it does not distinguish between the affine case and the projective case and (iii) it can be linked with the joint EVD of the multiplication tables, with MHR and with a higher-order INDSCAL model. Chapter 4 will relate the topics to an even more general tensor decomposition.

Chapter 4

Connections between Sets of Polynomial Equations and the Block Term Decomposition

So far, we have limited ourselves to systems of polynomial equations with simple roots. This chapter argues that the related third-order tensor CPD needs to be understood as a mere special case of a third-order tensor BTD when also constraint (i) in Fig. 3.1 is dropped. Section 4.1 will formulate this more general connection. To develop insight, the emphasis is on the affine case. With a little thought, the results incorporate the projective case as well. Section 4.2 will further establish a connection between the general result and some properties of tensor rank cited in Chapter 2. Finally, Section 4.3 will conclude with algorithms and experiments.

4.1 Roots with Multiplicities

Let $\mathcal{F} = \{f_i\}_{i=1}^s$ be a set of s polynomial equations in n variables x_1, x_2, \dots, x_n that has $m_0 \leq m$ disjoint roots $\mathbf{x}^{(k)}$ with multiplicity $\mu_k \geq 1, 1 \leq k \leq m_0$. Recall from Section 2.1.1 that if $\mu_k > 1$, also $\partial_{\mathbf{j}}[\mathbf{x}^{(k)}](r)$ with $\mathbf{0} \neq \mathbf{j} \in \mathbb{N}^n$ are needed to completely characterize a residue class $[r] \in \mathcal{C}^n / \langle \mathcal{F} \rangle$. Since $\text{null}(\mathbf{M}(d^*)) \cong \mathcal{C}^n / \langle \mathcal{F} \rangle$, multivariate Vandermonde vectors as well as their derivatives, *i.e.* $\left\{ \partial_{\mathbf{j}_{k,l}}[\mathbf{v}_k] \right\}_{l=0}^{\mu_k-1}$ ¹ with both $\mathbf{j}_{k,l} = \mathbf{0}$ and $\mathbf{j}_{k,l} \neq \mathbf{0}$, will constitute a basis for the null space of the Macaulay matrix:

$$\mathbf{M}(d) \begin{pmatrix} \partial_{\mathbf{j}_{k,0}}[\mathbf{v}_k] & \partial_{\mathbf{j}_{k,1}}[\mathbf{v}_k] & \dots & \partial_{\mathbf{j}_{k,\mu_k-1}}[\mathbf{v}_k] \end{pmatrix} \triangleq \mathbf{M}(d) \tilde{\mathbf{V}}_k = \mathbf{0}. \quad (4.1)$$

The differential functionals defined by $\{\mathbf{j}_{k,l}\}_{l=0}^{\mu_k-1}$ are referred to as the *multiplicity structure* of the root $\mathbf{x}^{(k)}$. Note that this multiplicity structure is not unique [23]: multiplying both sides in (4.1) by a linear transformation matrix $\mathbf{T} \in \mathbb{C}^{\mu_k \times \mu_k}$ yields

$$\mathbf{M}(d) \tilde{\mathbf{V}}_k \mathbf{T} = \mathbf{M}(d) \left(\tilde{\mathbf{V}}_k \mathbf{T} \right) = \mathbf{M}(d) \tilde{\mathbf{W}}_k = \mathbf{0}.$$

¹In the projective case, $\mathbf{j} \in \mathbb{N}^{n+1}$ and $\mathbf{v}_k \in \mathbb{C}^{q(d)}$ needs to be interpreted as $\mathbf{v}_k^h \in \mathbb{C}^{q(d)}$.

4. CONNECTIONS BETWEEN SETS OF POLYNOMIAL EQUATIONS AND THE BLOCK TERM DECOMPOSITION

If $\mu_k = 1$, $\tilde{\mathbf{V}}_k = \mathbf{v}_k \in \mathbb{C}^{q(d)}$ in (3.1) and in that case the “multiplicity” structure of $\mathbf{x}^{(k)}$ is unique (up to a scalar). If not, each $\tilde{\mathbf{V}}_k \in \mathbb{C}^{q(d) \times \mu_k}$ is a “multivariate Vandermonde *plus* derivative” matrix²:

$$\left(\tilde{\mathbf{V}}_k\right)_{l+1} = \partial_{\mathbf{j}_{k,l}}[\mathbf{v}_k], \quad 0 \leq l \leq \mu_k - 1, \quad 1 \leq k \leq m_0 \quad \text{and} \quad \sum_{k=1}^{m_0} \mu_k = m.$$

We can collect the $\{\tilde{\mathbf{V}}_k\}_{k=1}^{m_0}$ in a matrix

$$\tilde{\mathbf{V}} = \begin{pmatrix} \tilde{\mathbf{V}}_1 & \dots & \tilde{\mathbf{V}}_{m_0} \end{pmatrix} \in \mathbb{C}^{q(d) \times m}, \quad (4.2)$$

which is now a full basis for $\text{null}(\mathbf{M}(d))$ instead of \mathbf{V} in (3.1). At this point, it is crucial to see that the newly introduced columns in $\tilde{\mathbf{V}}$ do *not* exhibit the multiplicative shift structure exploited in (3.7); we cannot obtain the CPD in (3.12) anymore.

Example 4.1.1. [24, Example 7] Consider the system of $s = 2$ polynomial equations in $n = 2$ variables

$$\begin{cases} f_1(x_1, x_2) = (x_2 - 2)^2 = 0 \\ f_2(x_1, x_2) = (x_1 - x_2 + 1)^2 = 0 \end{cases}$$

where $d_1 = d_2 = 2$, so $d^* = d_1 + d_2 - n = 2$ and $m = d_1 \cdot d_2 = 4$, but $m_0 = 1$: the system has one (affine) root $\mathbf{x}^{(1)} = (1 \ 2)^T$ with multiplicity $\mu_1 = 4$. It can be verified that a (possible) basis for $\text{null}(\mathbf{M}(d^*)) = \text{null}(\mathbf{M}(2))$ is defined by the following (non-unique) multiplicity structure of the root $\mathbf{x}^{(1)}$:

$$\tilde{\mathbf{V}} = \tilde{\mathbf{V}}_1 = \begin{pmatrix} \partial_{\mathbf{j}_{1,0}}[\mathbf{v}_1] & \partial_{\mathbf{j}_{1,1}}[\mathbf{v}_1] & \partial_{\mathbf{j}_{1,2}}[\mathbf{v}_1] & \partial_{\mathbf{j}_{1,3}}[\mathbf{v}_1] \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ x_1^{(1)} & 1 & 0 & 0 \\ x_2^{(1)} & 0 & 1 & 0 \\ x_1^{(1)2} & 2x_1^{(1)} & 0 & 2 \\ x_1^{(1)}x_2^{(1)} & x_2^{(1)} & x_1^{(1)} & 1 \\ x_2^{(1)2} & 0 & 2x_2^{(1)} & 0 \end{pmatrix}.$$

where $\partial_{\mathbf{j}}$ is replaced with $\partial_{\mathbf{j}_{1,j_2}}$ for brevity. Whereas

$$\tilde{\mathbf{V}}_1([1 \ 2 \ 3], 1) \cdot x_1^{(1)} = \begin{pmatrix} 1 \\ x_1^{(1)} \\ x_2^{(1)} \end{pmatrix} x_1^{(1)} = \begin{pmatrix} x_1^{(1)} \\ x_1^{(1)2} \\ x_1^{(1)}x_2^{(1)} \end{pmatrix} = \tilde{\mathbf{V}}_1([2 \ 4 \ 5], 1),$$

we have that, e.g., $(\tilde{\mathbf{V}}_1)_2$ does not exhibit this multiplicative shift structure:

$$\tilde{\mathbf{V}}_1([1 \ 2 \ 3], 2) \cdot x_1^{(1)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} x_1^{(1)} = \begin{pmatrix} 0 \\ x_1^{(1)} \\ 0 \end{pmatrix} \neq \begin{pmatrix} 1 \\ 2x_1^{(1)} \\ x_2^{(1)} \end{pmatrix} = \tilde{\mathbf{V}}_1([2 \ 4 \ 5], 2).$$

² $\tilde{\mathbf{V}}_k$ is closely related to a so-called *confluent Vandermonde matrix* — see Appendix D.

Before we can come to a generalization of the CPD in (3.12), which is going to be the BTB in (4.7) in the soon-to-follow Theorem 4.1.1, we need some definitions. For a concise derivation of the result in Theorem 4.1.1, the reader can resort to Appendix D. The appendix re-interprets the spatial smoothing-based decomposition of the null space of the Macaulay matrix as a third-order tensor BTB with Hankel structure in its first two modes³. If $\mu_k = 1$, all Hankel matrices have rank 1. If there are $\mu_k > 1$, some have rank > 1 . The definitions below essentially serve to ensure that all factor matrices in the BTB have full column rank. First, let

$$\mathbf{K} = \tilde{\mathbf{V}}\mathbf{C}^T \in \mathbb{C}^{q(d) \times m} \quad (4.3)$$

be the usual numerical basis for null $(\mathbf{M}(d))$ and partition the invertible transformation matrix \mathbf{C} to match the partition in (4.2):

$$\mathbf{C} = \begin{pmatrix} \mathbf{C}_1 & \dots & \mathbf{C}_{m_0} \end{pmatrix} \in \mathbb{C}^{m \times m} \quad (4.4)$$

with $\mathbf{C}_k \in \mathbb{C}^{m \times \mu_k}$. Second, let $\mathbf{S}_{I_1^{(j)}}^{(j)}$ be the row selection matrix that selects all rows of $\mathbf{K}(d)$ onto which the rows of $\tilde{\mathbf{V}}(d - I_1^{(j)} + 1)$ ⁴ are mapped after multiplication with $\{x_j^\alpha\}_{\alpha=1}^{I_1^{(j)}-1}$, e.g., $\mathbf{S}_2^{(1)} = \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(1)}$. As in Example 4.1.2 then, define the multiplicity $\mu_k^{(j)}$ of a root $\mathbf{x}^{(k)}$ in x_j as

$$\mu_k^{(j)} \triangleq \max_{0 \leq l \leq \mu_k - 1} \mathbf{j}_{k,l}(j)^5 + 1, \quad 1 \leq k \leq m_0, \quad 0 \leq j \leq n.$$

Now take $I_1^{(j)} = \max(2, \max_{1 \leq k \leq m_0} \mu_k^{(j)})$, where 2 is the bare minimum to construct via $\mathbf{S}_2^{(j)}$ the spatial smoothing-based CPD in Chapter 3 if all the multiplicities are 1. Lastly, define the maximum $\bar{I}_1 \triangleq \max_{0 \leq j \leq n} I_1^{(j)}$.

Example 4.1.2. *To keep all the necessary definitions tactile, consider the system in Example 4.1.1 again. The root $\mathbf{x}^{(1)}$ has multiplicities*

$$\mu_1^{(1)} = \max_{0 \leq l \leq 3} \mathbf{j}_{1,l}(1) + 1 = \max\{0, 1, 0, 2\} + 1 = 2 + 1 = 3,$$

$$\mu_1^{(2)} = \max_{0 \leq l \leq 3} \mathbf{j}_{1,l}(2) + 1 = \max\{0, 0, 1, 1\} + 1 = 1 + 1 = 2$$

and, implicitly, $\mu_0^{(1)} = \max_l \{0\} + 1 = 1$ in x_1 , x_2 and x_0 respectively. Since $m_0 = 1$, $I_1^{(1)} = \mu_1^{(1)} = 3$, $I_1^{(2)} = \mu_1^{(2)} = 2$ and $I_1^{(0)} = \max(2, \mu_1^{(0)}) = 2$. Lastly, $\bar{I}_1 = \max_{0 \leq j \leq 2} I_1^{(j)} = \max\{2, 3, 2\} = 3$.

³The re-interpretation generalizes (3.12) like (2.12) generalizes the spatial smoothing in (2.11).

⁴In the projective case, $\tilde{\mathbf{V}}^h(d - I_1^{(j)} + 1)$ contains all rows of degree $\leq d - I_1^{(j)} + 1$ in x_j . In $I_1^{(j)}$, the subscript refers to the first dimension of a third-order tensor — see Theorem 4.1.1.

⁵To be precise, $\mathbf{j}_{k,l}(j)$ is the maximal derivative in x_j occurring in $\mathbf{j}_{k,l}$, e.g., $\mathbf{j}_{1,3}(1) = 2$ in Example 4.1.1.

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Appendix D shows that if one takes each $I_1^{(j)}$ as above, such that the first dimension of \mathcal{Y} in (4.6) is $I_1 = \sum_{j=0}^n (I_1^{(j)} - 1)$, and if one takes the degree d and the second dimension of \mathcal{Y} , I_2 , such as to adhere to the rather technical condition

$$\max \left(\max_{1 \leq k \leq m_0} \mu_k, q(d^* - \bar{I}_1 + 1) \right) \leq I_2 = q(d - \bar{I}_1 + 1), \quad (4.5)$$

then the result in Theorem 4.1.1 holds true.

Theorem 4.1.1 (Central Theorem). *Let $\mathbf{K}(d) \in \mathbb{C}^{q(d) \times m}$ be as in (4.3) and let $I_1^{(j)}$ in $\left\{ \mathbf{S}_{I_1^{(j)}}^{(j)} \right\}_{j=0}^n$, I_1 , I_2 and d have their values from above. Then the third-order tensor $\mathcal{Y} \in \mathbb{C}^{I_1 \times I_2 \times m}$, whose matricization is given by*

$$\mathbf{Y}_{[1,2;3]} = \begin{pmatrix} \mathbf{S}_{I_1^{(0)}}^{(0)} \mathbf{K}(d) \\ \mathbf{S}_{I_1^{(1)}}^{(1)} \mathbf{K}(d) \\ \vdots \\ \mathbf{S}_{I_1^{(n)}}^{(n)} \mathbf{K}(d) \end{pmatrix}, \quad (4.6)$$

admits the canonical BTD

$$\mathcal{Y} = \sum_{k=1}^{m_0} \mathcal{G}_k \cdot_1 \mathbf{A}_{k,I_1} \cdot_2 \mathbf{B}_{k,I_2} \cdot_3 \mathbf{C}_k \quad (4.7)$$

in which

1. the core tensors $\mathcal{G}_k \in \mathbb{C}^{\mu_k \times \mu_k \times \mu_k}$ are composed of upper-triangular $\mathbf{T}_{k,i_1} \in \mathbb{C}^{\mu_k \times \mu_k}$:

$$\mathbf{G}_{k[2;1,3]} = \begin{pmatrix} \mathbf{I}_{\mu_k} & \mathbf{T}_{k,2} & \dots & \mathbf{T}_{k,\mu_k} \end{pmatrix}$$

2. $\mathbf{A}_{k,I_1} \in \mathbb{C}^{I_1 \times \mu_k}$ equals

$$\begin{pmatrix} 1 & \mathbf{0}_{1 \times I_1^{(1)} - 1} & \mathbf{0}_{1 \times I_1^{(2)} - 1} & \dots & \mathbf{0}_{1 \times I_1^{(n)} - 1} \\ x_{1,k} & 1! \binom{1}{1} 1 & 0 & \dots & 0 \\ x_{1,k}^2 & 1! \binom{2}{1} x_{1,k} & 2! \binom{2}{2} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{1,k}^{I_1^{(1)} - 1} & 1! \binom{I_1^{(1)} - 1}{1} x_{1,k}^{I_1^{(1)} - 2} & \dots & \mathbf{0}_{1 \times I_1^{(2)} - 1} & \dots & \mathbf{0}_{1 \times I_1^{(n)} - 1} \\ x_{2,k} & \mathbf{0}_{1 \times I_1^{(1)} - 1} & 1! \binom{1}{1} 1 & \dots & \mathbf{0}_{1 \times I_1^{(n)} - 1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{n,k}^{I_1^{(n)} - 1} & \mathbf{0}_{1 \times I_1^{(1)} - 1} & \mathbf{0}_{1 \times I_1^{(2)} - 1} & \dots & (I_1^{(n)} - 1)! \binom{I_1^{(n)} - 1}{I_1^{(n)} - 1} x_{n,k}^0 \end{pmatrix}$$

in the affine case⁶

⁶If $\exists k' : x_0^{(k')} = 0$ and $\exists j' : \forall k : x_{j'}^{(k)} \neq 0$, one can switch the roles of x_0 and $x_{j'}$ to derive Theorem 4.1.1 and to rewrite \mathbf{A}_{k,I_1} in the projective case.

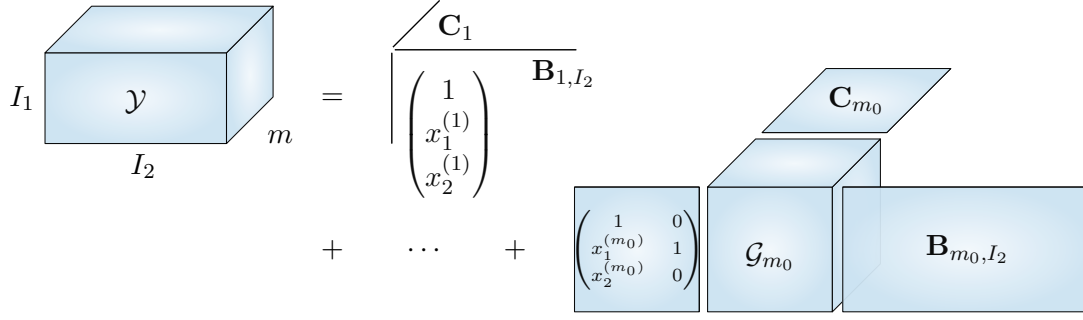


Figure 4.1: Visualization of (4.7) for the third-order tensor $\mathcal{Y} \in \mathbb{C}^{I_1 \times I_2 \times m}$ in (4.6) with $n = 2$, $\mu_1 = 1$ and $\mu_{m_0} = \mu_{m_0}^{(1)} = 2$.

3. $\mathbf{B}_{k,I_2} = \tilde{\mathbf{V}}(d - \bar{I}_1 + 1) \in \mathbb{C}^{I_2 \times \mu_k}$ and

4. $\mathbf{C}_k \in \mathbb{C}^{m \times \mu_k}$ is as in (4.4).

In words, Theorem 4.1.1 states that if we manage to get the degree d and the dimensions I_1 and I_2 based on the multiplicities right, the third-order tensor \mathcal{Y} consisting of $I_1 \geq n + 1$ (horizontal) slices (cf. Fig. 3.4) admits the canonical BTD in Fig. 4.1. Each of the $m_0 \leq m$ terms in the BTD reveals in its first factor matrix \mathbf{A}_{k,I_1} a (potentially multiple) root $\mathbf{x}^{(k)}$ and nonzero blocks of derivatives in the x_j . (3.12) in Fig. 3.5 arises now as a special case of (4.7) in Fig. 4.1 with $\mathcal{G}_k = 1$, $\mathbf{A}_{k,1} = (\mathbf{A})_k$ and $\mathbf{B}_{k,q(d-1)} = (\mathbf{B}(d-1))_k$, $1 \leq k \leq m_0 = m^7$.

Example 4.1.3. Consider the system in Example 4.1.1 again. Take $\bar{I}_1 = 3$, $I_1 = 1 + 2 + 1 = 4$, $d = 4$ and $I_2 = q(d - \bar{I}_1 + 1) = q(4 - 3 + 1) = q(2) = 6 \geq \mu_1 = 4$. From (4.7), we have that \mathcal{Y} in (4.6) admits the canonical BTD⁸

$$\mathcal{Y} = \mathcal{G}_1 \cdot_1 \mathbf{A}_{1,4} \cdot_2 \mathbf{B}_{1,6} \cdot_3 \mathbf{C} \quad (4.8)$$

in which

$$\mathbf{G}_{1[2;1,3]} = \left(\begin{array}{cccc|cccc|cccc|cccc} 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right),$$

$$\mathbf{A}_{1,4} = \left(\begin{array}{c|cc|c} 1 & 0 & 0 & 0 \\ \hline x_1^{(1)} & 1 & 0 & 0 \\ x_1^{(1)2} & 2x_1^{(1)} & 2 & 0 \\ \hline x_2^{(1)} & 0 & 0 & 1 \end{array} \right) \in \mathbb{C}^{4 \times 4}$$

and $\mathbf{B}_{1,6} = \tilde{\mathbf{V}}_1(2) \in \mathbb{C}^{6 \times 4}$. Indeed, the BTD (4.7) expresses a generalization of the multiplicative shift structure explored in Example 4.1.1.

⁷As an exercise, verify that I_1 and I_2 too become their counterparts in Chapter 3.

⁸For a derivation of (4.8), see Example D.2.1.

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To seal the connections, we give that the BTD of the third-order tensor \mathcal{Y} in (4.7) can be interpreted as the *joint triangularization* of the n multiplication tables in Corollary 3.1.1. Corollary 4.1.1 is an update of Corollary 3.1.1. \mathcal{H} is the same in both, but establishing the final equality is more involved here.

Corollary 4.1.1. *Let the system $\mathcal{F} = \{f_i\}_{i=1}^n$ of n polynomials in n variables x_1, x_2, \dots, x_n have $m_0 \leq m$ disjoint roots with multiplicity $\mu_k \geq 1, 1 \leq k \leq m_0$ and let $\mathbf{H}(d)$ be the column echelon basis of null $(\mathbf{M}(d))$. The slices $\{\mathcal{H}(j, :, :)\}_{j=1}^n$ of the third-order tensor*

$$\mathbf{H}_{[1,2;3]} = \begin{pmatrix} \hat{\mathbf{S}}_2^{(1)} \mathbf{H}(d) \\ \vdots \\ \hat{\mathbf{S}}_2^{(n)} \mathbf{H}(d) \end{pmatrix} \in \mathbb{C}^{(n \cdot m) \times m}$$

where $\hat{\mathbf{S}}_2^{(j)}$ denotes the row selection matrix that selects the rows of $\mathbf{H}(d)$ onto which the m standard monomials are mapped after multiplication with x_j and where d is taken according to the condition preceding Theorem 4.1.1, are equal to the multiplication tables $\{\mathbf{A}_{x_j}\}_{j=1}^n$ w.r.t. the normal set basis for $\mathbb{C}^n / \langle \mathcal{F} \rangle$.

Proof. The derivation of (4.7) does not rely on the specific choice $\mathbf{K}(d) = \tilde{\mathbf{V}}(d) \mathbf{C}^T$ that was made for the basis of null $(\mathbf{M}(d))$ ⁹, so the canonical BTD (4.7) holds for $\mathbf{K}(d) = \mathbf{H}(d)$ as well. Let $\hat{\mathbf{B}}_{k,I_2} \in \mathbb{C}^{m \times \mu_k}$ contain the rows of $\mathbf{B}_{k,I_2} \in \mathbb{C}^{I_2 \times \mu_k}$ that correspond to the m standard monomials. Then we have that

$$\begin{aligned} \text{vec}(\mathcal{H}(j, :, :))^T &= \left(0 \mid \mathbf{0}_{1 \times I_1^{(1)} - 1} \mid \cdots \mid 1 \mid \mathbf{0}_{1 \times I_1^{(j)} - 2} \mid \cdots \mid \mathbf{0}_{1 \times I_1^{(n)} - 1} \right) \mathbf{H}_{[1;3,2]} \\ &= (\mathbf{I}_{I_1})_s^T \sum_{k=1}^{m_0} \mathbf{A}_{k,I_1} \mathbf{G}_{k[1;3,2]} \left(\mathbf{C}_k \otimes \hat{\mathbf{B}}_{k,I_2} \right)^T = \sum_{k=1}^{m_0} \mathbf{A}_{k,I_1}(s, :) \mathbf{G}_{k[1;3,2]} \left(\mathbf{C}_k \otimes \hat{\mathbf{B}}_{k,I_2} \right)^T \\ &= \sum_{k=1}^{m_0} \left(x_j^{(k)} \cdot \mathbf{G}_{k[1;3,2]}(1, :) + 1 \cdot \mathbf{G}_{k[1;3,2]}(s, :) \right) \left(\mathbf{C}_k \otimes \hat{\mathbf{B}}_{k,I_2} \right)^T \end{aligned}$$

where the last equality is a simplification due to $I_1 - 2$ zeros in $\mathbf{A}_{k,I_1}(s, :)$ and s is such that $\mathbf{A}_{k,I_1}(s, 1) = x_{j,k} = x_j^{(k)}$. Let $\tilde{\mathbf{V}} = \mathbf{H}\mathbf{U}$, then, analogous to the proof of Corollary 3.1.1, $(\hat{\mathbf{B}}_{1,I_2} \ \cdots \ \hat{\mathbf{B}}_{m_0,I_2}) = \mathbf{U}$ and $\mathbf{C}^T = \mathbf{U}^{-1}$. Tensorization gives

$$\begin{aligned} \mathcal{H}(j, :, :) &= \sum_{k=1}^{m_0} \hat{\mathbf{B}}_{k,I_2} \left(x_j^{(k)} \cdot \mathcal{G}_k(1, :, :) + 1 \cdot \mathcal{G}_k(s, :, :) \right) \mathbf{C}_k^T \\ &= \sum_{k=1}^{m_0} \hat{\mathbf{B}}_{k,I_2} \underbrace{\left(x_j^{(k)} \mathbf{I}_{\mu_k} + \mathbf{T}_{k,s} \right)}_{\triangleq \mathbf{T}_{x_j,k}} \mathbf{C}_k^T = \mathbf{U} \begin{pmatrix} \mathbf{T}_{x_j,1} & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \mathbf{T}_{x_j,m_0} \end{pmatrix} \mathbf{U}^{-1} = \mathbf{A}_{x_j} \end{aligned}$$

where the last equality is implied by Theorem 2.1.2. □

⁹See Appendix D.

Example 4.1.4. Consider the polynomial equation in $n = 1$ variable x

$$f(x) = (x - \alpha)^2 = x^2 - 2\alpha x + \alpha^2 = 0$$

of degree $m = d_1 = 2$, but with $m_0 = 1$: f has one disjoint root $x^{(1)} = \alpha$ with multiplicity $\mu_1 = 2$. We have that

$$\tilde{\mathbf{V}}_1(2) = \begin{pmatrix} \partial_0[\mathbf{v}_1(2)] & \partial_1[\mathbf{v}_1(2)] \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \\ \alpha^2 & 2\alpha \end{pmatrix} \in \mathbb{C}^{3 \times 2}.$$

Take $I_1 = I_1^{(1)} = \max_{0 \leq l \leq 1} \mathbf{j}_{1,l}(1) + 1 = 2$ and $d = m = 2$, such that $I_2 = q(d - I_1 + 1) = q(2 - 2 + 1) = 2 \geq \mu_1$. $\mathbf{Y}_{[1,2;3]}$ in (4.6) can be constructed from $\mathbf{H}(2)$ instead of $\mathbf{K}(2)$ as well. \mathcal{Y} then reveals the multiplication table \mathbf{A}_x w.r.t. the normal set $\{1, x\}$:

$$\mathbf{Y}_{[1,2;3]} = \begin{pmatrix} \begin{pmatrix} \mathbf{I}_2 & \mathbf{0}_{2 \times 1} \end{pmatrix} \mathbf{H} \\ \begin{pmatrix} \mathbf{0}_{2 \times 1} & \mathbf{I}_2 \end{pmatrix} \mathbf{H} \end{pmatrix} = \begin{pmatrix} \underline{\mathbf{H}} \\ \overline{\mathbf{H}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ -\alpha^2 & 2\alpha \end{pmatrix} = \begin{pmatrix} \mathbf{I}_2 \\ \mathbf{A}_x \end{pmatrix} \in \mathbb{C}^{(2,2) \times 2}.$$

First, we know from (4.7) and the proof of Corollary 4.1.1 that \mathcal{Y} admits the canonical BTD

$$\mathcal{Y} = \mathcal{G}_1 \cdot_1 \mathbf{A}_{1,2} \cdot_1 \mathbf{B}_{1,2} \cdot_1 \mathbf{C} \quad (4.9)$$

in which

$$\mathbf{A}_{1,2} = \mathbf{B}_{1,2} = \tilde{\mathbf{V}}_1(1) = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{G}_{1[2;1,3]} = \left(\begin{array}{cc|cc} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{array} \right). \quad (4.10)$$

Second, \mathbf{A}_x has $m_0 = 1$ disjoint eigenvalue $x^{(1)} = \alpha$ with algebraic multiplicity $\mu_1 = 2$, but with geometric multiplicity 1. \mathbf{A}_x is not diagonalizable, but satisfies a Jordan canonical form

$$\mathbf{A}_x = \mathbf{U} \mathbf{T} \mathbf{U}^{-1} \quad (4.11)$$

where

$$\mathbf{T} = \begin{pmatrix} \alpha & 1 \\ 0 & \alpha \end{pmatrix} \quad \text{and} \quad \mathbf{U} = \begin{pmatrix} -\alpha & 1 \\ -\alpha^2 & 0 \end{pmatrix}$$

are an upper-triangular matrix with diagonal elements $x^{(1)} = \alpha$ and a matrix whose columns span an invariant subspace of dimension $\mu_1 = 2$, respectively.

The factor matrices in a BTD are only determined up to a linear transformation. An equally valid decomposition of \mathcal{Y} in (4.6) is therefore

$$\mathcal{Y} = \sum_{k=1}^{m_0} \tilde{\mathcal{G}}_k \cdot_1 \tilde{\mathbf{A}}_{k,I_1} \cdot_2 \tilde{\mathbf{B}}_{k,I_2} \cdot_3 \tilde{\mathbf{C}}_k$$

in which

$$\tilde{\mathcal{G}}_k = \mathcal{G}_k \cdot_1 \left(\mathbf{M}_k^{(1)} \right)^{-1} \cdot_2 \left(\mathbf{M}_k^{(2)} \right)^{-1} \cdot_3 \left(\mathbf{M}_k^{(3)} \right)^{-1},$$

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$\tilde{\mathbf{A}}_{k,I_1} = \mathbf{A}_{k,I_1} \mathbf{M}_k^{(1)} \in \mathbb{C}^{I_1 \times \mu_k}$, $\tilde{\mathbf{B}}_{k,I_2} = \mathbf{B}_{k,I_2} \mathbf{M}_k^{(2)} \in \mathbb{C}^{I_2 \times \mu_k}$, $\tilde{\mathbf{C}}_k = \mathbf{C}_k \mathbf{M}_k^{(3)} \in \mathbb{C}^{m \times \mu_k}$ and $\mathbf{M}_k^{(1)}, \mathbf{M}_k^{(2)}, \mathbf{M}_k^{(3)} \in \mathbb{C}^{\mu_k \times \mu_k}$ are invertible transformation matrices. The interpretation is as follows: although the multiplicity structure of a root $\mathbf{x}^{(k)}$ is not unique, but only determined up to a linear transformation with the invertible transformation matrix $\mathbf{T} \sim \mathbf{M}_k^{(n)} \in \mathbb{C}^{\mu_k \times \mu_k}$, the subspaces in the terms of the canonical BTB (4.7) are unique¹⁰.

4.2 Connection with Border Rank and Typical Rank

Writing the decomposition of the null space of the Macaulay matrix as a BTB sheds a new light on two properties of tensor rank from Chapter 2.

Border Rank

Recall from Section 2.2.2 that the computation of a rank- R CPD of a third-order tensor $\mathcal{Y} \in \mathbb{C}^{I \times I \times 2}$ where $r_{\mathcal{Y}} > R$, but where \mathcal{Y} has *border rank* R , yields some sort of diverging rank-1 terms. [39] demonstrates that the matrix $\mathbf{Y}_1^{-1} \mathbf{Y}_2$ consisting of the frontal slices of \mathcal{Y} is not diagonalizable, but satisfies a Jordan canonical form. [39] further proves Theorem 2.2.2: it is possible to decompose \mathcal{Y} into a third-order generalization of the Jordan form — as long as there are no groups of more than 4 diverging rank-1 terms.

Example 4.2.1 shows that Example 4.1.4 was actually able to independently come to \mathcal{G} in Theorem 2.2.2 for $R = 2$ diverging rank-1 terms. Similarly, Example 4.1.3 showed the generalization for \mathcal{G} in Theorem 2.2.2 for $R = 4$ diverging rank-1 terms.

Example 4.2.1. Consider the polynomial equation in $n = 1$ variable x in Example 4.1.4 again. The matrix $(\mathbf{Y}_1)^{-1} \mathbf{Y}_2 = \mathbf{I}_2^{-1} \mathbf{A}_x = \mathbf{A}_x$ consisting of the frontal slices of \mathcal{Y} is not diagonalizable, but satisfies the Jordan canonical form (4.11). Further, the canonical BTB (4.9) is a third-order generalization of the Jordan canonical form: \mathcal{G}_1 in (4.10) equals \mathcal{G} in (2.8) and $r_{\mathcal{G}_1} = r_{\mathcal{Y}} = 3$. In fact, we can rewrite (4.9) as

$$\mathcal{Y} = \begin{pmatrix} 1 \\ \alpha \end{pmatrix} \otimes \begin{pmatrix} 1 \\ \alpha \end{pmatrix} \otimes \mathbf{c}_1 + \begin{pmatrix} 1 \\ \alpha \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \mathbf{c}_2 + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ \alpha \end{pmatrix} \otimes \mathbf{c}_2,$$

which is, for a proper choice of basis for the null space of the Macaulay matrix, and, consequently, a proper choice of \mathbf{C} , precisely the border rank-2 tensor $\mathcal{X} = \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{v} + \mathbf{u} \otimes \mathbf{v} \otimes \mathbf{u} + \mathbf{v} \otimes \mathbf{u} \otimes \mathbf{u}$. in Example 2.2.2.

We come to the conclusion that, if $1 \leq m_0 < m$,

- a “naively fitted” m -term CPD to the third-order tensor $\mathcal{Y} \in \mathbb{C}^{(n+1) \times q(d-1) \times m}$ in (3.12) yields m_0 groups of μ_k diverging rank-1 terms in the k th group, if $\mu_k > 1$;
- no difficulties arise as long as we do not try to break the matching m_0 blocks of multilinear rank $(\mu_k \times \mu_k \times \mu_k)$ in the BTB in (4.7) — see Example 4.3.1.

¹⁰Similar properties hold for the Jordan canonical form in, e.g., Example 4.1.4.

Typical Rank

Recall from Section 2.2.2 that a third-order tensor $\mathcal{G} \in \mathbb{R}^{2 \times 2 \times 2}$ has two *typical ranks* $r_{\mathcal{G}} = 2$ or $r_{\mathcal{G}} = 3$ over $\mathbb{F} = \mathbb{R}$ — whereas there is only one typical rank $r_{\mathcal{Y}} = 2$ (the *generic rank*) if $\mathbb{F} = \mathbb{C}$.

If a set of polynomial equations has real coefficients and thus complex conjugated roots, one can w.l.o.g. combine a pair of terms in (3.12) corresponding to a pair of complex conjugated roots: the result is a BTD like the one in (4.7) where the core tensors $\mathcal{G} \in \mathbb{R}^{2 \times 2 \times 2}$ — see Example 4.2.2. One can combine pairs of simple and real roots in the same way¹¹. Say all roots are simple, but we do express \mathcal{Y} as a BTD with multilinear rank- $(2 \times 2 \times 2)$ terms. Inspection of the terms afterwards learns that

- if a term corresponds to a pair of complex conjugated roots, $\mathcal{G} \in \mathbb{R}^{2 \times 2 \times 2}$ has the generic rank 2 over \mathbb{C} , but the typical rank 3 over \mathbb{R} ;
- if a term corresponds to a pair of simple and real roots, $\mathcal{G} \in \mathbb{R}^{2 \times 2 \times 2}$ has rank 2 over *both* \mathbb{C} and \mathbb{R} , and it is possible to decompose the block term further over $\mathbb{F} = \mathbb{R}$.

Example 4.2.2. Consider the univariate polynomial equation

$$f(x) = x^2 - 2x + 2 = 0$$

of degree $m = d_1 = 2$. The coefficients in $\mathbf{f} \in \mathbb{R}^{m+1}$ are real, so f has $m = 2$ complex conjugated roots $x^{(1)} = 1 + i$ and $x^{(2)} = 1 - i$. At $d = d^* + 1 = 2$, \mathcal{Y} in (3.12) is constructed from $\mathbf{K} = \mathbf{V}\mathbf{C}^T \in \mathbb{R}^{3 \times 2}$ for this univariate polynomial equation as follows:

$$\mathbf{Y}_{[1,2;3]} = \left(-\frac{\begin{pmatrix} \mathbf{I}_2 & \mathbf{0}_{2 \times 1} \\ \mathbf{0}_{2 \times 1} & \mathbf{I}_2 \end{pmatrix} \mathbf{K}}{\begin{pmatrix} \mathbf{V} \\ \overline{\mathbf{V}} \end{pmatrix}} \right) \mathbf{C}^T = \begin{pmatrix} 1 & 1 \\ 1+i & 1-i \\ 1+i & 1-i \\ 2i & -2i \end{pmatrix} \mathbf{C}^T \in \mathbb{R}^{(2 \cdot 2) \times 2}.$$

Because all roots are simple, we know from (3.12) that \mathcal{Y} admits the CPD

$$\mathcal{Y} = \llbracket \mathbf{A}, \mathbf{A}, \mathbf{C} \rrbracket = \llbracket \mathbf{V}, \mathbf{V}, \mathbf{C} \rrbracket. \quad (4.12)$$

Note that $\mathbf{v}_2 = \mathbf{v}_1^*$, and that the same holds for the columns of \mathbf{A} and \mathbf{C} ¹². We can rewrite (4.12) as a BTD

$$\mathcal{Y} = \mathcal{G} \cdot_1 \mathbf{A} \cdot_2 \mathbf{A} \cdot_3 \mathbf{C}$$

in which

$$\mathbf{G}_{[1;3,2]} = \left(\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right).$$

¹¹See (4.16).

¹²Every entry in \mathbf{V} is a monomial, and $(\mathbf{x}^*)^\alpha = (\mathbf{x}^\alpha)^*$. \mathbf{A} is just $\mathbf{V}(1:2,:)$. $\mathbf{c}_2 = \mathbf{c}_1^*$ is needed to have only real entries in \mathbf{K} : $\mathbf{K}(i_1, i_2) = \mathbf{v}_1(i_1)\mathbf{c}_1(i_2) + \mathbf{v}_2(i_1)\mathbf{c}_2(i_2) = \mathbf{v}_1(i_1)\mathbf{c}_1(i_2) + \mathbf{v}_1^*(i_1)\mathbf{c}_1^*(i_2) = \mathbf{v}_1(i_1)\mathbf{c}_1(i_2) + (\mathbf{v}_1(i_1)\mathbf{c}_1(i_2))^* \in \mathbb{R}$.

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Clearly, $r_{\mathcal{Y}} = r_{\mathcal{G}} = 2$: the generic rank for $\mathcal{Y} \in \mathbb{R}^{2 \times 2 \times 2}$ over $\mathbb{F} = \mathbb{C}$. An equally valid decomposition of \mathcal{Y} in (4.12) is

$$\mathcal{Y} = \tilde{\mathcal{G}} \cdot_1 \tilde{\mathbf{A}}^{(1)} \cdot_2 \tilde{\mathbf{A}}^{(2)} \cdot_3 \tilde{\mathbf{C}}$$

in which $\tilde{\mathbf{A}}^{(1)} = \mathbf{A}\mathbf{M}^{(1)}$, $\tilde{\mathbf{A}}^{(2)} = \mathbf{A}\mathbf{M}^{(2)}$, $\tilde{\mathbf{C}} = \mathbf{C}\mathbf{M}^{(3)} \in \mathbb{C}^{2 \times 2}$,

$$\tilde{\mathcal{G}} = \mathcal{G} \cdot_1 (\mathbf{M}^{(1)})^{-1} \cdot_2 (\mathbf{M}^{(2)})^{-1} \cdot_3 (\mathbf{M}^{(3)})^{-1}$$

and $\mathbf{M}^{(1)}, \mathbf{M}^{(2)}, \mathbf{M}^{(3)} \in \mathbb{C}^{2 \times 2}$ are invertible transformation matrices. Take

$$\mathbf{M}^{(1)} = \mathbf{M}^{(2)} = \mathbf{M}^{(3)} = \mathbf{M} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2i} \\ \frac{1}{2} & -\frac{1}{2i} \end{pmatrix},$$

such that $\tilde{\mathbf{A}}^{(1)}, \tilde{\mathbf{A}}^{(2)}, \tilde{\mathbf{C}} \in \mathbb{R}^{2 \times 2}$ are (constrained to be) real, then

$$\tilde{\mathbf{G}}_{1[1;3,2]} = \left(\begin{array}{cc|cc} 2 & 0 & 0 & -2 \\ 0 & -2 & -2 & 0 \end{array} \right)$$

with $r_{\tilde{\mathcal{G}}} = 3$: $\mathcal{Y} \in \mathbb{R}^{2 \times 2 \times 2}$ has the typical rank $r_{\mathcal{Y}} = 3$ over $\mathbb{F} = \mathbb{R}$.

4.3 Algorithms

This section hints at some multivariate polynomial root-finding algorithms that put the theoretic insights in the previous sections to the fore.

4.3.1 A Multivariate Polynomial Subspace-Finding Algorithm

Theorem 4.1.1 is constructive in nature: it hints at the polynomial “subspace-finding” procedure by means of a BTB in Algorithm 4.1. `poly_btd` is a Matlab implementation of Algorithm 4.1. If $\mu_k = 1, 1 \leq k \leq m_0$, Algorithm 4.1 is Algorithm 3.1 (`poly_cpd`)¹³. Some additional remarks on Algorithm 4.1 are in order.

Input. A prerequisite to compute the BTB (4.7) in Theorem 4.1.1 is that the size of the core tensors $\mathcal{G}_k \in \mathbb{C}^{\mu_k \times \mu_k \times \mu_k}$, *i.e.* the multiplicities μ_k are known beforehand. The connection with border rank in Section 4.2 is helpful: before fitting a generalization of the Jordan form, [38] starts with identifying groups of diverging rank-1 terms in a “naively fitted” CPD, *e.g.*, using a proper collinearity criterion on the columns of the factor matrices. Here, we could return early from Algorithm 3.1 with these m_0 identified groups, the size of which corresponds to the $\{\mu_k\}_{k=1}^{m_0}$.

Step 1. A prerequisite to use the correct $I_1^{(j)}, I_1, I_2$ and d in Theorem 4.1.1 is that the multiplicity structure of the roots is known. This is infeasible in practice. Note that, per definition, $I_1^{(j)} \leq \max_{1 \leq k \leq m_0} \mu_k, 0 \leq j \leq n$, so by taking every $I_1^{(j)} = I$ in Step 6, the condition preceding Theorem 4.1.1 is certainly met.

Step 2. Consequently, $\bar{I}_1 = I$. By taking $d \geq d^*$ and such that $I_2 = q(d - \bar{I}_1 + 1) = q(d - I + 1) \geq I = \max_{1 \leq k \leq m_0} \mu_k$, (4.5) is met too.

Step 8-9. Like in Algorithm 3.1, compression is possible (as long as $r_{\tilde{\mathbf{B}}_{k,I_2}} \geq I$) and, *e.g.*, an NLS type algorithm can compute the BTB [35].

¹³No implementation of Algorithm 4.1 builds on the SD method in `poly_sd` — see Appendix F.

Algorithm 4.1 BTD for Multivariate Polynomial Subspace-Finding

Input: A system $f_i \in \mathcal{C}_{d_i}^n, 1 \leq i \leq s = n$, in the $n + 1$ projective unknowns $x_j \in \mathbb{C}, 0 \leq j \leq n$, with $m_0 \leq m$ roots, and their multiplicities $\mu_k, 1 \leq k \leq m_0$.

Output: The subspaces $\{\tilde{\mathbf{A}}_{k,I_1}\}_{k=1}^{m_0}$.

- 1: $I \leftarrow \max(2, \max_{1 \leq k \leq m_0} \mu_k)$.
- 2: Take $d \geq d^*$ and such that $I_2 = q(d - I + 1) \geq I$.
- 3: Construct the Macaulay matrix $\mathbf{M}(d)$.
- 4: $\mathbf{K} \leftarrow \text{null}(\mathbf{M}(d))$.
- 5: **for** $0 \leq j \leq n$ **do**
- 6: $\mathcal{Y}(j+1, :, :) \leftarrow \mathbf{S}_I^{(j)} \mathbf{K}$.
- 7: Compute the SVD $\mathbf{Y}_{[2;1,3]} = \mathbf{U}^{(2)} \mathbf{S}^{(2)} \mathbf{U}^{(1,3)H}$
- 8: $\hat{\mathcal{Y}} \leftarrow \mathcal{Y} \cdot_2 \hat{\mathbf{U}}^{(2)H}$
- 9: Compute the m_0 -term BTD (4.7) of $\hat{\mathcal{Y}}$ in which $\mathcal{G}_k \in \mathbb{C}^{\mu_k \times \mu_k \times \mu_k}, 1 \leq k \leq m_0$.
- 10: **return** $\{\tilde{\mathbf{A}}_{k,I_1}\}_{k=1}^{m_0}$

4.3.2 Numerical Experiments

Appendix H exemplifies how to use `poly_btd`. In this section, we share some results.

No Diverging Rank-1 Terms

Our experiments (e.g., in Example 4.3.1) confirm the conclusion in Section 4.2, namely that fitting the BTD in (4.7) instead of the m -term CPD in (3.12) resolves the difficulty of diverging rank-1 terms if there are multiple roots.

Example 4.3.1. Consider the system of $s = 2$ polynomial equations in $n = 2$ variables in Example 1.1.1 again. The system has $m_0 = 3 < m = 4$ disjoint (and affine) roots:

$$\mathbf{x}^{(1)} = \begin{pmatrix} x_1^{(1)} & x_2^{(1)} \end{pmatrix}^T = \begin{pmatrix} 0 & 0 \end{pmatrix}^T \quad \text{and} \quad \begin{pmatrix} x_1^{(2,3)} & x_2^{(2,3)} \end{pmatrix}^T = \begin{pmatrix} 2 & \pm\sqrt{2} \end{pmatrix}^T$$

with multiplicity $\mu_1 = 2$ and $\mu_{2,3} = 1$ (Fig. 1.1a). E.g.,

$$\tilde{\mathbf{V}}(2) = \left(\tilde{\mathbf{V}}_1(2) \mid \mathbf{v}_2(2) \mid \mathbf{v}_3(2) \right) = \left(\partial_{00}[\mathbf{v}_1] \quad \partial_{10}[\mathbf{v}_1] \mid \partial_{00}[\mathbf{v}_2] \mid \partial_{00}[\mathbf{v}_3] \right) \in \mathbb{C}^{q(2) \times m}$$

where $\partial_{\mathbf{j}} \in \mathbb{N}^2$ is again written as $\partial_{j_1 j_2}$ and where

$$\tilde{\mathbf{V}}_1(2) = \begin{pmatrix} 1 & 0 \\ x_1^{(1)} & 1 \\ x_2^{(1)} & 0 \\ x_1^{(1)2} & 2x_1^{(1)} \\ x_1^{(1)} x_2^{(1)} & x_2^{(1)} \\ x_2^{(1)2} & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{C}^{q(2) \times \mu_1}$$

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is a possible basis for $\text{null}(\mathbf{M}(d^*)) = \text{null}(\mathbf{M}(2))$. We have that

$$\mu_1^{(1)} = \max_{0 \leq l \leq 1} \mathbf{j}_{1,l}(1) + 1 = \max\{0, 1\} + 1 = 1 + 1 = 2,$$

$$\mu_1^{(2)} = \max_{0 \leq l \leq 1} \mathbf{j}_{1,l}(2) + 1 = \max\{0, 0\} + 1 = 0 + 1 = 1,$$

$\mu_{2,3}^{(1)} = \mu_{2,3}^{(2)} = 1$ and, implicitly, every $\mu_k^{(0)} = 1$. As $I_1^{(j)} = \max\left(2, \max_{1 \leq k \leq 3} \mu_k^{(j)}\right)$, every $I_1^{(j)} = 2$, $\bar{I} = \max_{0 \leq j \leq 2} I_1^{(j)} = 2$ and $I_1 = \sum_{j=0}^n (I_1^{(j)} - 1) = (n+1) \cdot 1 = 3$. It suffices to take $d = d^* = 2$ such that $I_2 = q(d - \bar{I}_1 + 1) = q(2 - 2 + 1) = q(1) = 3 \geq \mu_1 = 2$. From (4.7), we have that $\mathcal{Y} \in \mathbb{C}^{3 \times 3 \times 4}$ in (4.6) admits the canonical BTD

$$\mathcal{Y} = \mathcal{G}_1 \cdot_1 \tilde{\mathbf{V}}_1(2) \cdot_2 \tilde{\mathbf{V}}_1(2) \cdot_3 \mathbf{C}_1 + \mathbf{v}_2(1) \otimes \mathbf{v}_2(1) \otimes \mathbf{C}_2 + \mathbf{v}_3(1) \otimes \mathbf{v}_3(1) \otimes \mathbf{C}_3$$

in which

$$\mathbf{G}_{1[2;1,3]} = \left(\begin{array}{cc|cc} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{array} \right). \quad (4.13)$$

We first run Algorithm 3.1 with $m = 4$ using an NLS type algorithm, until the relative change in objective function $< 10^{-9}$ or a maximum of 500 iterations is reached. The convergence is shown in Fig. 4.2: it is slow. A collinearity criterion [39, (3.4)] identifies 1 group of $\mu_1 = 2$ diverging rank-1 terms¹⁴.

We then run Algorithm 4.1 with $m_0 = 4 - 1 = 3$ and the identified, correct μ_k using NLS and convergence criterion 10^{-9} . If we hadn't know the multiplicity structure of $\mathbf{x}^{(1)}$, Steps 1-2 in Algorithm 4.1 would prescribe $I = 2$, $d = 2$ and $I_2 = 2$ as well. Since $I_2 = 2 < m = 4$, there is no need for compression in Step 7. The immediate convergence in Step 9 is shown in Fig. 4.2. Algorithm 3.1 finds $\mathbf{x}^{(2)}$ and $\mathbf{x}^{(3)}$ with forward error $\mathcal{O}(10^{-9})$, and the normalized

$$\tilde{\mathbf{A}}_{1,3} = \begin{pmatrix} 1.000 & 1.000 \\ 0.9723 & 0.4435 \\ 0.0000 & 0.0000 \end{pmatrix} = \tilde{\mathbf{V}}_1(2) \mathbf{M}_1^{(1)}.$$

Note that the result of an optimization-based NLS type algorithm can depend on its random initialization.

As explained before, the $\tilde{\mathbf{A}}_{k,I_1}$ with $\mu_k > 1$ are subject to multilinear transformation indeterminacies due to the non-unique multiplicity structure of the multiple roots. The canonical \mathbf{A}_{k,I_1} could be recovered by way of imposing the right constraints on (4.7). We have, e.g., found $\mathbf{A}_{1,3}$ in Example 4.3.1 up to a predefined tolerance by fixing \mathcal{G}_1 in (4.13) using the structured data fusion framework in Tensorlab — but due to the many multilinear transformations that are possible, we have also found that fixing \mathcal{G} is not sufficient in general.

¹⁴In the best 4-term approximation after running an ALS algorithm 10 times with random initialization and convergence criterion 10^{-9} , the absolute value of the cosine between these 2 vectorized rank-1 terms $\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}$ is $0.9311 > 0.90$.

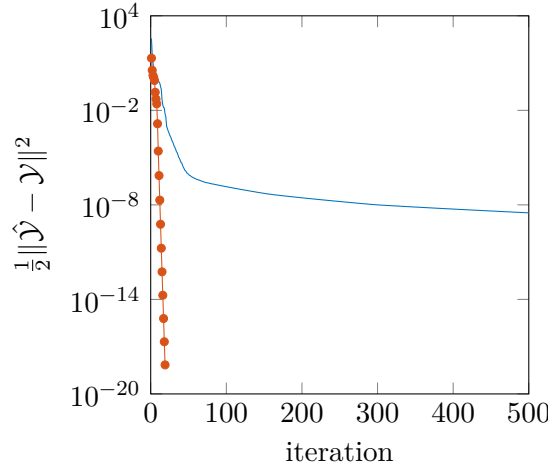


Figure 4.2: Convergence of Algorithm 3.1 (`poly_cpd`) (—) and Algorithm 4.1 (`poly_btd`) (—) using NLS on $\mathcal{Y} \in \mathbb{C}^{3 \times 3 \times 4}$ in Example 4.3.1 as a function of the iteration step. $\hat{\mathcal{Y}}$ is the approximation of the optimization algorithm.

A Recursive Polynomial Root-Finding Algorithm

Algorithm 4.1 is not a polynomial root-finding algorithm. The terms in the BTD

$$\mathcal{Y} = \sum_{k=1}^{m_0} \tilde{\mathcal{G}}_k \cdot_1 \tilde{\mathbf{A}}_{k,I_1} \cdot_2 \tilde{\mathbf{B}}_{k,I_2} \cdot_3 \tilde{\mathbf{C}}_k \quad (4.14)$$

in Step 9 only reveal the *subspaces* defined by the “multivariate Vandermonde plus derivative” matrices

$$\tilde{\mathbf{V}}_k = \begin{pmatrix} \partial_{\mathbf{j}_{k,0}}[\mathbf{v}_k] & \dots & \partial_{\mathbf{j}_{k,\mu_l-1}}[\mathbf{v}_k] \end{pmatrix} \in \mathbb{C}^{q(d) \times \mu_k}, \quad 1 \leq k \leq m_0,$$

that represent $\mathbf{x}^{(k)}$ (with multiplicity μ_k) in the null space of the Macaulay matrix. Without hard constraints, $\mathbf{x}^{(k)}$ cannot be read off directly.

In the generic case in Chapter 3, *i.e.* if $\mu_k = 1, 1 \leq k \leq m_0 = m$, $\tilde{\mathbf{V}}_k = \mathbf{v}_k \in \mathbb{C}^{q(d)}$ and the m_0 multilinear rank- $(\mu_k \times \mu_k \times \mu_k)$ terms in (4.14) become m rank-1 terms in a CPD

$$\mathcal{Y} = \sum_{k=1}^m \mathbf{a}_k \otimes \mathbf{b}_k(d-1) \otimes \mathbf{c}_k \in \mathbb{C}^{(n+1) \times q(d-1) \times m} \quad (4.15)$$

in which \mathbf{a}_k *does* reveal $\mathbf{x}^{(k)}$. Say one combines every $\nu = 2$ terms in (4.15) to rewrite (4.15) as a BTD¹⁵:

$$\mathcal{Y} = \sum_{l=1}^{\lfloor m/2 \rfloor} \mathcal{G}_l \cdot_1 \mathbf{A}_l \cdot_2 + \mathbf{B}_l(d-1) \cdot_3 \mathbf{C}_l + \delta_{1,m \bmod 2} \mathbf{a}_m \otimes \mathbf{b}_m(d-1) \otimes \mathbf{c}_m$$

¹⁵Recall that we did this in Example 4.2.2 for a pair of complex conjugated simple roots.

4. CONNECTIONS BETWEEN SETS OF POLYNOMIAL EQUATIONS AND THE BLOCK TERM DECOMPOSITION

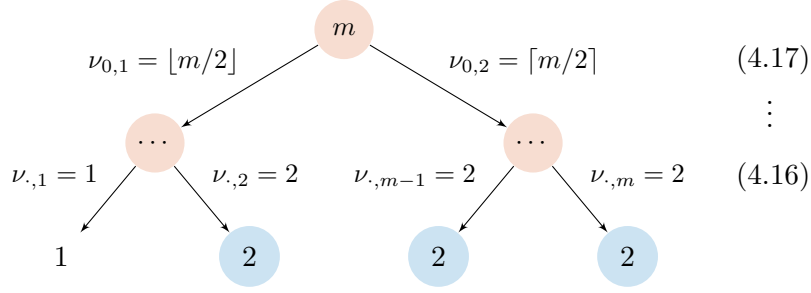


Figure 4.3: A recursive polynomial root-finding scheme that uses **BTD**s at the top levels and **CPD**s at the leaves of rank- R tensors $\hat{\mathcal{Y}}^{(i,l)} \in \mathbb{C}^{(n+1) \times R \times R}$. R is depicted in each node. $\nu_{i,l}$ is the size of a block term in the BTM at a parent node at level i that passes as $\hat{\mathcal{Y}}^{(i+1,l)} \in \mathbb{C}^{(n+1) \times R \times R}$ (where $R = \nu_{i,l}$) to a child node at level $i + 1$.

in which

$$\mathbf{G}_{l[1;3,2]} = \left(\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right) \in \mathbb{C}^{\nu \times (\nu \cdot \nu)}, \quad 1 \leq l \leq \lfloor m/2 \rfloor,$$

$\mathbf{A}_l = (\mathbf{a}_{2l-1} \quad \mathbf{a}_{2l}) \in \mathbb{C}^{(n+1) \times \nu}$, $\mathbf{B}_l(d-1) = (\mathbf{b}_{2l-1}(d-1) \quad \mathbf{b}_{2l}(d-1)) \in \mathbb{C}^{q(d-1) \times \nu}$ and $\mathbf{C}_l = (\mathbf{c}_{2l-1} \quad \mathbf{c}_{2l}) \in \mathbb{C}^{m \times \nu}$. δ_{ij} is the Kronecker delta: $\delta_{ij} = 1$ if $i = j$ and 0 otherwise. Without constraints, an equally valid BTM is

$$\mathcal{Y} = \sum_{l=1}^{\lfloor m/2 \rfloor} \tilde{\mathcal{G}}_l \cdot_1 \tilde{\mathbf{A}}_l \cdot_2 \tilde{\mathbf{B}}_l(d-1) \cdot_3 \tilde{\mathbf{C}}_l + \delta_{1, m \bmod 2} \mathbf{a}_m \otimes \mathbf{b}_m(d-1) \otimes \mathbf{c}_m \quad (4.16)$$

in which $\tilde{\cdot}$ indicates that \mathcal{G}_l has undergone the usual multilinear transformations. The terms in (4.16) reveal the *subspaces* defined by the multivariate Vandermonde matrices

$$\bar{\mathbf{V}}_l = (\mathbf{v}_{2l-1} \quad \mathbf{v}_{2l}) \in \mathbb{C}^{q(d) \times \nu}, \quad 1 \leq l \leq \lfloor m/2 \rfloor,$$

i.e. $\bar{\mathbf{V}}_l$ represents $\mathbf{x}^{(2l-1)}$ and $\mathbf{x}^{(2l)}$ (each with multiplicity 1) in the null space of $\mathbf{M}(d)$. Of course, there is no reason (i) not to use a different size $\nu \neq 2$ for \mathcal{G}_l — possibly varying as ν_l from one term to the other, or (ii) not to merge the terms in (4.16) even further, such that, eventually, we rewrite

$$\mathcal{Y} = \sum_{l=1}^2 \tilde{\mathcal{G}}_l \cdot_1 \tilde{\mathbf{A}}_l \cdot_2 \tilde{\mathbf{B}}_l(d-1) \cdot_3 \tilde{\mathbf{C}}_l \quad (4.17)$$

where $\nu_1 = \lfloor m/2 \rfloor$ and $\nu_2 = \lceil m/2 \rceil$.

The converse of the bottom-up reasoning (4.15)-(4.17) is the top-down scheme (4.17)-(4.15) depicted in Fig. 4.3. The scheme suggests a *recursive* root-finding algorithm. Start with a compressed¹⁶ $\hat{\mathcal{Y}}^{(0,1)} \in \mathbb{C}^{(n+1) \times R \times R} = \mathcal{Y} \in \mathbb{C}^{(n+1) \times m \times m}$ in (4.6), which embodies all $R = m$ roots. Compute the BTM (4.17), *e.g.*, using an

¹⁶Step 7 in Algorithm 3.1.

NLS type algorithm. Descend to the next level and run the same procedure on both terms in (4.17): on $\hat{\mathcal{Y}}^{(1,1)} \in \mathbb{C}^{(n+1) \times R \times R}$, which embodies $R = \nu_{0,1} = \lfloor m/2 \rfloor$ roots, and on $\hat{\mathcal{Y}}^{(1,2)} \in \mathbb{C}^{(n+1) \times R \times R}$, which embodies $R = \nu_{0,2} = \lceil m/2 \rceil$ roots. Repeat this $\mathcal{O}(\log_2 m)$ times, until each CPD at the leaves reveals $R = \nu_{\cdot,l} = 2$ roots left. The columns of the obtained factor matrices $\tilde{\mathbf{A}}_l$, $\tilde{\mathbf{B}}_l(d-1)$ and $\tilde{\mathbf{C}}_l$ in (4.16) could thereby serve as an initialization at a lower level. `mergesolve` is a Matlab implementation of the scheme. Example 4.3.2 contains a numerical example.

Example 4.3.2. Consider the system of $s = 2$ polynomial equations in $n = 2$ variables with $m = 4$ simple (and affine) roots in Example 1.1.4 again. Fig. 4.4b repeats the zero level curves in Fig. 1.4a. We construct $\mathcal{Y} \in \mathbb{C}^{3 \times 4 \times 4}$ from $\mathbf{K}(d^* + 1) = \mathbf{K}(3)$ as in (4.6) and we compress the tensor. We then run `mergesolve` in Matlab using NLS and convergence criterion 10^{-6} for both the BTD and the CPD. As $m = 4$, the BTD at level 0 in Fig. 4.3 already uses $\nu_{0,1} = \nu_{0,2} = m/2 = 2$. Fig. 1.4a superimposes the convergence of the resp. $\nu_{0,1} = 2$ and $\nu_{0,2} = 2$ columns of the first factor matrices $\tilde{\mathbf{A}}_1$ and $\tilde{\mathbf{A}}_2$ in the successive BTD (NLS) iterates from a random initialization to the subspaces (lines) in \mathbb{C}^2 spanned by

$$\mathbf{A}_1 = \overline{\mathbf{V}}_1(2:3, :) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{A}_2 = \overline{\mathbf{V}}_2(2:3, :) = \begin{pmatrix} 3 & 4 \\ -2 & -5 \end{pmatrix}.$$

Note that the upper-left converged column of $\tilde{\mathbf{A}}_2$ is kept outside Fig. 4.4b for visibility. Next, the CPDs converge fast (Fig. 4.4a) along these subspaces (Fig. 4.4b) to the sought for roots.

We suggest the reader to take a moment to fully digest Fig. 4.3 and Fig. 4.4. The root node in Fig. 4.3 represents in fact the m -dimensional *null space* of the Macaulay matrix. The lower-level nodes represent increasingly lower- R -dimensional *nested subspaces* $\subseteq \mathbb{C}^{n^{17}}$ that provide an increasingly finer-grained view on the roots $\mathbf{x} \in \mathbb{C}^n$ of a set of polynomial equations. Due to many NLS runs, the recursive approach does not compete with Algorithm 3.1 in the matter of computational cost. It is more interesting conceptually. One could zoom in on a cluster of roots in one block term. One could even apply the recursive algorithm in conjunction with Algorithm 4.1. The latter would then be a leaf that represents the μ_k -dimensional subspace defined by a μ_k -fold root $\mathbf{x}^{(k)}$ — instead of the rank-1 terms in a CPD in the simple leaves.

In this respect, recall Section 3.2.2: solving a set of s (homogeneous) polynomial equations boils down to searching for another set of m (homogeneous) polynomials — Fig. 4.3 is a recursive search.

4.4 Conclusion

This chapter has taken the multilinear algebra framework in Chapter 3 for formulating and solving a multivariate polynomial root-finding problem to the next level. The framework appears even more flexible: with the inclusion of the BTD, multilinear

¹⁷ \mathbb{C}^{n+1} in the projective case.

4. CONNECTIONS BETWEEN SETS OF POLYNOMIAL EQUATIONS AND THE BLOCK TERM DECOMPOSITION

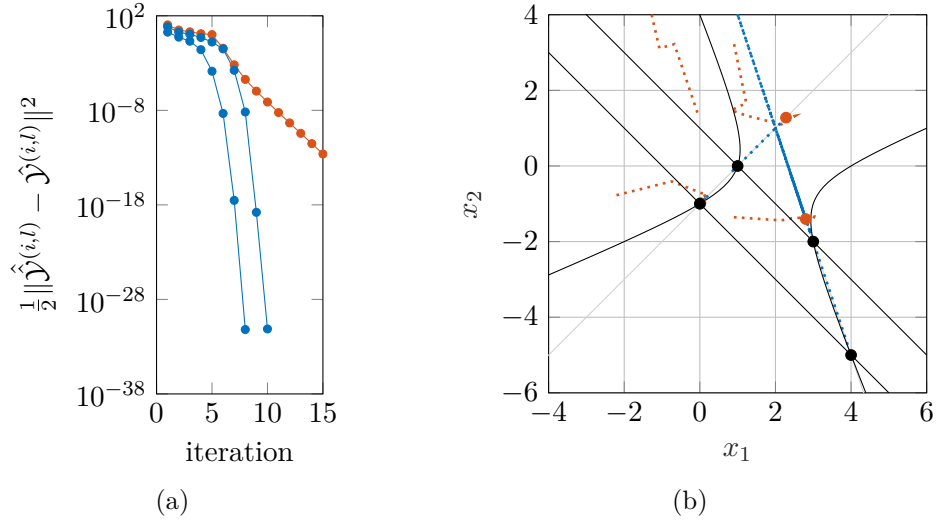


Figure 4.4: (a) Convergence of one BTM at level 0 (—) and two CPDs at the leaves (—) in Fig. 4.3 (`mergesolve`) on $\hat{\mathcal{Y}}$ in Example 4.3.2 as a function of the iteration step. (b) The zero level curves of the system (—) and the convergence from a random initialization to the subspaces (.....) and from the subspaces to the roots (.....) projected on the affine space \mathbb{C}^2 .

algebra is able to detect various (possibly nested) structures in the null space of the Macaulay matrix. The third-order tensor BTM in (4.7) is a natural Hankel generalization of the simple spatial smoothing-based third-order tensor CPD in (3.12) to detect multiple roots. The BTM boils down to the CPD if all roots happen to be simple. Not only is the third-order tensor BTM (i) a generalization of the CPD, it is also (ii) a useful tool to gain a better understanding of the properties border rank and typical rank associated with that CPD and it is (iii) related to the joint triangularization of the multiplication tables. With the proven link in Corollary 4.1.1 between Stetter's Central Theorem of NPA and our Central Theorem 4.1.1, we have come full circle.

Chapter 5

Conclusion and Future Work

The previous chapters have established many connections between sets of polynomial equations, decompositions of higher-order tensors and multidimensional harmonic retrieval. This chapter summarizes and hints at future work.

5.1 Conclusion

Connections between univariate polynomial root-finding, linear algebra and 1D HR are well-known. In this text, we have adopted a bottom-up approach to establish connections between their higher-order generalizations: 0-dimensional sets of multivariate polynomial equations, multilinear algebra and MHR¹.

If a set of polynomial equations has only simple roots, we have relied on the shift-invariance properties and spatial smoothing in each mode in MHR. A multivariate Vandermonde basis for the null space of the system's Macaulay matrix $\mathbf{M}(d)$ exhibits that same shift-invariance property. A third-order tensor CPD arises as the result of implementing spatial smoothing in each variable. The first factor matrix in the CPD reveals the roots of the system. We have built on CPD uniqueness conditions and relaxed MHR uniqueness conditions to show that the third-order tensor CPD, and therefore, the obtained roots, are easily (generically) unique if $d \geq d^*$. At $d = d^* + 1$, the CPD can be interpreted as the joint diagonalization of the multiplication tables in NPA. Surpassing the (Vandermonde) MHR model ($x_0 = 1$) yields a natural homogeneous interpretation of the CPD ($x_0 \neq 1$) in which the scaling ambiguities of the CPD coincide with the scaling ambiguities in the projective space. Short, it has become clear that there is no reason to treat the affine case any differently than the projective case in a multilinear algebra framework.

If the set of polynomial equations has also multiple roots, we cannot rely on the multiplicative shift structure of a full basis for the null space of $\mathbf{M}(d)$ anymore. A well-known “generalization” in signal processing of simple spatial smoothing is hankelization. Hankelization allows us to obtain a general third-order tensor BTD for the null space of $\mathbf{M}(d)$ that incorporates multiple roots in the Central Theorem 4.1.1. If all roots are simple, the BTD reduces to the CPD again. This connection

¹Appendix I gives a schematic.

helps to understand some remarkable properties of the CPD, *e.g.*, border rank and typical rank, better. The BTD can be linked to the joint triangularization of the multiplication tables in NPA. Finally, the (non-unique) factor matrices in a BTD introduce the notion of “subspaces of roots”, embedded in the null space of $\mathbf{M}(d)$.

5.2 Future Work

Below, we formulate three suggestions for future work.

- Section 1.2 touches the isomorphism between homogeneous polynomials and symmetric higher-order tensors. A newly discovered connection is the one between the BTD in Theorem 4.1.1 for sets with multiple roots and the third-order generalization of the Jordan canonical form for tensors that have a certain border rank. Future work might investigate more loosened conditions under which this generalization is valid, or an extension to groups of many diverging rank-1 terms, by means of sets of polynomial equations with (many) multiple roots.
- Tensor methods suffer from the curse of dimensionality: if the number of modes or entries of a higher-order tensor increases, algorithms tend to become slow. However, the real curse of dimensionality in this thesis resides in $q(d)$, which equals the dimension of \mathcal{C}_d^n , the number of columns of $\mathbf{M}(d)$ and the number of rows of $\mathbf{K}(d)$. As n and d grow, $\mathbf{M}(d)$ becomes prohibitively large. We have mentioned the effect on computation time as well as the recursive orthogonalization scheme [2, Algorithm 4.2] and the compression in Algorithm 3.1 to partly overcome it, but a clear need for fast algorithms that exploit the sparsity of the Macaulay matrix, *e.g.*, Krylov-like methods, remains.
- The connections in this thesis open the world of tensor computations and complex optimization to multivariate polynomial root-finding. First, ever-improving tensor algorithms might start competing with traditional, *e.g.*, homotopy continuation-based methods to solve (over-constrained) sets of polynomial equations. Second, future work might further investigate the effect of imposing constraints on the optimization-based computation of the CPD and the BTD to improve the identifiability of the roots. Third, it might be interesting to see whether, *e.g.*, clusters of roots of no interest can be discarded early in the recursive polynomial root-finding scheme.

Although we have already implemented and illustrated the potential of algorithms in Matlab, the main contribution of this thesis is the unraveling of fundamental connections, which could serve as a firm basis for future algorithms. And that was only a matter of “putting on the right glasses”.

Appendices

Appendix A

Linear Algebra

This appendix gives an overview of basic notions from linear algebra (Section A.1), the singular value decomposition (Section A.2) and other matrix decompositions (Section A.3) that support a good understanding of the material in this thesis.

A.1 Algebraic Foundations

A vector $\mathbf{a} \in \mathbb{F}^{I_1}$ is an element of an I_1 -dimensional vector space over the field \mathbb{F} . The field \mathbb{F} could be \mathbb{R} , the set of the real numbers, or \mathbb{C} , the set of the complex numbers. A vector can be seen as a 1-dimensional array of I_1 entries: $(\mathbf{a})_{i_1} = \mathbf{a}(i_1) = a_{i_1} \in \mathbb{C}$, $1 \leq i_1 \leq I_1$. $\omega(\mathbf{a})$ is the number of nonzero entries of \mathbf{a} .

An $I_1 \times I_2$ matrix $\mathbf{A} \in \mathbb{C}^{I_1 \times I_2}$ is a 2-dimensional array, consisting of entries $(\mathbf{A})_{i_1, i_2} = \mathbf{A}(i_1, i_2) = a_{i_1, i_2}$ with row index i_1 , $1 \leq i_1 \leq I_1$ and column index i_2 , $1 \leq i_2 \leq I_2$. $(\mathbf{A})_{i_2} = \mathbf{A}(:, i_2) = \mathbf{a}_{i_2}$ denotes the i_2 th column of \mathbf{A} . $\mathbf{A}(i_{1,1} : i_{2,1}, i_{1,2} : i_{2,2})$ is a submatrix of the original matrix \mathbf{A} for which the first index runs from $i_{1,1}$ to $i_{2,1}$ and the second index runs from $i_{1,2}$ to $i_{2,2}$. A square matrix \mathbf{D} is a diagonal matrix if it has nonzero elements on its diagonal only, *i.e.* $d_{i_1, i_2} = 0$ if $i_1 \neq i_2$. If $\mathbf{D} \in \mathbb{C}^{I \times I}$ is a diagonal matrix with the vector \mathbf{d} on its diagonal, we write $\mathbf{D} = \text{diag}(\mathbf{d})$. $\mathbf{I}_I = \text{diag}(\mathbf{1}) \in \mathbb{C}^{I \times I}$ denotes the identity matrix of order I , where $\mathbf{1} \in \mathbb{C}^I$ is the vector of all ones. A symmetric matrix \mathbf{A} is a matrix that is invariant under permutation of its row and column indexes, *i.e.* $\mathbf{A} = \mathbf{A}^T \Leftrightarrow a_{i_1, i_2} = a_{i_2, i_1}$. The matrix $\mathbf{A} \in \mathbb{C}^{I_1 \times I_2}$ can be thought of as the representation of a linear mapping f from the vector space \mathbb{C}^{I_2} to \mathbb{C}^{I_1} :

$$f : \mathbb{C}^{I_2} \rightarrow \mathbb{C}^{I_1} : \mathbf{x} \mapsto \mathbf{A}\mathbf{x}. \quad (\text{A.1})$$

A fundamental concept in linear algebra is then the concept of the *rank* of a matrix.

Definition A.1.1 (matrix rank). *The rank $r_{\mathbf{A}}$ of a matrix \mathbf{A} is the dimension of the column space of \mathbf{A} .*

Note that Definition A.1.1 is only one possible definition for the rank of a matrix. The matrix rank can be defined in multiple ways:

- (i) The rank $r_{\mathbf{A}} \in \mathbb{N}$ of a matrix \mathbf{A} is the dimension of the range space of the linear mapping (A.1). As

$$\text{range}(f) = \{\mathbf{y} \in \mathbb{C}^{I_1} | \exists \mathbf{x} \in \mathbb{C}^{I_2} : \mathbf{y} = \mathbf{A}\mathbf{x}\} = \text{span}(\{\mathbf{a}_1, \dots, \mathbf{a}_{I_2}\}) \triangleq \text{col}(\mathbf{A}),$$

the rank is indeed given by $\text{colrank}(\mathbf{A}) \triangleq \dim \text{col}(\mathbf{A})$, as in Definition A.1.1. If the columns of $\mathbf{B} \in \mathbb{C}^{I_1 \times R}$ constitute a basis for $\text{col}(\mathbf{A})$, then $r_{\mathbf{A}} = R$ means that R is the minimal number for which $\mathbf{A} = \mathbf{B}\mathbf{C}^T$, where $\mathbf{C} \in \mathbb{C}^{I_2 \times R}$. The decomposition $\mathbf{A} = \mathbf{B}\mathbf{C}^T$ is *not unique*. For any invertible matrix $\mathbf{M} \in \mathbb{C}^{R \times R}$, $\mathbf{A} = \mathbf{B}\mathbf{M}\mathbf{M}^{-1}\mathbf{C}^T = \mathbf{B}\mathbf{M}(\mathbf{C}\mathbf{M}^{-T})^T$ is another valid decomposition. One can also define the row space of \mathbf{A} , $\text{row}(\mathbf{A}) = \text{col}(\mathbf{A}^T)$, and likewise, $\text{rowrank}(\mathbf{A}) \triangleq \dim \text{row}(\mathbf{A})$. Because $\mathbf{A} = \mathbf{B}\mathbf{C}^T \Leftrightarrow \mathbf{A}^T = \mathbf{C}\mathbf{B}^T$, a fundamental result from linear algebra is that $\text{colrank}(\mathbf{A}) = \text{rowrank}(\mathbf{A}) = r_{\mathbf{A}}$ ¹.

- (ii) By noting that $\mathbf{A} = \mathbf{B}\mathbf{C}^T$ can alternatively be written as $\mathbf{A} = \sum_{r=1}^R \mathbf{b}_r \mathbf{c}_r^T$, $r_{\mathbf{A}}$ is the minimal number of *rank-1 terms* that yield \mathbf{A} in a linear combination.

In the matrix case, views (i) and (ii) coincide.

A.2 The Singular Value Decomposition

Closely related to matrix rank, the *singular value decomposition* (SVD) is a widely used matrix decomposition, both conceptually and for computational purposes [42].

Theorem A.2.1 (SVD). [13, Theorem 1] Every complex matrix $\mathbf{A} \in \mathbb{C}^{I_1 \times I_2}$ can be written as the product

$$\mathbf{A} = \mathbf{U}^{(1)} \mathbf{S} \mathbf{U}^{(2)H} \quad (\text{A.2})$$

in which

1. $\mathbf{U}^{(1)} = \begin{pmatrix} \mathbf{u}_1^{(1)} & \dots & \mathbf{u}_{I_1}^{(1)} \end{pmatrix} \in \mathbb{C}^{I_1 \times I_1}$ is a unitary matrix,
2. $\mathbf{U}^{(2)} = \begin{pmatrix} \mathbf{u}_1^{(2)} & \dots & \mathbf{u}_{I_2}^{(2)} \end{pmatrix} \in \mathbb{C}^{I_2 \times I_2}$ is a unitary matrix,
3. $\mathbf{S} \in \mathbb{C}^{I_2 \times I_2}$ is a diagonal matrix with the properties of

(i) *pseudodiagonality*:

$$\mathbf{S} = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_{\min(I_1, I_2)}),$$

(ii) *ordering*:

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{\min(I_1, I_2)} \geq 0$$

The σ_r are the singular values of \mathbf{A} and the $\mathbf{u}_r^{(1)}$ and $\mathbf{u}_r^{(2)}$ are the r th left and right singular vector respectively.

¹Among other proofs, one proof relies on the SVD — see Theorem A.2.1.

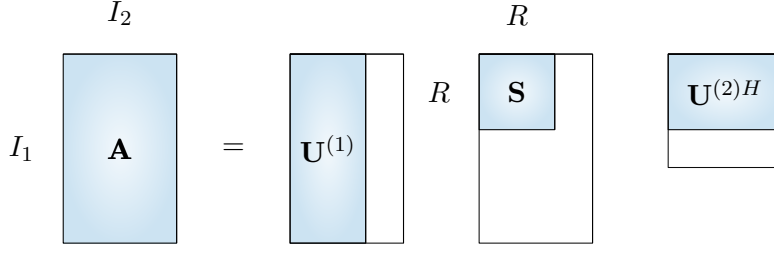


Figure A.1: Visualization of the matrix SVD.

Fig. A.1 visualizes the matrix SVD. Note that the decomposition $\mathbf{A} = \mathbf{U}^{(1)} \mathbf{S} \mathbf{U}^{(2)H}$ is unique due to the constraints given in Theorem A.2.1. The SVD has many other interesting properties. First, its relation with matrix rank is that it is *rank-revealing*: the rank $r_{\mathbf{A}}$ of the matrix \mathbf{A} is the largest number R for which $\sigma_R > 0$. Note that always $R \leq \min(I_1, I_2)$. Second, per the Eckart–Young theorem, the *best rank- k approximation* $\hat{\mathbf{A}}$ of a given matrix \mathbf{A} in the least-squares sense is given by its truncated SVD

$$\hat{\mathbf{A}} = \arg \min_{\mathbf{L} \in \mathbb{C}^{I_1 \times I_2}, r_{\mathbf{L}} \leq k} \|\mathbf{A} - \mathbf{L}\|^2 = \mathbf{U}^{(1)}(:, 1:k) \cdot \mathbf{S}(1:k, 1:k) \cdot \mathbf{U}^{(2)}(:, 1:k)^H$$

Since $\sigma_r = 0$ when $r > R$, it follows that $\hat{\mathbf{A}} = \mathbf{A}$ when $k \geq R$ (Fig. A.1).

A.3 Decompositions of a Square Matrix

The matrix decompositions below are frequently referred to in this thesis.

Definition A.3.1 (eigenvalue, eigenvector). [42, p. 181] Let $\mathbf{A} \in \mathbb{C}^{I \times I}$ be a square complex matrix. $\mathbf{0} \neq \mathbf{x} \in \mathbb{C}^I$ is an eigenvector of \mathbf{A} and $\lambda \in \mathbb{C}$ the corresponding eigenvalue if

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}.$$

Theorem A.3.1 (EVD). [42, Theorem 24.5] Let $\mathbf{A} \in \mathbb{C}^{I \times I}$ be a square complex matrix. If all eigenvectors of \mathbf{A} are linearly independent, \mathbf{A} is nondefective and its eigenvalue decomposition (EVD) exists:

$$\mathbf{A} = \mathbf{X} \mathbf{\Lambda} \mathbf{X}^{-1},$$

where $\mathbf{X} = (\mathbf{x}_1 \dots \mathbf{x}_I) \in \mathbb{C}^{I \times I}$ and $\mathbf{\Lambda} = \text{diag}(\boldsymbol{\lambda}) \in \mathbb{C}^{I \times I}$.

Definition A.3.2 (Jordan canonical form). [39, p. 625] Let $\mathbf{A} \in \mathbb{C}^{I \times I}$ be a square complex matrix. If not all eigenvectors of \mathbf{A} are linearly independent, \mathbf{A} is defective and can be written in Jordan canonical form:

$$\mathbf{A} = \mathbf{P} \mathbf{J} \mathbf{P}^{-1},$$

where $\mathbf{P} = (\mathbf{p}_1 \dots \mathbf{p}_I) \in \mathbb{C}^{I \times I}$ contains the principal vectors of \mathbf{A} and $\mathbf{J} \in \mathbb{C}^{I \times I}$ is the block diagonal form in which each block

$$\mathbf{J}_j = \begin{pmatrix} \lambda_j & 1 & 0 & \dots & 0 \\ 0 & \lambda_j & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & 1 \\ 0 & \dots & \dots & 0 & \lambda_j \end{pmatrix}.$$

Appendix B

Multilinear Algebra

This appendix gives an overview of basic multilinear algebra tools in Section B.1. Section B.2 will define the multilinear singular value decomposition (MLSVD). Besides the canonical polyadic decomposition (CPD) discussed in Chapter 2, which is closely related to the tensor rank in Definition 2.2.5, the MLSVD is another important higher-order tensor decomposition, closely related to the multilinear rank in Definition 2.2.2. Section B.3 and B.4 will cover the relation between the MLSVD and the multilinear rank and between the multilinear rank and the tensor rank, respectively.

B.1 Higher-Order Tensors

An N th-order tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ is an array, indexed by three or more indexes: the (i_1, i_2, \dots, i_N) th entry of \mathcal{A} is denoted by $(\mathcal{A})_{i_1, i_2, \dots, i_N} = \mathcal{A}(i_1, i_2, \dots, i_N) = a_{i_1, i_2, \dots, i_N} \in \mathbb{C}$, $1 \leq i_n \leq I_n$, $1 \leq n \leq N$. N is the *order* of the tensor: the number of dimensions (*modes*). Capitals I_n are used for the dimensions, *i.e.* the upper bound on the set of mode- n indexes. Subtensors are lower-order parts of the original tensor, obtained when one or more indexes are fixed: a mode- n *fiber* $\mathbf{a}_{i_1, i_2, \dots, i_{n-1}, i_{n+1}, \dots, i_N} = (\mathcal{A})_{i_1, i_2, \dots, i_{n-1}, :, i_{n+1}, \dots, i_N}$ is a vector obtained when fixing all but the n th index and a matrix *slice* is obtained when fixing all but two indexes $\mathbf{A}_{i_1, i_2, \dots, i_{m-1}, i_{m+1}, \dots, i_{n-1}, i_{n+1}, \dots, i_N} = (\mathcal{A})_{i_1, i_2, \dots, i_{m-1}, :, i_{m+1}, \dots, i_{n-1}, :, i_{n+1}, \dots, i_N}$. A symmetric tensor is a tensor of which the entries are invariant under any permutation of the indexes. The manipulation of a higher-order tensor often requires its reshaping into a vector or a matrix.

Definition B.1.1 (vectorization). $\text{vec}(\mathcal{A}) = \mathbf{a}_{[N, N-1, \dots, 1]} \in \mathbb{C}^{I_N I_{N-1} \dots I_1}$ is the *vectorization* of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ whose entry

$$a_j = a_{i_1, i_2, \dots, i_N}$$

with

$$j = i_1 + \sum_{k=2}^N (i_k - 1) \left[\prod_{l=1}^{k-1} I_l \right].$$

According to Definition B.1.1, the vectorization of a matrix $\mathbf{A} \in \mathbb{C}^{I_1 \times I_2}$ is obtained by vertically stacking the columns of \mathbf{A} .

Definition B.1.2 (matricization).

$$\mathbf{A}_{(n)} = \mathbf{A}_{[n; \bullet]} = \mathbf{A}_{[n; N, N-1, \dots, n+1, n-1, \dots, 1]} \in \mathbb{C}^{I_n \times I_N I_{N-1} \dots I_{n+1} I_{n-1} \dots I_1}$$

is the mode- n matricization of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ whose entry

$$a_{i_n, j} = a_{i_1, i_2, \dots, i_N}$$

with

$$j = 1 + \sum_{k=1, k \neq n}^N (i_k - 1) \left[\prod_{l=1, l \neq n}^{k-1} I_l \right].$$

According to Definition B.1.2, the mode-1 matricization $\mathbf{A}_{[1;3,2]}$ of a third-order tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ is obtained by horizontally stacking the mode-1 fibers of \mathcal{A} into a matrix, where i_2 varies fastest along the second dimension of $\mathbf{A}_{[1;3,2]}$.

Example B.1.1. Consider the third-order tensor $\mathcal{A} \in \mathbb{C}^{3 \times 3 \times 3}$ defined by

$$\begin{cases} a_{1,1,1} = a_{2,2,1} = a_{2,2,2} = a_{3,3,2} = 1 \\ a_{1,1,3} = -a_{3,3,3} = 2 \end{cases}$$

and $a_{i_1, i_2, i_3} = 0$ elsewhere. Its mode-1 matricization $\mathbf{A}_{(1)} = \mathbf{A}_{[1;3,2]}$ is given by

$$\mathbf{A}_{(1)} = \left(\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -2 \end{array} \right).$$

Definition B.1.1 allows for the easy view of $\mathbb{C}^{I_1 \times I_2}$ and, more generally $\mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$, as a vector space. In addition to the elementwise addition and scalar multiplication, an outer product, a n -mode product, an inner product and a vector norm are defined.

Definition B.1.3 (outer product). The outer product $\mathcal{C} = \mathcal{A} \otimes \mathcal{B}$ of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_M}$ and a tensor $\mathcal{B} \in \mathbb{C}^{J_1 \times J_2 \times \dots \times J_N}$ yields a tensor $\mathcal{C} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_M \times J_1 \times J_2 \times \dots \times J_N}$ with entries

$$(\mathcal{C})_{i_1, i_2, \dots, i_M, j_1, j_2, \dots, j_N} \triangleq a_{i_1, i_2, \dots, i_M} b_{j_1, j_2, \dots, j_N}.$$

Example B.1.2. The outer product of vectors $\mathbf{u}^{(n)} \in \mathbb{C}^{I_n}, 1 \leq n \leq N$ yields a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ with entries

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

Definition B.1.4 (n -mode product). The n -mode product $\mathcal{C} = \mathcal{A} \cdot_n \mathbf{B}$ of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ and a matrix $\mathbf{B} \in \mathbb{C}^{J \times I_n}$ yields a tensor $\mathcal{C} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_{n-1} \times J \times I_{n+1} \times \dots \times I_N}$ with entries

$$(\mathcal{C})_{i_1, i_2, \dots, i_{n-1}, j, i_{n+1}, \dots, i_N} \triangleq \sum_{i_n=1}^{I_n} a_{i_1, i_2, \dots, i_n, \dots, i_N} b_{j, i_n}.$$

According to Definition B.1.2 and B.1.4, the n -mode product of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ and a matrix $\mathbf{B} \in \mathbb{C}^{J \times I_n}$ has the matrix representation $\mathbf{C}_{(n)} = \mathbf{B} \mathbf{A}_{(n)}$, i.e. taking the n -mode product amounts to the multiplication of all mode- n fibers of \mathcal{A} with \mathbf{B} .

Example B.1.3. Suppose that

$$\mathbf{A}_{[1;2]} \triangleq \mathbf{A} = \mathbf{U}^{(1)} \mathbf{S}_{[1;2]} \mathbf{U}^{(2)T} \Leftrightarrow \mathbf{A}_{[2;1]} \triangleq \mathbf{A}^T = \mathbf{U}^{(2)} \mathbf{S}_{[2;1]} \mathbf{U}^{(1)T}.$$

Using the n -mode product, this can be rewritten as $\mathbf{A} = \mathbf{S} \cdot_1 \mathbf{U}^{(1)} \cdot_2 \mathbf{U}^{(2)}$.

Using Definition B.1.4, the third-order tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times I_3}$ can also be thought of as the representation of a bilinear mapping f from the vector space \mathbb{C}^{I_2} and \mathbb{C}^{I_3} to \mathbb{C}^{I_1}

$$f_1 : \mathbb{C}^{I_2} \times \mathbb{C}^{I_3} \rightarrow \mathbb{C}^{I_1} : (\mathbf{x}, \mathbf{y}) \mapsto \mathcal{A} \cdot_2 \mathbf{x} \cdot_3 \mathbf{y} \quad (\text{B.1})$$

with a straightforward generalization to the N th-order case.

Example B.1.4. The matrix multiplication of two matrices $\mathbf{B}_1, \mathbf{B}_2 \in \mathbb{C}^{2 \times 2}$ yields the matrix $\mathbf{C} \in \mathbb{C}^{2 \times 2}$. Each entry of \mathbf{C} is a bilinear form¹ of the entries of \mathbf{B}_1 and \mathbf{B}_2

$$\text{vec}(\mathbf{C}) = \mathcal{A} \cdot_2 \text{vec}(\mathbf{B}_1) \cdot_3 \text{vec}(\mathbf{B}_2),$$

where each matrix slice $\mathcal{A}(i_1, :, :)$, $1 \leq i_1 \leq 4$ holds the coefficients that produce the i_1 th entry of $\text{vec}(\mathbf{C})$.

Given the vector $\mathbf{x} \in \mathbb{C}^{I+1}$, with a vector $\mathbf{a} \in \mathbb{C}^{I+1}$, we can associate the linear form $\mathbf{a}^T \mathbf{x} \in \mathcal{P}_1^I$. Likewise, with a symmetric matrix $\mathbf{A} \in \mathbb{R}^{(I+1) \times (I+1)}$, we can associate the quadratic form $\mathbf{x}^T \mathbf{A} \mathbf{x} \in \mathcal{P}_2^I$. A symmetric third-order tensor $\mathcal{A} \in \mathbb{C}^{(I+1) \times (I+1) \times (I+1)}$ can be thought of as the representation of a cubic form $\mathcal{A} \cdot_1 \mathbf{x} \cdot_2 \mathbf{x} \cdot_3 \mathbf{x} \in \mathcal{P}_3^I$. The space of third-order symmetric tensors is isomorphic with the space of cubic homogeneous polynomials [9]. There is a straightforward generalization to the N th-order case. Fig. B.1 visualizes the idea.

Example B.1.5. Consider the third-order symmetric tensor $\mathcal{A} \in \mathbb{C}^{2 \times 2 \times 2}$ defined by

$$a_{1,1,1} = a_{1,1,2} = a_{1,2,1} = a_{2,1,1} = 1$$

¹The decomposition of this bilinear mapping forms the basis of Strassen's algorithm for the multiplication of two matrices [33, Chapter 1, p. 5].

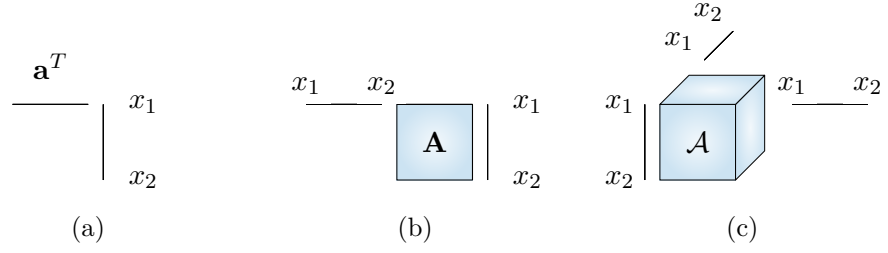


Figure B.1: Visualization of (a) a linear form, (b) a quadratic form and (c) a cubic form in two variables x_1 and x_2 .

and $a_{i_1, i_2, i_3} = 0$ elsewhere. Given $\mathbf{x} = (x_1 \ x_2)^T$, with \mathcal{A} , we can associate the cubic form

$$x_1^3 + 3x_1^2x_2 \in \mathcal{P}_3^1,$$

which is a homogeneous multivariate polynomial of degree 3 in x_1 and x_2 .

Definition B.1.5 (inner product). The inner product of two tensors $\mathcal{A}, \mathcal{B} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ is

$$\langle \mathcal{A}, \mathcal{B} \rangle \triangleq \sum_{i_1=1}^{I_1} \sum_{i_2=1}^{I_2} \dots \sum_{i_N=1}^{I_N} a_{i_1, i_2, \dots, i_N} b_{i_1, i_2, \dots, i_N}^*.$$

Definition B.1.6 (Frobenius norm). The Frobenius norm of a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ is

$$\|\mathcal{A}\| \triangleq \sqrt{\langle \mathcal{A}, \mathcal{A} \rangle}.$$

Two other (matrix) products are frequently used in this thesis. We mention them here for the sake of completeness.

Definition B.1.7 (Kronecker product). The Kronecker product $\mathbf{C} = \mathbf{A} \otimes \mathbf{B}$ of $\mathbf{A} \in \mathbb{C}^{I_1 \times I_2}$ and $\mathbf{B} \in \mathbb{C}^{J_1 \times J_2}$ yields a matrix $\mathbf{C} \in \mathbb{C}^{I_1 J_1 \times I_2 J_2}$

$$\mathbf{C} \triangleq \begin{pmatrix} a_{1,1}\mathbf{B} & \dots & a_{1,I_2}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{I_1,1}\mathbf{B} & \dots & a_{I_1,I_2}\mathbf{B} \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \otimes \mathbf{b}_1 & \mathbf{a}_1 \otimes \mathbf{b}_2 & \dots & \mathbf{a}_{I_2} \otimes \mathbf{b}_{J_2-1} & \mathbf{a}_{I_2} \otimes \mathbf{b}_{J_2} \end{pmatrix}.$$

Example B.1.6. The Kronecker product $\mathbf{b} \otimes \mathbf{a}$ is equal to the rank-1 matrix $\mathbf{a}\mathbf{b}^T$.

Definition B.1.8 (Khatri–Rao product). The Khatri–Rao product $\mathbf{C} = \mathbf{A} \odot \mathbf{B}$ of $\mathbf{A} \in \mathbb{C}^{I_1 \times K}$ and $\mathbf{B} \in \mathbb{C}^{J_1 \times K}$ yields a matrix $\mathbf{C} \in \mathbb{C}^{I_1 J_1 \times K}$ with columns

$$\mathbf{c}_k \triangleq \mathbf{a}_k \otimes \mathbf{b}_k.$$

B.2 The Multilinear Singular Value Decomposition

If one thinks of a tensor as the representation of a multilinear mapping (B.1), it becomes clear that the entries of a tensor are defined with respect to the chosen bases in N vector spaces, say $\mathbb{C}^{I_1}, \mathbb{C}^{I_2}, \dots, \mathbb{C}^{I_N}$. A change of basis in one or more of these vector spaces then corresponds to a higher-order tensor decomposition that can possibly reveal interesting properties of the tensor. The Tucker model in [43] implements a change of bases (coordinate transformation) by decomposing a tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ into a *core tensor* $\mathcal{G} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ multiplied by a $I_n \times I_n$ matrix along each mode.

$$\begin{aligned} \mathcal{A} &= \mathcal{G} \cdot_1 \mathbf{U}^{(1)} \cdot_2 \mathbf{U}^{(2)} \cdot_3 \dots \cdot_N \mathbf{U}^{(N)} \\ &= \sum_{i_1=1}^{I_1} \sum_{i_2=1}^{I_2} \dots \sum_{i_N=1}^{I_N} (\mathcal{G})_{i_1, i_2, \dots, i_N} \mathbf{u}_{i_1}^{(1)} \otimes \mathbf{u}_{i_2}^{(2)} \otimes \dots \otimes \mathbf{u}_{i_N}^{(N)}. \end{aligned}$$

The Tucker decomposition is not unique². Building on the Tucker model, a convincing generalization of the matrix SVD is the *multilinear singular value decomposition* (MLSVD).

Theorem B.2.1 (MLSVD). [13, Theorem 2] *Every complex tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ can be written as the product*

$$\mathcal{A} = \mathcal{S} \cdot_1 \mathbf{U}^{(1)} \cdot_2 \mathbf{U}^{(2)} \cdot_3 \dots \cdot_N \mathbf{U}^{(N)}, \quad (\text{B.2})$$

in which

1. $\mathbf{U}^{(n)} = \begin{pmatrix} \mathbf{u}_1^{(n)} & \dots & \mathbf{u}_{I_n}^{(n)} \end{pmatrix} \in \mathbb{C}^{I_n \times I_n}$ is a unitary matrix,
2. $\mathcal{S} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ is a complex tensor of which the subtensors $\mathcal{S}_{i_n=\alpha}$, obtained when fixing the n th index to α , have the properties of

(i) *all-orthogonality:*

$$\langle \mathcal{S}_{i_n=\alpha}, \mathcal{S}_{i_n=\beta} \rangle = 0, \alpha \neq \beta$$

(ii) *ordering:*

$$\|\mathcal{S}_{i_n=1}\| \geq \|\mathcal{S}_{i_n=2}\| \geq \dots \geq \|\mathcal{S}_{i_n=n}\| \geq 0. \quad (\text{B.3})$$

The Frobenius norms $\|\mathcal{S}_{i_n=i}\|$, denoted by $\sigma_i^{(n)}$, are the mode- n singular values of \mathcal{A} and $\mathbf{u}_i^{(n)}$ is a mode- n singular vector.

Fig. B.2 visualizes the MLSVD of a third-order tensor. The interpretation is the following: for every tensor \mathcal{A} , it is possible to find orthogonal transformations such that $\mathcal{S} = \mathcal{A} \cdot_1 \mathbf{U}^{(1)H} \cdot_2 \mathbf{U}^{(2)H} \cdot_3 \dots \cdot_N \mathbf{U}^{(N)H}$ is all-orthogonal and ordered. This orthogonal transformations, and therefore also decomposition (B.2), are unique on similar conditions as the matrix SVD (Theorem A.2.1) due to the constraints given

²The same argument as for the matrix case applies here.

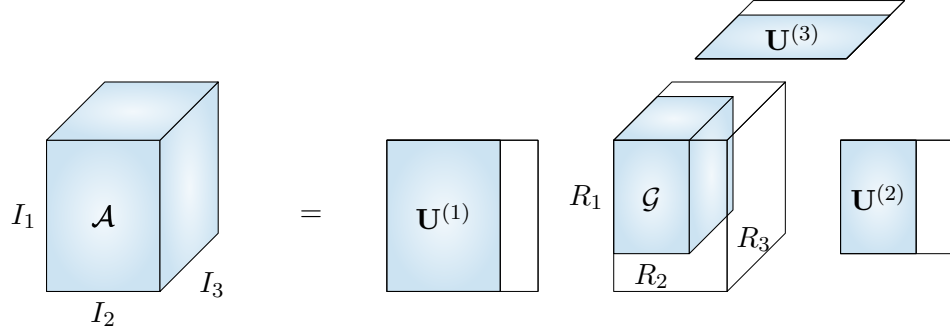


Figure B.2: Visualization of the MLSVD.

in Theorem B.2.1. Note that the diagonality of \mathcal{S} in (A.2) is lost. Comparing the degrees of freedom of a diagonalization (B.2) and the number of constraints, *i.e.* the number of elements of \mathcal{A} , we have that $\sum_{n=1}^N I_n^2 + \min(I_1, I_2, \dots, I_N) < \prod_{n=1}^N I_i$ for N sufficiently large, and one cannot expect the core tensor to be diagonal in general. In the matrix case, $I_1^2 + I_2^2 + \min(I_1, I_2) > I_1 I_2$ and one needs additional constraints to enforce uniqueness. As diagonality implies orthogonality, Theorem A.2.1 is in fact a special case of Theorem B.2.1.

B.3 Connections between the MLSVD and the Multilinear Rank

The MLSVD generalizes some other properties of the matrix SVD as well. First, it is *multilinear rank-revealing* (Definition 2.2.2).

Example B.3.1. Consider again the third-order tensor \mathcal{A} in Example B.1.1. Its mode-1, mode-2 and mode-3 matricizations are given by

$$\begin{aligned} \mathbf{A}_{(1)} &= \left(\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array} \middle| \begin{array}{ccc} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{array} \right), \\ \mathbf{A}_{(2)} &= \left(\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array} \middle| \begin{array}{ccc} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{array} \right), \\ \mathbf{A}_{(3)} &= \left(\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 2 & 0 & 0 & 0 & 0 & 0 \end{array} \middle| \begin{array}{ccc} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -2 \end{array} \right). \end{aligned}$$

$R_1 = 3$ and $R_2 = 3$, but as $\mathbf{A}_{(3)}(:, 9) = \mathbf{A}_{(3)}(:, 5) - \mathbf{A}_{(3)}(:, 1)$, $R_3 = 2$ only. The multilinear rank $\text{rank}_{\boxplus}(\mathcal{A}) = (3, 3, 2)$.

It is shown in [13] that the N sets of mode- n singular values $\sigma_{i_n}^{(n)}$, $1 \leq n \leq N$, are in fact the singular values of the mode- n matricizations $\mathbf{A}_{(n)}$ and that the mode- n singular vectors $\mathbf{u}_i^{(n)}$ are the corresponding left singular vectors. This establishes the multilinear rank-revealing property of the MLSVD. This also shows how to compute the core tensor: $\mathcal{S} = \mathcal{A} \cdot_1 \mathbf{U}^{(1)H} \cdot_2 \mathbf{U}^{(2)H} \cdot_3 \dots \cdot_N \mathbf{U}^{(N)H}$ where $\mathbf{U}^{(n)}$ is obtained from the SVD of $\mathbf{A}_{(n)}$.

Corollary B.3.1. *Let r_n be equal to the highest index for which $\|\mathcal{S}_{i_n=r_n}\| > 0$ in (B.3). Then one has*

$$R_n = r_n.$$

Proof. $R_n \triangleq \dim \text{col}(\mathbf{A}_{(n)}) = r_{\mathbf{A}_{(n)}} = \max\{i_n \mid \sigma_{i_n}^{(n)} > 0\} = \max\{i_n \mid \|\mathcal{S}_{i_n}\| > 0\} \triangleq r_n.$ \square

When the third-order tensor \mathcal{A} is regarded as the representation of the bilinear mapping $f_1 : \mathbb{C}^{I_2} \times \mathbb{C}^{I_3} \rightarrow \mathbb{C}^{I_1}$ in (B.1), the mode-1 rank of \mathcal{A} is effectively $\dim \text{range}(f_1)$. More generally, the mode- n rank is $\dim \text{range}(f_n)$ with

$$f_n : \mathbb{C}^{I_1 \times I_2 \times \dots \times I_{n-1} \times I_{n+1} \times \dots \times I_N} \rightarrow \mathbb{C}^{I_n}.$$

Furthermore, the dominant subspace of the mode- n subspace $\text{range}(f_n)$ is generated by the first part of the factor matrix $\mathbf{U}^{(n)}$.

The MLSVD (B.2) can equivalently be written as the product

$$\mathcal{A} = \mathcal{S} \cdot_1 \mathbf{U}^{(1)} \cdot_2 \mathbf{U}^{(2)} \cdot_3 \dots \cdot_N \mathbf{U}^{(N)}$$

in which $\mathbf{U}^{(n)} \in \mathbb{C}^{I_n \times R_n}$ and $\mathcal{S} \in \mathbb{C}^{R_1 \times R_2 \times \dots \times R_N}$ (Fig. B.2). The Eckart-Young theorem does *not* generalize to the higher-order case though. Let the tensor $\hat{\mathcal{A}}$ be defined by discarding the smallest nonzero mode- n singular values $\sigma_{i_n}^{(n)}$, $I'_n + 1 \leq i_n \leq R_n$, $1 \leq n \leq N$, *i.e.* truncate the corresponding parts of \mathcal{S} and $\mathbf{U}^{(n)}$. [13, p. 1269] gives an example which shows that $\hat{\mathcal{A}}$ is in general not the best multilinear rank- $(I'_1, I'_2, \dots, I'_N)$ approximation. It is still a good approximation and it can be used as a starting point for enhancing optimization procedures [32].

B.4 Connections between the Multilinear Rank and the Tensor Rank

For a matrix $\mathbf{X} \in \mathbb{C}^{I \times J}$, $R = r_{\mathbf{X}} \leq \min(I, J)$. Comparing the degrees of freedom in (2.7) and the number of equations, one should have $(I + J + K - 2)R \geq IJK$ ³ and therefore $R \geq \lceil \frac{IJK}{I+J+K-2} \rceil$, which could be as high as $\min(IJ, JK, IK)$ in general.

Theorem B.4.1. *For a third-order rank- R tensor $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ with multilinear rank $\text{rank}_{\boxplus}(\mathcal{X}) = (R_1, R_2, R_3)$,*

$$\max(R_1, R_2, R_3) \leq R \leq \min(R_1 R_2, R_2 R_3, R_1 R_3).$$

³One can always scale \mathbf{a}_r and \mathbf{b}_r and counter-scale \mathbf{c}_r , explaining the term $-2R$ in the degrees of freedom of (2.7).

Proof. Since $\text{rank}_{\boxplus}(\mathcal{X}) = (R_1, R_2, R_3)$, the MLSVD of \mathcal{X} is

$$\mathcal{X} = \mathcal{G} \cdot_1 \mathbf{U}^{(1)} \cdot_2 \mathbf{U}^{(2)} \cdot_3 \mathbf{U}^{(3)}$$

where $\mathcal{G} \in \mathbb{C}^{R_1 \times R_2 \times R_3}$. Write the matrix $\mathbf{G}_{r_3} = \tilde{\mathbf{A}}_{r_3} \tilde{\mathbf{B}}_{r_3}^T$ for some $\tilde{\mathbf{A}}_{r_3}, \tilde{\mathbf{B}}_{r_3}$ having at most $\min(R_1, R_2)$ columns. Write $\tilde{\mathbf{A}} \triangleq (\tilde{\mathbf{A}}_1 \dots \tilde{\mathbf{A}}_{R_3})$, $\tilde{\mathbf{B}} \triangleq (\tilde{\mathbf{B}}_1 \dots \tilde{\mathbf{B}}_{R_3})$ and $\tilde{\mathbf{C}} \triangleq (\mathbf{I}_{R_3 \times R_3} \otimes \mathbf{1}_{1 \times \min(R_1, R_2)})$ where $\mathbf{1}_{1 \times \min(R_1, R_2)}$ is a $1 \times \min(R_1, R_2)$ vector of all ones, having at most $\min(R_1 R_3, R_2 R_3)$ columns. Now $\mathcal{G} = \llbracket \tilde{\mathbf{A}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}} \rrbracket$ and, upon a change of basis,

$$\mathcal{X} = \llbracket \mathbf{U}^{(1)} \tilde{\mathbf{A}}, \mathbf{U}^{(2)} \tilde{\mathbf{B}}, \mathbf{U}^{(3)} \tilde{\mathbf{C}} \rrbracket$$

is a $\min(R_1 R_3, R_2 R_3)$ -term PD of \mathcal{X} . By relying on role symmetry, this establishes the upper bound.

For the lower bound, assume that we have found the matrices \mathbf{A} , \mathbf{B} and \mathbf{C} such that the R -term CPD (2.7) holds. We have that

$$\mathbf{X}_{(1)} = \mathbf{X}_{[1;3,2]} = \begin{pmatrix} \mathbf{X}_1 & \dots & \mathbf{X}_K \end{pmatrix} = \mathbf{A} \begin{pmatrix} \mathbf{D}_1(\mathbf{C})\mathbf{B} & \dots & \mathbf{D}_K(\mathbf{C})\mathbf{B} \end{pmatrix}.$$

Because $\mathbf{A} \in \mathbb{C}^{I \times R}$, it follows that $R \geq R_1$ in order to have $\text{colrank}(\mathbf{X}_{(1)}) = R_1$, and analogously, $R \geq R_2$ and $R \geq R_3$. \square

Theorem B.4.1 suggests to consider the multilinear rank first when investigating the rank of a tensor.

Example B.4.1. Consider again the third-order tensor \mathcal{A} in Example B.1.1. The multilinear rank $\text{rank}_{\boxplus}(\mathcal{A}) = (3, 3, 2)$, so $R = r_{\mathcal{A}}$ should satisfy

$$\max(3, 3, 2) \leq R \leq \min(3 \cdot 3, 3 \cdot 2, 3 \cdot 2) \Leftrightarrow 3 \leq R \leq 6.$$

Since the PD for \mathcal{A} in Example 2.2.1 has 3 terms, $R = 3$ and the PD in Example 2.2.1 is a CPD.

Appendix C

Uniqueness of the Canonical Polyadic Decomposition

Chapter 2 discusses the canonical polyadic decomposition (CPD). This appendix holds some background for the reader who is interested in the CPD uniqueness conditions referred to in Chapter 3.

C.1 Uniqueness Conditions

First, the CPD is always subject to trivial permutation and scaling indeterminacies.

Definition C.1.1 (essential uniqueness). *Let $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ be a rank- R tensor. The CPD of \mathcal{X} is essentially unique if*

$$\mathcal{X} = [\mathbf{A}, \mathbf{B}, \mathbf{C}] = [\tilde{\mathbf{A}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}]$$

implies that there exist a permutation matrix $\mathbf{\Pi} \in \mathbb{C}^{R \times R}$ and nonsingular diagonal matrices $\mathbf{\Lambda}_\mathbf{A} \in \mathbb{C}^{R \times R}$, $\mathbf{\Lambda}_\mathbf{B} \in \mathbb{C}^{R \times R}$ and $\mathbf{\Lambda}_\mathbf{C} \in \mathbb{C}^{R \times R}$ such that

$$\tilde{\mathbf{A}} = \mathbf{A}\mathbf{\Pi}\mathbf{\Lambda}_\mathbf{A}, \quad \tilde{\mathbf{B}} = \mathbf{B}\mathbf{\Pi}\mathbf{\Lambda}_\mathbf{B}, \quad \tilde{\mathbf{C}} = \mathbf{C}\mathbf{\Pi}\mathbf{\Lambda}_\mathbf{C}, \quad \text{and} \quad \mathbf{\Lambda}_\mathbf{A}\mathbf{\Lambda}_\mathbf{B}\mathbf{\Lambda}_\mathbf{C} = \mathbf{I}_R.$$

For brevity, we have dropped the “essential” part in the text. Similar to generic rank, we will further say that the CPD is *generically* unique if the uniqueness conditions hold with probability 1 for \mathbf{A} , \mathbf{B} and \mathbf{C} sampled at random from a continuous probability distribution.

Definition C.1.2 (generic uniqueness). [19, p. 1568] *Let μ be the Lebesgue measure on $\mathbb{C}^{I \times R} \times \mathbb{C}^{J \times R} \times \mathbb{C}^{K \times R}$. The CPD of a rank- R tensor $\in \mathbb{C}^{I \times J \times K}$ is generically unique if*

$$\mu \{(\mathbf{A}, \mathbf{B}, \mathbf{C}) \mid \text{the CPD } [\mathbf{A}, \mathbf{B}, \mathbf{C}] \text{ is not unique}\} = 0.$$

Definition C.1.3 (Kruskal rank). *The Kruskal rank $k_{\mathbf{A}}$ of a matrix \mathbf{A} is the largest number k such that any subset of k columns of \mathbf{A} is linearly independent.*

Evidently, we have that $k_{\mathbf{A}} \leq r_{\mathbf{A}}$, but the equality does not hold in general.

Example C.1.1. *Consider*

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \in \mathbb{C}^{2 \times 3},$$

which has $r_{\mathbf{A}} = 2$, but $k_{\mathbf{A}} = 1$.

Theorem C.1.1 contains a *necessary* uniqueness condition.

Theorem C.1.1. [37, p. 530] *Let $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ be a rank- R tensor ($R > 1$) that admits a CPD $\mathcal{X} = \llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket$, with $\mathbf{A} \in \mathbb{C}^{I \times R}$, $\mathbf{B} \in \mathbb{C}^{J \times R}$ and $\mathbf{C} \in \mathbb{C}^{K \times R}$, then it is necessary for uniqueness of \mathbf{A} , \mathbf{B} and \mathbf{C} that*

$$\begin{aligned} \min(r_{\mathbf{A} \odot \mathbf{B}}, r_{\mathbf{B} \odot \mathbf{C}}, r_{\mathbf{A} \odot \mathbf{C}}) &= R, \\ \min(k_{\mathbf{A}}, k_{\mathbf{B}}, k_{\mathbf{C}}) &\geq 2. \end{aligned}$$

Following are necessary and/or *sufficient* uniqueness conditions. Theorem C.1.2 repeats Theorem 2.2.1.

Theorem C.1.2 (two factor matrices have full column rank). [36, p. 530] *Let $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ admit a PD $\mathcal{X} = \llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket$, where $\mathbf{A} \in \mathbb{C}^{I \times R}$ and $\mathbf{B} \in \mathbb{C}^{J \times R}$ have full column rank, then $r_{\mathcal{X}} = R$ and the CPD of \mathcal{X} is unique iff $k_{\mathbf{C}} \geq 2$. Generically, this is satisfied if $R \leq \min(I, J)$ and $K \geq 2$.*

The proof of Theorem C.1.2 proves particularly insightful in Chapter 3. We shall not give a complete proof here, but we will instead validate the “if” (\Leftarrow) part¹ for $\mathcal{X} \in \mathbb{C}^{I \times J \times 2}$, where $R \leq \min(I, J)$. Generically, all matrices involved have rank R then. Write $\mathbf{D}_1 = \mathbf{D}_1(\mathbf{C})$ and $\mathbf{D}_2 = \mathbf{D}_2(\mathbf{C})$ for brevity and

$$\mathbf{X}_1 = \mathbf{A}\mathbf{D}_1\mathbf{B}^T \text{ and } \mathbf{X}_2 = \mathbf{A}\mathbf{D}_2\mathbf{B}^T \Leftrightarrow \begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{A}\mathbf{D}_1 \\ \mathbf{A}\mathbf{D}_2 \end{pmatrix} \mathbf{B}^T.$$

Using the SVD $\mathbf{U}\mathbf{S}\mathbf{V}^T = \begin{pmatrix} \mathbf{X}_1^T & \mathbf{X}_2^T \end{pmatrix}^T$, we have that there exists an invertible matrix $\mathbf{M} \in \mathbb{C}^{R \times R}$ such that

$$\mathbf{U} = \begin{pmatrix} \mathbf{U}_1 \\ \mathbf{U}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{A}\mathbf{D}_1 \\ \mathbf{A}\mathbf{D}_2 \end{pmatrix} \mathbf{M}.$$

Define

$$\mathbf{R}_1 \triangleq \mathbf{U}_1^T \mathbf{U}_1 = \mathbf{M}^T (\mathbf{A}\mathbf{D}_1)^T \mathbf{A}\mathbf{D}_1 \mathbf{M} \triangleq \mathbf{Q}\mathbf{D}_1 \mathbf{M},$$

¹The “only if” (\Rightarrow) part follows from Theorem C.1.1.

$$\mathbf{R}_2 \triangleq \mathbf{U}_1^T \mathbf{U}_2 = \mathbf{M}^T (\mathbf{A} \mathbf{D}_1)^T \mathbf{A} \mathbf{D}_2 \mathbf{M} \triangleq \mathbf{Q} \mathbf{D}_2 \mathbf{M},$$

then it follows that

$$(\mathbf{R}_1^{-1} \mathbf{R}_2) \mathbf{M}^{-1} = \mathbf{M}^{-1} \mathbf{D}_1^{-1} \mathbf{Q}^{-1} \mathbf{Q} \mathbf{D}_2 \mathbf{M} \mathbf{M}^{-1} = \mathbf{M}^{-1} (\mathbf{D}_1^{-1} \mathbf{D}_2),$$

where, w.l.o.g., it is assumed that the first row of \mathbf{C} has no zero element², such that \mathbf{D}_1 is invertible. \mathbf{M}^{-1} holds the eigenvectors of $\mathbf{R}_1^{-1} \mathbf{R}_2$ and $\mathbf{D}_1^{-1} \mathbf{D}_2$ holds the corresponding eigenvalues. If $k_{\mathbf{C}} \geq 2$, \mathbf{C} does not have collinear columns and the eigenvalues in $(\mathbf{D}_1(\mathbf{C}))^{-1} \mathbf{D}_2(\mathbf{C})$ are simple. We can then recover the eigenvectors in \mathbf{M}^{-1} up to permutation and scaling indeterminacies, from which the factor matrices follow. This reasoning shows that, if the conditions in Theorem C.1.2 are satisfied, the computation of the CPD reduces to a joint EVD [14].

Example C.1.2. Consider again the third-order tensor \mathcal{A} in Example B.1.1. In Example 2.2.1, a 3-term CPD for \mathcal{A} was given:

$$\mathcal{A} = \llbracket \mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \mathbf{U}^{(3)} \rrbracket$$

where

$$\mathbf{U}^{(1)} = \mathbf{I}_3, \quad \mathbf{U}^{(2)} = \mathbf{I}_3, \quad \mathbf{U}^{(3)} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 2 & 0 & -2 \end{pmatrix}.$$

Obviously, $\mathbf{A} = \mathbf{U}^{(1)}$ and $\mathbf{B} = \mathbf{U}^{(2)}$ have full column rank, and $k_{\mathbf{C}} = r_{\mathbf{C}} = 2$, so Theorem 2.2.1 guarantees that this CPD is unique.

Let $C_n^k = \binom{n}{k}$.

Definition C.1.4 (compound matrix). The k th compound matrix $\mathcal{C}_k(\mathbf{A}) \in \mathbb{C}^{C_I^k \times C_R^k}$ of $\mathbf{A} \in \mathbb{C}^{I \times R}$ is the matrix containing the determinants of all $k \times k$ submatrices of \mathbf{A} , arranged with the submatrix index sets in lexicographic order.

Definition C.1.5 defines conditions (Cm) and (Um) which depend on $m \in \mathbb{N}$.

Definition C.1.5. [18, p. 879] Let $\mathbf{A} \in \mathbb{C}^{I \times R}$, $\mathbf{B} \in \mathbb{C}^{J \times R}$ and $\mathbf{d} \in \mathbb{C}^R$.

$$\mathcal{C}_m(\mathbf{A}) \odot \mathcal{C}_m(\mathbf{B}) \text{ has full column rank;} \quad (\text{Cm})$$

$$\left\{ \begin{array}{l} r_{\mathbf{A} \text{Diag}(\mathbf{d}) \mathbf{B}^T} \leq m-1 \Leftrightarrow (\mathcal{C}_m(\mathbf{A}) \odot \mathcal{C}_m(\mathbf{B})) \hat{\mathbf{d}}^m = \mathbf{0} \\ \hat{\mathbf{d}}^m = \begin{pmatrix} d_1 \dots d_m & \dots & d_{R-m+1} \dots d_R \end{pmatrix}^T \in \mathbb{C}^{C_R^m} \end{array} \right. \Rightarrow \hat{\mathbf{d}}^m = \mathbf{0} \quad (\text{Um})$$

It is clear that (Cm) \Rightarrow (Um), i.e. (Um) is more relaxed.

²If the first row of \mathbf{C} has a zero element, we could consider $\mathbf{R}_2^{-1} \mathbf{R}_1$ instead. An entire zero column in \mathbf{C} is excluded if $k_{\mathbf{C}} \geq 2$.

Theorem C.1.3 (one factor matrix has full column rank (i)). [36, p. 530] Let $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ admit a PD $\mathcal{X} = \llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket$, where $\mathbf{C} \in \mathbb{C}^{K \times R}$ has full column rank, then $r_{\mathcal{X}} = R$ and the CPD of \mathcal{X} is unique iff condition (U2) is satisfied. Generically, this is satisfied iff $R \leq K$ and $R \leq (I-1)(J-1)$.

The uniqueness condition in Theorem C.1.3 might be hard to check. The easier-to-check uniqueness in Theorem C.1.4 is only sufficient.

Theorem C.1.4 (one factor matrix has full column rank (ii)). [10, p. 652] Let $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ admit a PD $\mathcal{X} = \llbracket \mathbf{A}, \mathbf{B}, \mathbf{C} \rrbracket$, where $\mathbf{C} \in \mathbb{C}^{K \times R}$ has full column rank, then $r_{\mathcal{X}} = R$ and the CPD of \mathcal{X} is unique if condition (C2) is satisfied. Generically, this is satisfied if $R \leq K$ and $\frac{R(R-1)}{2} \leq \frac{I(I-1)}{2} \frac{J(J-1)}{2}$.

Appendix D

Derivation of the Decomposition of the Null Space of the Macaulay Matrix as a BTD

This appendix contains a derivation of the result in Theorem 4.1.1. To develop insight, Section D.1 will first cover the univariate case, *i.e.* the case where the number of variables $n = 1$. Following is the multivariate case, which is essentially nothing but (a coupled version of) the univariate case — although the notation is somewhat more involved. Finally, Section D.2 will establish the desired result.

D.1 A Decomposition in rank- $(L_r, L_r, 1)$ terms

D.1.1 Univariate Case

Consider the univariate polynomial root-finding problem (like in Example 1.1.2)

$$f(x) = 0$$

where $f \in \mathcal{C}_m^1$. Let $x^{(k)}, 1 \leq k \leq m_0 = m$, be the disjoint roots of f with multiplicity $\mu_k = 1$. The null space of the coefficient “matrix” \mathbf{f}^T contains m Vandermonde-structured vectors. Let

$$\mathbf{V} = \begin{pmatrix} \mathbf{v}_1 & \dots & \mathbf{v}_m \end{pmatrix} \in \mathbb{C}^{(m+1) \times m}$$

be such a full Vandermonde basis for $\text{null}(\mathbf{f}^T)$, where

$$\mathbf{v}_k = (\mathbf{V})_k = \begin{pmatrix} 1 & x^{(k)} & \dots & x^{(k)m} \end{pmatrix}^T \in \mathbb{C}^{m+1}, \quad 1 \leq k \leq m,$$

is a Vandermonde vector. Let $\mathbf{K} \in \mathbb{C}^{(m+1) \times m}$ be a numerical basis related to \mathbf{V} by

$$\mathbf{K} = \mathbf{V}\mathbf{C}^T$$

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where \mathbf{C}^T is an invertible transformation matrix. By exploiting the multiplicative shift structure contained in the Vandermonde matrix \mathbf{V} , we obtain

$$\mathbf{Y}_{[1,2;3]} = \begin{pmatrix} \mathbf{K} \\ \mathbf{K} \end{pmatrix} = \begin{pmatrix} \mathbf{V} \\ \mathbf{V} \end{pmatrix} \mathbf{C}^T = (\mathbf{V}^{(2)} \odot \mathbf{V}) \mathbf{C}^T \in \mathbb{C}^{(2 \cdot m) \times m} \quad (\text{D.1})$$

where

$$\mathbf{V}^{(2)} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ x^{(1)} & x^{(2)} & \dots & x^{(m)} \end{pmatrix}.$$

(D.1) is (3.11) for the univariate polynomial equation¹, which is just the 1D HR model (2.13). Each $(\mathbf{V}^{(2)} \odot \mathbf{V})_k$ is a vectorized $(2 \times m)$ rank-1 Hankel matrix² — say \mathbf{H}_k . After reshaping (D.1) into a third-order tensor model, (D.1) can equivalently be seen as an m -term “rank-1 Hankel decomposition” of null (\mathbf{f}^T) :

$$\mathcal{Y} = \sum_{k=1}^m \mathbf{H}_k \otimes \mathbf{c}_k \in \mathbb{C}^{2 \times m \times m} \quad (\text{D.2})$$

where

$$\mathbf{H}_k = \begin{pmatrix} 1 & x^{(k)} & \dots & x^{(k)m-1} \\ x^{(k)} & x^{(k)2} & \dots & x^{(k)m} \end{pmatrix} \in \mathbb{C}^{2 \times m}, \quad 1 \leq k \leq m.$$

More generally, if $\mu_k \geq 1, 1 \leq k \leq m_0$, and that the number of disjoint roots $m_0 \leq m$, we have that $f(x^{(k)}) = f'(x^{(k)}) = \dots = f^{(\mu_k-1)}(x^{(k)}) = 0$, or equivalently,

$$\begin{aligned} \mathbf{f}^T \tilde{\mathbf{V}}_k &\triangleq \mathbf{f}^T \begin{pmatrix} \partial_0[\mathbf{v}_k] & \partial_1[\mathbf{v}_k] & \dots & \partial_{\mu_k-1}[\mathbf{v}_k] \end{pmatrix} \\ &= \mathbf{f}^T \begin{pmatrix} 1 & 0 & \dots & 0 \\ x^{(k)} & 1 & \dots & 0 \\ x^{(k)2} & 2x^{(k)} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ x^{(k)m} & 1! \binom{m}{1} x^{(k)m-1} & \dots & (\mu_k-1)! \binom{m}{\mu_k-1} x^{(k)m-\mu_k+1} \end{pmatrix} = \mathbf{0}^T, 1 \leq k \leq m_0. \end{aligned}$$

Bringing the $\tilde{\mathbf{V}}_k \in \mathbb{C}^{m \times \mu_k}$ together,

$$\tilde{\mathbf{V}} = \begin{pmatrix} \tilde{\mathbf{V}}_1 & \dots & \tilde{\mathbf{V}}_{m_0} \end{pmatrix} \in \mathbb{C}^{m \times m}$$

is a full “Vandermonde plus derivative” basis for null (\mathbf{f}^T) . We partition

$$\mathbf{C} = \begin{pmatrix} \mathbf{C}_1 & \dots & \mathbf{C}_{m_0} \end{pmatrix} \in \mathbb{C}^{m \times m}$$

¹See also Example 3.1.2.

²See also (2.11).

accordingly and we define $\mathbf{c}_{k,l} \triangleq (\mathbf{C}_k)_{l+1}$. The m -term “rank-1 Hankel decomposition” (D.2) changes to

$$\mathcal{Y} = \sum_{k=1}^{m_0} \sum_{l=0}^{\mu_k-1} \tilde{\mathbf{H}}_{k,l} \otimes \mathbf{c}_{k,l} \in \mathbb{C}^{I_1 \times I_2 \times m} \quad (\text{D.3})$$

where each $\tilde{\mathbf{H}}_{k,l} \in \mathbb{C}^{I_1 \times I_2}$ is the hankelization of $\partial_l[\mathbf{v}_k]$:

$$\tilde{\mathbf{H}}_{k,l} = \begin{pmatrix} l! \binom{0}{l} x^{(k)-l} & l! \binom{1}{l} x^{(k)1-l} & \dots & l! \binom{I_2-1}{l} x^{(k)I_2-1-l} \\ l! \binom{1}{l} x^{(k)1-l} & l! \binom{2}{l} x^{(k)2-l} & \dots & l! \binom{I_2}{l} x^{(k)I_2-l} \\ \vdots & \vdots & \ddots & \vdots \\ l! \binom{I_1-1}{l} x^{(k)I_1-1-l} & l! \binom{I_1}{l} x^{(k)I_1-l} & \dots & l! \binom{I_1+I_2-2}{l} x^{(k)I_1+I_2-l-2} \end{pmatrix} \in \mathbb{C}^{I_1 \times I_2},$$

$$0 \leq l \leq \mu_k - 1, \quad 1 \leq k \leq m,$$

and $x^{(k)\alpha} = 0$ if $\alpha < 0$. [25] shows that the Hankel matrix $\tilde{\mathbf{H}}_{k,l}$ has *exactly rank* $l+1$ and admits the factorization³

$$\tilde{\mathbf{H}}_{k,l} = \tilde{\mathbf{V}}_{k,l,I_1} \cdot \mathbf{G}_l \cdot \tilde{\mathbf{V}}_{k,l,I_2}^T$$

where $\mathbf{G}_l = \text{antidiag}(\mathbf{g}_l) \in \mathbb{C}^{(l+1) \times (l+1)}$ with $(\mathbf{g}_l)_s = \binom{l}{s-1}$, $1 \leq s \leq l+1$ ⁴, and where

$$\tilde{\mathbf{V}}_{k,l,I} = \begin{pmatrix} \left(\frac{d}{dx}\right)^0 1 & \left(\frac{d}{dx}\right)^1 1 & \dots & \left(\frac{d}{dx}\right)^l 1 \\ \left(\frac{d}{dx}\right)^0 x^1 & \left(\frac{d}{dx}\right)^1 x^1 & \dots & \left(\frac{d}{dx}\right)^l x^1 \\ \vdots & \vdots & \ddots & \vdots \\ \left(\frac{d}{dx}\right)^0 x^{I-1} & \left(\frac{d}{dx}\right)^1 x^{I-1} & \dots & \left(\frac{d}{dx}\right)^l x^{I-1} \end{pmatrix}_{x=x^{(k)}} \quad (\text{D.4})$$

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$$\begin{aligned} (\tilde{\mathbf{H}}_{k,l})_{i_1,i_2} &= \sum_{s=1}^{l+1} (\tilde{\mathbf{V}}_{k,l,I_1})_{i_1,s} (\mathbf{g}_l)_s (\tilde{\mathbf{V}}_{k,l,I_2})_{i_2,l-s+2} \\ &= \sum_{s=1}^{l+1} \left(\frac{d}{dx}\right)^{s-1} x^{i_1-1} \binom{l}{s-1} \left(\frac{d}{dx}\right)^{l-s+1} x^{i_2-1} \\ &= \sum_{s=1}^{l+1} (s-1)! \binom{i_1-1}{s-1} x^{i_1-s} \binom{l}{s-1} (l-s+1)! \binom{i_2-1}{l-s+1} x^{i_2-l+s-2} \\ &= l! x^{i_1+i_2-l-2} \sum_{s=0}^l \binom{i_1-1}{s} \binom{i_2-1}{l-s} \\ &= l! x^{i_1+i_2-l-2} \binom{i_1-1+i_2-1}{l} \end{aligned}$$

where the last equality is by the Chu-Vandermonde identity in combinatorics and where for brevity $x = x^{(k)}$.

⁴ \mathbf{G}_l is thus a square matrix of order $l+1$ with the l th row of Pascal’s triangle on its antidiagonal.

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is called a *confluent Vandermonde matrix* of order $l + 1$. Note that $\tilde{\mathbf{V}}_{k,l,m} = \tilde{\mathbf{V}}_k(:, 1 : l + 1)$.

It becomes clear now why we have silently replaced the (dimensions of the) $(2 \times m)$ Hankel matrix \mathbf{H}_k by the $(I_1 \times I_2)$ Hankel matrix $\tilde{\mathbf{H}}_{k,l}$ with $I_1 + I_2 = m + 2$: $\min(I_1, I_2) \geq \mu_k$, $1 \leq k \leq m_0$, is necessary for every $\tilde{\mathbf{H}}_{k,l}$ to effectively have rank $1 \leq l + 1 \leq \mu_k$ ⁵. (D.3) becomes

$$\mathcal{Y} = \sum_{k=1}^{m_0} \sum_{l=0}^{\mu_k-1} \mathbf{G}_l \cdot_1 \tilde{\mathbf{V}}_{k,l,I_1} \cdot_2 \tilde{\mathbf{V}}_{k,l,I_2} \cdot_3 \mathbf{c}_{k,l} \triangleq \sum_{r=1}^m \tilde{\mathbf{H}}_r \otimes \mathbf{c}_r \in \mathbb{C}^{I_1 \times I_2 \times m} \quad (\text{D.5})$$

which is an m -term BTB of \mathcal{Y} ⁶. If $\mu_k = 1$, $1 \leq k \leq m_0$, $\tilde{\mathbf{H}}_r = \tilde{\mathbf{H}}_{k,0} = \mathbf{H}_k$ is a rank-1 Hankel matrix again and the m -term BTB boils down to the m -term CPD (D.2).

Example D.1.1. Consider the univariate polynomial equation

$$f(x) = (x - \alpha)^2 = 0$$

of degree $m = 2$, but with $m_0 = 1$: f has one root $x^{(1)} = \alpha$ with multiplicity $\mu_1 = 2$. We can construct

$$\mathbf{Y}_{[1,2;3]} = \begin{pmatrix} \frac{\partial_0[\mathbf{v}_1]}{\partial_0[\mathbf{v}_1]} & \frac{\partial_1[\mathbf{v}_1]}{\partial_1[\mathbf{v}_1]} \end{pmatrix} \mathbf{C}^T = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \\ \alpha & 1 \\ \alpha^2 & 2\alpha \end{pmatrix} \mathbf{C}^T \in \mathbb{C}^{(2 \cdot 2) \times 2}$$

where $I_1 = I_2 = 2 \geq \mu_1$. \mathcal{Y} admits an $m = 2$ -term BTB (D.5) in rank- $(L_r, L_r, 1)$ terms with $1 \leq L_r = l + 1 \leq \mu_1 = 2$:

$$\begin{aligned} \mathcal{Y} &= 1 \cdot_1 \tilde{\mathbf{V}}_{1,1,2} \cdot_2 \tilde{\mathbf{V}}_{1,1,2} \cdot_3 \mathbf{c}_{1,1} + \mathbf{G}_1 \cdot_1 \tilde{\mathbf{V}}_{1,2,2} \cdot_2 \tilde{\mathbf{V}}_{1,2,2} \cdot_3 \mathbf{c}_{1,2} \\ &= \begin{pmatrix} 1 \\ \alpha \end{pmatrix} 1 \begin{pmatrix} 1 & \alpha \end{pmatrix} \otimes \mathbf{c}_1 + \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix}^T \otimes \mathbf{c}_2. \end{aligned} \quad (\text{D.6})$$

Uniqueness

Definition 2.2.7 introduces the BTB of a higher-order tensor, with the CPD and the MLSVD as particular cases. Another particular case is a decomposition of a third-order tensor $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ in a sum of rank- $(L_r, L_r, 1)$ terms:

$$\mathcal{X} = \sum_{r=1}^R \mathbf{E}_r \otimes \mathbf{c}_r \quad (\text{D.7})$$

where $\mathbf{E}_r \in \mathbb{C}^{I \times J}$ is a rank- r matrix and $\mathbf{c}_r \in \mathbb{C}^K$ is a nonzero vector, $1 \leq r \leq R$. Note the correspondence between the right-hand side of (D.5) and (D.7) now.

⁵Or: $\mathbf{V}^{(2)}$ is not sufficient if $\exists k : \mu_k > 2$.

⁶(D.5) is a BTB in so-called rank- $(L_r, L_r, 1)$ terms — see (D.7) and [12]. Note that $\tilde{\mathbf{H}}_{k,l}$ and $\tilde{\mathbf{H}}_r$ represent the same matrices, but in (D.5) they emphasize a decomposition in m rank- $(L_r, L_r, 1)$ terms.

Theorem D.1.1 (necessary uniqueness condition for (D.7)). [12, Theorem 2.4] Let $\mathcal{X} \in \mathbb{C}^{I \times J \times K}$ be a third-order tensor that admits a decomposition in rank- $(L_r, L_r, 1)$ terms of the form (D.7). Define $\mathbf{E}(\mathbf{w}) = \sum_{r=1}^R w_r \mathbf{E}_r$. Then it is necessary for essential uniqueness of decomposition (D.7) that for every \mathbf{w} with $\omega(\mathbf{w}) \geq 2$, we have that $r_{\mathbf{E}(\mathbf{w})} > \max_{r|w_r \neq 0} (L_r)$.

Corollary D.1.1. Let $\mathcal{Y} \in \mathbb{C}^{(I_1 \times I_2 \times m)}$ admit a decomposition in rank- $(L_r, L_r, 1)$ -terms of the form (D.5). If $\exists k : \mu_k > 1$, then this decomposition is not unique⁷.

Proof. If $\mu_k > 1$, we can without loss of generality take $\mathbf{E}_1 = \tilde{\mathbf{H}}_1 = \tilde{\mathbf{H}}_{k,0}$ ($L_1 = 1$) and $\mathbf{E}_2 = \tilde{\mathbf{H}}_2 = \tilde{\mathbf{H}}_{k,1}$ ($L_2 = 2$). Note that

$$\text{col}(\tilde{\mathbf{H}}_{k,0}) = \text{col}(\tilde{\mathbf{V}}_{k,0,I_1}) = \text{col}\left(\left(\tilde{\mathbf{V}}_{k,1,I_1}\right)_1\right) \subset \text{col}(\tilde{\mathbf{V}}_{k,1,I_1}) = \text{col}(\tilde{\mathbf{H}}_{k,1}).$$

If we then take $\mathbf{E}(\mathbf{w}) = w_1 \mathbf{E}_1 + w_2 \mathbf{E}_2 = 1 \cdot \mathbf{H}_{k,0} + 1 \cdot \mathbf{H}_{k,1}$, $\text{col}(\mathbf{E}(\mathbf{w})) = \text{col}(\tilde{\mathbf{H}}_{k,1})$ and $r_{\mathbf{E}(\mathbf{w})} = 2 \not> 2 = L_2 = \max\{L_1, L_2\}$, such that the decomposition cannot be unique per Theorem D.1.1. \square

The non-uniqueness stems from the fact that $\tilde{\mathbf{V}}_k$ is only unique *after* we impose the “Vandermonde plus derivative” structure: any other linear, but non-“Vandermonde plus derivative” combination of the $\{\partial_l[\mathbf{v}_k]\}_{l=0}^{\mu_k-1}$ would constitute an equally valid basis for the null space of the “matrix” \mathbf{f}^T ⁸.

D.1.2 Multivariate Case

Please, take a bird’s eye view on Section D.1.1 again. We have re-interpreted the spatial smoothing-based CPD (D.1) of null (\mathbf{f}^T) as a third-order tensor decomposition involving rank-1 Hankel matrices (D.2). If $\mu_k \geq 1$, the decomposition involves Hankel matrices of rank ≥ 1 or equivalently, it is a BTD involving confluent Vandermonde matrices (D.5). A similar line of reasoning applies in the multivariate case.

For this purpose, consider the multivariate set of n polynomial equations

$$\begin{cases} f_1(x_1, x_2, \dots, x_n) = 0 \\ \vdots \\ f_n(x_1, x_2, \dots, x_n) = 0 \end{cases}$$

where $f_i \in \mathcal{C}_{d_i}^n$, $1 \leq i \leq n$. First, let $\mathbf{x}^{(k)} = \left(x_1^{(k)} \ x_2^{(k)} \ \dots \ x_n^{(k)}\right)^T$, $1 \leq k \leq m_0 = m$, be its disjoint roots with multiplicity $\mu_k = 1$. $m = \prod_{i=1}^n d_i$ is the Bézout number

⁷Although the overall decomposition is not unique, one can employ part of the proof of [12, Theorem 2.4] to show that the root-revealing factor matrix $\mathbf{E}_1 = \tilde{\mathbf{V}}_{k,1,I}$ is uniquely determined.

⁸Section D.2 will suggest to combine the two terms in (D.6) into *one* block term to eliminate the non-uniqueness encountered in Corollary D.1.1 and to obtain a third-order generalization of the Jordan canonical form (Definition A.3.2) — see Example 4.1.4.

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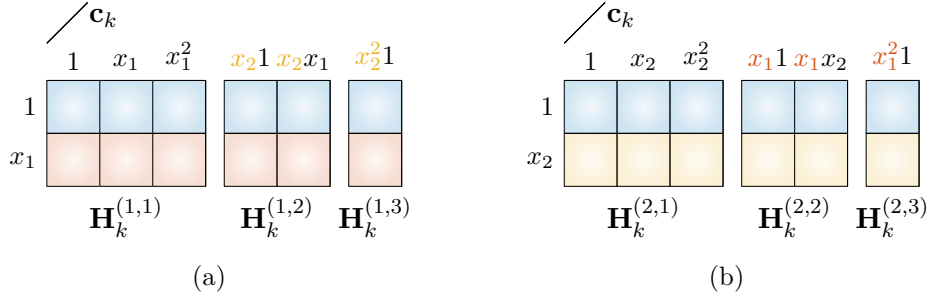


Figure D.1: The k th term in the third-order tensor $\mathcal{Y}^{(j)}$ (up to $\mathbf{P}^{(j)}$) in (D.9) with $n = 2$, $d = 3$, (a) $j = 1$ and (b) $j = 2$.

of the system. The null space of its Macaulay matrix $\mathbf{M}(d)$ contains m multivariate Vandermonde vectors. Let

$$\mathbf{V} = \begin{pmatrix} \mathbf{v}_1 & \dots & \mathbf{v}_m \end{pmatrix} \in \mathbb{C}^{q(d) \times m}$$

be such a multivariate Vandermonde basis for $\text{null}(\mathbf{M}(d))$ where

$$\mathbf{v}_k = \left(1 \quad x_1^{(k)} \quad x_2^{(k)} \quad \dots \quad x_1^{(k)2} \quad x_1^{(k)}x_2^{(k)} \quad \dots \quad x_{n-1}^{(k)}x_n^{(k)d-1} \quad x_n^{(k)d} \right)^T \in \mathbb{C}^{q(d)}$$

is a multivariate Vandermonde vector with its entries ordered by the degree negative lexicographic order. Once more, we use \mathbf{K} for a numerical basis related to \mathbf{V} via \mathbf{C} . By exploiting the multiplicative shift structure contained in the j th variable in \mathbf{V} , we obtain (3.8):

$$\mathbf{Y}^{(j)} = \begin{pmatrix} \underline{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)} \mathbf{K} \\ \overline{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)} \mathbf{K} \end{pmatrix} = \left(\mathbf{V}^{(2,j)} \odot \mathbf{B}(d-1) \right) \mathbf{C}^T \in \mathbb{C}^{(2 \cdot q(d-1)) \times m}, \quad 1 \leq j \leq n, \quad (\text{D.8})$$

where

$$\mathbf{V}^{(2,j)} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ x_j^{(1)} & x_j^{(2)} & \dots & x_j^{(m)} \end{pmatrix} \quad \text{and} \quad \mathbf{B}(d-1) = \mathbf{V}(d-1).$$

Due to a multivariate Vandermonde rather than a genuine Vandermonde structure in \mathbf{v}_k , $\left(\mathbf{V}^{(2,j)} \odot \mathbf{B}(d-1) \right)_k$ is *no longer* a vectorized Hankel matrix. However, its matricization can be reordered and partitioned into several horizontally stacked Hankel matrices: one for each unique monomial combination of the other variables (Fig. D.1). Reshaping (D.8) into a third-order tensor yields the “horizontally stacked rank-1 Hankel decomposition”

$$\begin{aligned} \mathcal{Y}^{(j)} &= \sum_{k=1}^m \mathbf{H}_k^{(j)} \otimes \mathbf{c}_k \\ &= \sum_{k=1}^m \begin{pmatrix} \mathbf{H}_k^{(j,1)} & \mathbf{H}_k^{(j,2)} & \dots & \mathbf{H}_k^{(j, \binom{n+d-2}{n-1})} \end{pmatrix} \mathbf{P}^{(j)} \otimes \mathbf{c}_k \in \mathbb{C}^{2 \times q(d-1) \times m} \quad (\text{D.9}) \end{aligned}$$

where $\mathbf{P}^{(j)} \in \mathbb{C}^{q(d-1) \times q(d-1)}$ is a column permutation matrix that mixes the columns of the $\mathbf{H}_k^{(j)}$ such that they are ordered by the degree negative lexicographic order. Each $\mathbf{H}_k^{(j,p)}$ is a (scaled) rank-1 Hankel matrix (Fig. D.1):

$$\mathbf{H}_k^{(j,p)} = \mathbf{x}^{(k)\alpha_p} \begin{pmatrix} 1 & x_j^{(k)} & \cdots & x_j^{(k)d-p} \\ x_j^{(k)} & x_j^{(k)2} & \cdots & x_j^{(k)d-p+1} \end{pmatrix} \in \mathbb{C}^{2 \times (d-p+1)}$$

where $\alpha_p(j) = 0, \quad 1 \leq p \leq \binom{n+d-2}{n-1} \quad \text{and} \quad 1 \leq k \leq m.$

More generally, if $\mu_k \geq 1, 1 \leq k \leq m_0$, and that the number of disjoint roots $m_0 \leq m$, multivariate Vandermonde vectors as well as their derivatives are needed in a basis for the null space of the Macaulay matrix:

$$\mathbf{M}(d) \begin{pmatrix} \partial_{\mathbf{j}_{k,0}}[\mathbf{v}_k] & \partial_{\mathbf{j}_{k,1}}[\mathbf{v}_k] & \cdots & \partial_{\mathbf{j}_{k,\mu_k-1}}[\mathbf{v}_k] \end{pmatrix} \triangleq \mathbf{M}(d)\tilde{\mathbf{V}}_k = \mathbf{0}.$$

The differential functionals defined by $\{\mathbf{j}_{k,l}\}_{l=0}^{\mu_k-1} \subset \mathbb{N}^n$ are called the *multiplicity structure* of the root $\mathbf{x}^{(k)}$. Recall from Section 4.1 that this multiplicity structure is not unique, but only determined up to a linear transformation. The multiplicity structure can imply a different multiplicity in each variable. To decouple the multivariate case to the well-understood univariate case, define the multiplicity $\mu_k^{(j)}$ of the root $\mathbf{x}^{(k)}$ in x_j as

$$\mu_k^{(j)} \triangleq \max_{0 \leq l \leq \mu_k-1} \mathbf{j}_{k,l}(j)^9 + 1 \leq \mu_k.$$

Example D.1.2. [24, Example 7] Consider the system of $s = 2$ polynomial equations in $n = 2$ variables

$$\begin{cases} f_1(x_1, x_2) = (x_2 - 2)^2 = 0 \\ f_2(x_1, x_2) = (x_1 - x_2 + 1)^2 = 0 \end{cases}$$

where $d_1 = d_2 = 2$, so $d^* = d_1 + d_2 - n = 2$ and $m = d_1 \cdot d_2 = 4$, but $m_0 = 1$: the system has one (affine) root $\mathbf{x}^{(1)} = \begin{pmatrix} 1 & 2 \end{pmatrix}^T$ with multiplicity $\mu_1 = 4$. It can be verified that a (possible) basis for $\text{null}(\mathbf{M}(d^*)) = \text{null}(\mathbf{M}(2))$ is defined by the following (non-unique) multiplicity structure of the root $\mathbf{x}^{(1)}$:

$$\tilde{\mathbf{V}}_1 = \begin{pmatrix} \partial_{\mathbf{j}_{1,0}}[\mathbf{v}_1] & \partial_{\mathbf{j}_{1,1}}[\mathbf{v}_1] & \partial_{\mathbf{j}_{1,2}}[\mathbf{v}_1] & \partial_{\mathbf{j}_{1,3}}[\mathbf{v}_1] \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ x_1^{(1)} & 1 & 0 & 0 \\ x_2^{(1)} & 0 & 1 & 0 \\ x_1^{(1)2} & 2x_1^{(1)} & 0 & 2 \\ x_1^{(1)}x_2^{(1)} & x_2^{(1)} & x_1^{(1)} & 1 \\ x_2^{(1)2} & 0 & 2x_2^{(1)} & 0 \end{pmatrix}.$$

⁹To be precise, $\mathbf{j}_{k,l}(j)$ is the maximal derivative in x_j occurring in $\mathbf{j}_{k,l}$, e.g., $\mathbf{j}_{1,3}(1) = 2$ in Example D.1.2.

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We have that $\mathbf{x}^{(1)}$ has multiplicity

$$\mu_1^{(1)} = \max_{0 \leq l \leq 3} \mathbf{j}_{1,l}(1) + 1 = \max \{0, 1, 0, 2\} + 1 = 2 + 1 = 3,$$

in x_1 , but multiplicity

$$\mu_1^{(2)} = \max_{0 \leq l \leq 3} \mathbf{j}_{1,l}(2) + 1 = \max \{0, 0, 1, 1\} + 1 = 1 + 1 = 2$$

in x_2 .

Like (D.2) changes to (D.3) in the univariate case when $\mu_k \geq 1$, the m -term “horizontally stacked rank-1 Hankel decompositions” (D.9) change to

$$\begin{aligned} \mathcal{Y}^{(j)} &= \sum_{k=1}^{m_0} \sum_{l=0}^{\mu_k-1} \tilde{\mathbf{H}}_{k,l}^{(j)} \otimes \mathbf{c}_{k,l} \\ &= \sum_{k=1}^{m_0} \sum_{l=0}^{\mu_k-1} \begin{pmatrix} \tilde{\mathbf{H}}_{k,l}^{(j,1)} & \tilde{\mathbf{H}}_{k,l}^{(j,2)} & \dots & \tilde{\mathbf{H}}_{k,l}^{(j, \binom{n+d-2}{n-1})} \end{pmatrix} \mathbf{P}^{(j)} \otimes \mathbf{c}_{k,l} \in \mathbb{C}^{I_1^{(j)} \times I_2^{(j)} \times m} \quad (\text{D.10}) \end{aligned}$$

where $\tilde{\mathbf{H}}_{k,l}^{(j)}$ is the hankelization that corresponds to $\partial_{\mathbf{j}_{k,l}}[\mathbf{v}_k]$. Because each Hankel matrix $\tilde{\mathbf{H}}_{k,l}^{(j,p)}$ in (D.10) is (a scaled) $\tilde{\mathbf{H}}_{k,l}$ in (D.3), each $\tilde{\mathbf{H}}_{k,l}^{(j,p)}$ has rank

$$r_{\tilde{\mathbf{H}}_{k,l}^{(j,p)}} = \min(\mathbf{j}_{k,l}(j) + 1, d - I_1^{(j)} - p + 3)^{10}$$

and each $\tilde{\mathbf{H}}_{k,l}^{(j,p)}$ admits a factorization involving confluent Vandermonde matrices $\tilde{\mathbf{V}}_{k,l,I}^{(j)}$ of order $r_{\tilde{\mathbf{H}}_{k,l}^{(j,p)}} \geq 1$ as defined in (D.4) — but where x needs to be replaced by x_j . After stacking the $\tilde{\mathbf{H}}_{k,l}^{(j,p)}$ together,

$$\tilde{\mathbf{H}}_{k,l}^{(j)} = \begin{pmatrix} \tilde{\mathbf{H}}_{k,l}^{(j,1)} & \tilde{\mathbf{H}}_{k,l}^{(j,2)} & \dots & \tilde{\mathbf{H}}_{k,l}^{(j, \binom{n+d-2}{n-1})} \end{pmatrix} \mathbf{P}^{(j)} \in \mathbb{C}^{I_1^{(j)} \times I_2^{(j)}}$$

has rank $r_{\tilde{\mathbf{H}}_{k,l}^{(j)}} = \mathbf{j}_{k,l}(j) + 1$ and admits a factorization involving a genuine confluent Vandermonde matrix of order $r_{\tilde{\mathbf{H}}_{k,l}^{(j)}}$ in its first mode and a “monomially rescaled, stacked and permuted multivariate confluent Vandermonde” matrix in its second mode¹¹. Note that we have once more replaced the (dimensions of the) $(2 \times q(d-1))$ Hankel matrix $\mathbf{H}_k^{(j)}$ by the $(I_1^{(j)} \times I_2^{(j)})$ Hankel matrix $\tilde{\mathbf{H}}_{k,l}^{(j)}$ with $I_2^{(j)} = q(d - I_1^{(j)} + 1)$: $\min(I_1^{(j)}, I_2^{(j)}) \geq \mu_k^{(j)}$ is necessary to effectively have

$$r_{\tilde{\mathbf{H}}_{k,l}^{(j)}} = \mathbf{j}_{k,l}(j) + 1 \leq \mu_k^{(j)}, \quad 0 \leq l \leq \mu_k - 1, \quad 1 \leq k \leq m_0^{12}.$$

¹⁰See Example D.1.3.

¹¹See Example D.1.4.

¹²Or: $\bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)}$ is not sufficient if $\exists k' : \mu_{k'}^{(j)} > 2$. $\bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)}$ is sufficient if $\forall k : \mu_k^{(j)} \leq 2$ and taken strictly, *no* spatial smoothing with $\bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(j)}$ is required if $\forall k : \mu_k^{(j)} = 1$, but this would not be very meaningful.

Example D.1.3. Consider the system in Example D.1.2 with $m = 4$ and with $m_0 = 1$ root with multiplicity $\mu_1 = 4$ again. Appending extra rows to $\tilde{\mathbf{V}}_1(2)$ yields the basis $\tilde{\mathbf{V}}_1(4)$.

From (D.10), we have that

$$\mathcal{Y}^{(1)} = \sum_{l=0}^{\mu_1-1} \tilde{\mathbf{H}}_{1,l}^{(1)} \otimes \mathbf{c}_{1,l}$$

where $\tilde{\mathbf{H}}_{1,0}^{(1)}$, $\tilde{\mathbf{H}}_{1,1}^{(1)}$, $\tilde{\mathbf{H}}_{1,2}^{(1)}$ and $\tilde{\mathbf{H}}_{1,3}^{(1)}$ correspond to $\partial_{00}[\mathbf{v}_1]$, $\partial_{10}[\mathbf{v}_1]$, $\partial_{01}[\mathbf{v}_1]$ and $(\partial_{20} + \partial_{11})[\mathbf{v}_1]$ and have rank 1, 2, 1 and 3 respectively:

$$\begin{aligned} \tilde{\mathbf{H}}_{1,0}^{(1)} &= \left(\begin{array}{ccc|ccc} 1 & x_1 & x_1^2 & x_2 & x_1x_2 & x_2^2 \\ x_1 & x_1^2 & x_1^3 & x_1x_2 & x_1^2x_2 & x_1x_2^2 \\ x_1^2 & x_1^3 & x_1^4 & x_1^2x_2 & x_1^3x_2 & x_1^2x_2^2 \end{array} \right) \mathbf{P}^{(1)}, \\ \tilde{\mathbf{H}}_{1,1}^{(1)} &= \left(\begin{array}{ccc|ccc} 0 & 1 & 2x_1 & 0 & x_2 & 0 \\ 1 & 2x_1 & 3x_1^2 & x_2 & 2x_1x_2 & x_2^2 \\ 2x_1 & 3x_1^2 & 4x_1^3 & 2x_1x_2 & 3x_1^2x_2 & 2x_1x_2^2 \end{array} \right) \mathbf{P}^{(1)}, \\ \tilde{\mathbf{H}}_{1,2}^{(1)} &= \left(\begin{array}{ccc|cc|c} 0 & 0 & 0 & 1 & x_1 & 2x_2 \\ 0 & 0 & 0 & x_1 & x_1^2 & 2x_1x_2 \\ 0 & 0 & 0 & x_1^2 & x_1^3 & 2x_1^2x_2 \end{array} \right) \mathbf{P}^{(1)} \end{aligned}$$

and

$$\begin{aligned} \tilde{\mathbf{H}}_{1,3}^{(1)} &= \left(\begin{array}{ccc|cc|c} 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 2 & 6x_1 & 0 & 2x_2 & 0 \\ 2 & 6x_1 & 12x_1^2 & 2x_2 & 6x_1x_2 & 2x_2^2 \end{array} \right) \mathbf{P}^{(1)} \\ &\quad + \left(\begin{array}{ccc|cc|c} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 2x_1 & 2x_2 \\ 0 & 0 & 0 & 2x_1 & 3x_1^2 & 4x_1x_2 \end{array} \right) \mathbf{P}^{(1)}. \end{aligned}$$

$x_j = x_j^{(1)}$ for brevity. Note that we have taken $d = 4$, $I_1^{(1)} = 3$ and $I_2^{(1)} = q(2) = q(d - I_1^{(1)} + 1) = q(4 - 3 + 1)$, such that $r_{\tilde{\mathbf{H}}_{1,3}^{(1)}} = \mu_1^{(1)} = 3 \leq \min(I_1^{(1)}, I_2^{(1)})$. It becomes clear that the rank of each block $\tilde{\mathbf{H}}_{1,l}^{(1,p)}$ is bounded by $d - I_1^{(1)} - p + 3$, e.g., $r_{\tilde{\mathbf{H}}_{1,l}^{(1,3)}} = 4 - 3 - 3 + 3 = 1, \forall l \in \{0, 1, 2, 3\}$.

We can construct $\mathcal{Y}^{(2)}$ in a completely analogous way, but then $I_1^{(2)} = 2$ suffices to have $r_{\tilde{\mathbf{H}}_{1,1}^{(2)}} = r_{\tilde{\mathbf{H}}_{1,3}^{(2)}} = \mu_1^{(2)} = 2 \leq I_1^{(2)} = 2$. We can now take $d = 3$ and $I_2^{(2)} = q(2)$.

Using the factorization in confluent Vandermonde matrices, (D.10) becomes an m -term BTD in rank- $(L_r, L_r, 1)$ terms:

$$\mathcal{Y}^{(j)} = \sum_{k=1}^{m_0} \sum_{l=0}^{\mu_k-1} \mathbf{G}_{k,l}^{(j)} \cdot_1 \tilde{\mathbf{V}}_{k,l,I_1^{(j)}}^{(j)} \cdot_2 \tilde{\mathbf{V}}_{k,l,I_2^{(j)}}^{(j)} \cdot_3 \mathbf{c}_{k,l} \triangleq \sum_{r=1}^m \tilde{\mathbf{H}}_r^{(j)} \otimes \mathbf{c}_r \in \mathbb{C}^{I_1^{(j)} \times I_2^{(j)} \times m} \quad (\text{D.11})$$

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in which $\mathbf{G}_{k,l}^{(j)}$ is a square matrix of order $r_{\tilde{\mathbf{H}}_{k,l}^{(j)}} = \mathbf{j}_{k,l}(j) + 1$ with binomial coefficients on its antidiagonal. $\tilde{\mathbf{V}}_{k,l,I_1^{(j)}}^{(j)}$ is a genuine Vandermonde matrix and $\tilde{\mathbf{V}}_{k,l,I_2^{(j)}}^{(j)}$ is a “monomially rescaled, stacked and permuted multivariate confluent Vandermonde” matrix. Note that $\tilde{\mathbf{H}}_{k,l}^{(j)}$ and $\tilde{\mathbf{H}}_r^{(j)}$ are the same, but (D.11) emphasizes the decomposition in m rank- $(L_r, L_r, 1)$ terms.

Example D.1.4. Consider the system in Example D.1.2 again. From (D.11), we have that $\mathcal{Y}^{(1)} \in \mathbb{C}^{3 \times q(2) \times m}$ admits an $m = 4$ -term BTD in rank- $(L_r, L_r, 1)$ terms with $1 \leq L_r = r_{\tilde{\mathbf{H}}_{1,r-1}^{(1)}} = \mathbf{j}_{1,r-1}(1) + 1 \leq \mu_1^{(1)} = 3$ and with $\mathbf{c}_r = \mathbf{c}_{1,r-1}$, $1 \leq r \leq 4$:

$$\mathcal{Y}^{(1)} = \sum_{r=1}^m \tilde{\mathbf{H}}_r^{(1)} \otimes \mathbf{c}_r \quad (\text{D.12})$$

in which

$$\begin{aligned} \tilde{\mathbf{H}}_1^{(1)} &= \begin{pmatrix} 1 \\ x_1 \\ x_1^2 \end{pmatrix} 1 \left(1 \mid x_1 \quad x_2 \mid x_1^2 \quad x_1 x_2 \quad x_2^2 \right), \\ \tilde{\mathbf{H}}_2^{(1)} &= \begin{pmatrix} 1 & 0 \\ x_1 & 1 \\ x_1^2 & 2x_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \mid x_1 \quad x_2 \mid x_1^2 \quad x_1 x_2 \quad x_2^2 \\ 0 \mid 1 \quad 0 \mid 2x_1 \quad x_2 \quad 0 \end{pmatrix}, \\ \tilde{\mathbf{H}}_3^{(1)} &= \begin{pmatrix} 1 \\ x_1 \\ x_1^2 \end{pmatrix} 1 \left(0 \mid 0 \quad 1 \mid 0 \quad x_1 \quad 2x_2 \right) \end{aligned}$$

and

$$\begin{aligned} \tilde{\mathbf{H}}_4^{(1)} &= \begin{pmatrix} 1 & 0 & 0 \\ x_1 & 1 & 0 \\ x_1^2 & 2x_1 & 2 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \mid x_1 \quad x_2 \mid x_1^2 \quad x_1 x_2 \quad x_2^2 \\ 0 \mid 1 \quad 0 \mid 2x_1 \quad x_2 \quad 0 \\ 0 \mid 0 \quad 0 \mid 2 \quad 0 \quad 0 \end{pmatrix} \\ &\quad + \begin{pmatrix} 1 & 0 \\ x_1 & 1 \\ x_1^2 & 2x_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \mid 0 \quad 1 \mid 0 \quad x_1 \quad 2x_2 \\ 0 \mid 0 \quad 0 \mid 0 \quad 1 \quad 0 \end{pmatrix}. \end{aligned}$$

For brevity $x_j = x_j^{(1)}$ again. The “monomially rescaled, stacked and permuted confluent multivariate Vandermonde” matrices in the second mode are in fact simply the columns of $\tilde{\mathbf{V}}_1(2)$ in Example D.1.2.

Similarly, $\mathcal{Y}^{(2)} \in \mathbb{C}^{2 \times q(2) \times m}$ from Example D.1.4 admits an $m = 4$ -term BTD in rank- $(L_r, L_r, 1)$ terms with $L_r = \mathbf{j}_{1,r-1}(2) + 1 \leq \mu_1^{(2)} = 2$:

$$\mathcal{Y}^{(2)} = \sum_{r=1}^m \tilde{\mathbf{H}}_r^{(2)} \otimes \mathbf{c}_r \quad (\text{D.13})$$

in which

$$\tilde{\mathbf{H}}_1^{(2)} = \begin{pmatrix} 1 \\ x_2 \end{pmatrix} 1 \left(\begin{array}{c|cc} 1 & x_1 & x_2 \\ \hline x_1^2 & x_1 x_2 & x_2^2 \end{array} \right),$$

$$\tilde{\mathbf{H}}_2^{(2)} = \begin{pmatrix} 1 \\ x_2 \end{pmatrix} 1 \left(\begin{array}{c|cc} 0 & 1 & 0 \\ \hline 2x_1 & x_2 & 0 \end{array} \right),$$

$$\tilde{\mathbf{H}}_3^{(2)} = \begin{pmatrix} 1 & 0 \\ x_2 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & x_1 & x_2 & x_1^2 & x_1 x_2 & x_2^2 \\ 0 & 0 & 1 & 0 & x_1 & 2x_2 \end{pmatrix}$$

and

$$\begin{aligned} \tilde{\mathbf{H}}_4^{(2)} = & \begin{pmatrix} 1 \\ x_2 \end{pmatrix} 1 \left(\begin{array}{c|ccc} 0 & 0 & 0 & 2 \\ \hline 0 & 0 & 0 & 0 \end{array} \right) \\ & + \begin{pmatrix} 1 & 0 \\ x_2 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 2x_1 & x_2 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \end{aligned}$$

The matrices in the second mode comprise again the columns of $\tilde{\mathbf{V}}_1(2)$.

It appears in Example D.1.4 that the $\{\mathcal{Y}^{(j)}\}_{j=1}^n$ in (D.12) and (D.13) have quite a lot in common. They do not only have their third factor matrix \mathbf{C} , but also their second factor matrices $\tilde{\mathbf{V}}_{k,l,I_2}^{(j)}$ and their first slice $\mathcal{Y}^{(j)}(1, :, :)$ in common. Like in Chapter 3, we could combine them along their first mode into one third-order tensor — say \mathcal{Y} .

We need to ensure common dimensions in the second mode first. Define

$$I_2 \triangleq \max \left(\max_{1 \leq j \leq n} I_2^{(j)}, q(d^* - \max_{1 \leq j \leq n} I_1^{(j)} + 1) \right)$$

and put every $I_2^{(j)} = I_2$, such that every $\tilde{\mathbf{V}}_{k,l,I_2}^{(j)} = \tilde{\mathbf{V}}'_{k,l,I_2}, 1 \leq j \leq n$.

Second, define the *total* multiplicity $\mu_{k,l}$ in $(\tilde{\mathbf{V}}_k)_{l+1} = \partial_{\mathbf{j}_{k,l}}[\mathbf{v}_k]$ over all variables as

$$\mu_{k,l} \triangleq \sum_{j=1}^n \mathbf{j}_{k,l}(j) + 1 \leq \mu_k.$$

As Example D.1.5 shows, we are now ready to combine (D.11) for $1 \leq j \leq n$ into one third-order tensor \mathcal{Y} and to remove the redundant slices to obtain a “simultaneous” m -term BTD in rank- $(L_r, L_r, 1)$ terms:

$$\mathcal{Y} = \sum_{k=1}^{m_0} \sum_{l=0}^{\mu_k-1} \mathbf{G}_{k,l} \cdot_1 \tilde{\mathbf{V}}_{k,l,I_1} \cdot_2 \tilde{\mathbf{V}}'_{k,l,I_2} \cdot_3 \mathbf{c}_{k,l} \triangleq \sum_{r=1}^m \tilde{\mathbf{H}}_r \otimes \mathbf{c}_r \in \mathbb{C}^{I_1 \times I_2 \times m} \quad (\text{D.14})$$

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in which $\mathbf{G}_{k,l} \in \mathbb{C}^{\mu_{k,l} \times \mu_{k,l}}$, $\tilde{\mathbf{V}}_{k,l,I_1} \in \mathbb{C}^{I_1 \times \mu_{k,l}}$ equals

$$\left(\begin{array}{c|ccc} 1 & \mathbf{0}_{1 \times \mathbf{j}_{k,l}(1)} & \mathbf{0}_{1 \times \mathbf{j}_{k,l}(2)} & \dots & \mathbf{0}_{1 \times \mathbf{j}_{k,l}(n)} \\ \hline x_{1,k} & 1! \binom{1}{1} 1 & 0 & \dots & 0 \\ x_{1,k}^2 & 1! \binom{2}{1} x_{1,k} & 2! \binom{2}{2} & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ x_{1,k}^{I_1^{(1)}-1} & 1! \binom{I_1^{(1)}-1}{1} x_{1,k}^{I_1^{(1)}-2} & \dots & & \dots \\ \hline x_{2,k} & \mathbf{0}_{1 \times \mathbf{j}_{k,l}(1)} & 1! \binom{1}{1} 1 & \dots & \mathbf{0}_{1 \times \mathbf{j}_{k,l}(n)} \\ \vdots & \vdots & \vdots & & \vdots \\ \vdots & \vdots & \vdots & & \vdots \\ \vdots & \vdots & \vdots & & \vdots \\ x_{1,k}^{I_1^{(n)}-1} & \mathbf{0}_{1 \times \mathbf{j}_{k,l}(1)} & \mathbf{0}_{1 \times \mathbf{j}_{k,l}(2)} & \dots & (\mathbf{j}_{k,l}(n))! \binom{I_1^{(n)}-1}{\mathbf{j}_{k,l}(n)} x_{n,k}^{I_1^{(n)}-1-\mathbf{j}_{k,l}(n)} \end{array} \right)$$

and $I_1 = \sum_{j=1}^n I_1^{(j)} - n + 1$. (D.14) is the generalization of (D.5) in the univariate case.

Example D.1.5. Consider the decompositions in Example D.1.4 of the system in Example D.1.2 again. Take $I_1 = I_1^{(1)} + I_1^{(2)} - n + 1 = 3 + 2 - 2 + 1 = 4$ and take $I_2 = \max(\max_{1 \leq j \leq 2} I_2^{(j)}, q(d^* - I_1^{(1)} + 1)) = \max(q(2), q(0)) = q(2) = 6$. We can combine (D.12) and (D.13) into a third-order tensor \mathcal{Y} that admits an $m = 4$ -term BTB in rank- $(L_r, L_r, 1)$ terms with $1 \leq L_r = \mu_{1,r-1} \leq \mu_1 = 4$:

$$\mathcal{Y} = \sum_{r=1}^m \tilde{\mathbf{H}}_r \otimes \mathbf{c}_r \quad (\text{D.15})$$

in which

$$\begin{aligned} \tilde{\mathbf{H}}_1 &= \left(\begin{array}{c|c} 1 & \\ \hline x_1 & \\ x_1^2 & \\ \hline x_2 & \end{array} \right) 1 \left(\begin{array}{c|cc|cc} 1 & x_1 & x_2 & x_1^2 & x_1 x_2 & x_2^2 \end{array} \right), \\ \tilde{\mathbf{H}}_2 &= \left(\begin{array}{c|c} 1 & \mathbf{0} \\ \hline x_1 & 1 \\ x_1^2 & 2x_1 \\ \hline x_2 & \mathbf{0} \end{array} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left(\begin{array}{c|cc|cc} 1 & x_1 & x_2 & x_1^2 & x_1 x_2 & x_2^2 \\ \hline 0 & 1 & 0 & 2x_1 & x_2 & 0 \end{array} \right), \\ \tilde{\mathbf{H}}_3 &= \left(\begin{array}{c|c} 1 & \mathbf{0} \\ \hline x_1 & \mathbf{0} \\ x_1^2 & \mathbf{0} \\ \hline x_2 & 1 \end{array} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left(\begin{array}{c|cc|cc} 1 & x_1 & x_2 & x_1^2 & x_1 x_2 & x_2 \\ \hline 0 & 0 & 1 & 0 & x_1 & 2x_2 \end{array} \right) \end{aligned}$$

and

$$\begin{aligned} \tilde{\mathbf{H}}_4 = & \left(\begin{array}{c|cc} 1 & 0 & 0 \\ \hline x_1 & 1 & 0 \\ x_1^2 & 2x_1 & 2 \\ \hline x_2 & 0 & 0 \end{array} \right) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & x_1 & x_2 & x_1^2 & x_1x_2 & x_2^2 \\ \hline 0 & 1 & 0 & 2x_1 & x_2 & 0 \\ \hline 0 & 0 & 0 & 2 & 0 & 0 \end{pmatrix} \\ & + \left(\begin{array}{c|cc} 1 & 0 & 0 \\ \hline x_1 & 1 & 0 \\ x_1^2 & 2x_1 & 0 \\ \hline x_2 & 0 & 1 \end{array} \right) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 2x_1 & x_2 & 0 \\ \hline 0 & 0 & 1 & 0 & x_1 & 2x_2 \\ \hline 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \end{aligned}$$

Once more, $x_j = x_j^{(1)}$ for brevity.

If $\mu_k = 1, 1 \leq k \leq m_0$, and $I^{(j)} = 2$ (> 1 for meaningful spatial smoothing), $\tilde{\mathbf{H}}_r = \tilde{\mathbf{H}}_{k,0}$ is a rank-1 Hankel matrix and the m -term BTB boils down to the m -term CPD (3.11).

Uniqueness

Although we will not derive it here, a similar result as in Corollary D.1.1 can be obtained for (D.14). The non-uniqueness of decomposition (D.14) stems from the non-uniqueness of the multiplicity structure of the roots.

D.2 A Block Term Decomposition

The m -term BTB in rank- $(L_r, L_r, 1)$ terms (D.14) from Section D.1 proves insightful, but it is not unique. One combination step remains. Indeed, we can combine the μ_k rank- $(\mu_{k,l}, \mu_{k,l}, 1)$ terms ($\mu_{k,l} \leq \mu_k$) that together correspond to a disjoint root $\mathbf{x}^{(k)}$. We rewrite the BTB for \mathcal{Y} in (D.14) as follows:

$$\mathcal{Y} = \sum_{k=1}^{m_0} \mathcal{G}_k \cdot_1 \mathbf{A}_{k,I_1} \cdot_2 \mathbf{B}_{k,I_2} \cdot_3 \mathbf{C}_k \in \mathbb{C}^{I_1 \times I_2 \times m} \quad (\text{D.16})$$

in which $\mathbf{A}_{k,I_1} \in \mathbb{C}^{I_1 \times \mu_k}$ equals

$$\left(\begin{array}{c|cccc} 1 & \mathbf{0}_{1 \times I_1^{(1)}-1} & \mathbf{0}_{1 \times I_1^{(2)}-1} & \cdots & \mathbf{0}_{1 \times I_1^{(n)}-1} \\ \hline x_{1,k} & 1! \binom{1}{1} 1 & 0 & \cdots & 0 \\ x_{1,k}^2 & 1! \binom{2}{1} x_{1,k} & 2! \binom{2}{2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{1,k}^{I_1^{(1)}-1} & 1! \binom{I_1^{(1)}-1}{1} x_{1,k}^{I_1^{(1)}-2} & \cdots & \mathbf{0}_{1 \times I_1^{(2)}-1} & \mathbf{0}_{1 \times I_1^{(n)}-1} \\ \hline x_{2,k} & \mathbf{0}_{1 \times I_1^{(1)}-1} & 1! \binom{1}{1} 1 & \cdots & \mathbf{0}_{1 \times I_1^{(n)}-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \hline x_{n,k}^{I_1^{(n)}-1} & \mathbf{0}_{1 \times I_1^{(1)}-1} & \mathbf{0}_{1 \times I_1^{(2)}-1} & \cdots & (I_1^{(n)}-1)! \binom{I_1^{(n)}-1}{I_1^{(n)}-1} x_{n,k}^0 \end{array} \right),$$

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and $\mathbf{B}_{k,I_2} = \tilde{\mathbf{V}}_k(d - \max_{1 \leq j \leq n} I_1^{(j)} + 1) \in \mathbb{C}^{I_2 \times \mu_k}$. The core tensors $\mathcal{G}_k \in \mathbb{C}^{\mu_k \times \mu_k \times \mu_k}$ in (D.16) have a particular structure.

Lemma D.2.1. *The core tensors $\mathcal{G}_k \in \mathbb{C}^{\mu_k \times \mu_k \times \mu_k}$ in (D.16) are composed of upper-triangular $\mathbf{T}_{k,i_1} \in \mathbb{C}^{\mu_k \times \mu_k}$:*

$$\mathbf{G}_{k[2;1,3]} = \begin{pmatrix} \mathbf{I}_{\mu_k} & \mathbf{T}_{k,2} & \dots & \mathbf{T}_{k,\mu_k} \end{pmatrix}$$

.

Proof. Sort the columns of \mathbf{A}_{k,I_1} and \mathbf{B}_{k,I_2} as we have consistently been doing in this appendix: grouped by x_j and by ascending $0 \leq l \leq \mu_k - 1$.

Suppose that an outer product $\left(\tilde{\mathbf{V}}_{k,l,I_1}\right)_1 \left(\tilde{\mathbf{V}}'_{k,l,I_2}\right)_s^T$ occurs in the $(l+1)$ th term in the k th group in (D.14). Because of the antidiagonals in $\mathbf{G}_{k,l}$, the occurrence of another outer product $\left(\tilde{\mathbf{V}}_{k,l,I_1}\right)_t (\mathbf{g}_l)_t \left(\tilde{\mathbf{V}}'_{k,l,I_2}\right)_u^T$ with $t > 1$ in that $(l+1)$ th term in the k th group $\Rightarrow u < s$. Hence, the slice $(\mathbf{G}_k)_{l+1} \triangleq \mathcal{G}_k(:, :, l+1)$ contains *only* nonzero entries $(\mathbf{G}_k)_{l+1}(t, u) \neq 0$ with $u < s$ if $t > 1$. Equivalently, the slices $\mathcal{G}_k(i_1, :, :)$ are upper-triangular¹³. \square

As we learn from Section 2.2.3, the core tensors and the factor matrices in a BTB are only unique up to linear transformations. The interpretation is as follows: although the multiplicity structure of a root $\mathbf{x}^{(k)}$ is not unique, the associated subspace $\text{span}(\tilde{\mathbf{V}}_k)$ is unique.

Example D.2.1. *Consider the decomposition in Example D.1.5 of the system in Example D.1.2 again. We can rewrite (D.15) as follows:*

$$\mathcal{Y} = \tilde{\mathcal{G}}_1 \cdot_1 \tilde{\mathbf{A}}_{1,4} \cdot_2 \tilde{\mathbf{B}}_{1,6} \cdot_3 \tilde{\mathbf{C}}_1$$

in which

$$\tilde{\mathbf{A}}_{1,4} = \left(\begin{array}{c|cc|c} 1 & 0 & 0 & 0 \\ x_1 & 1 & 0 & 0 \\ x_1^2 & 2x_1 & 2 & 0 \\ \hline x_2 & 0 & 0 & 1 \end{array} \right) \mathbf{M}^{(1)} \in \mathbb{C}^{4 \times 4},$$

$$x_j = x_j^{(1)}, \tilde{\mathbf{B}}_{1,6} = \tilde{\mathbf{V}}_1(2) \mathbf{M}^{(2)} \in \mathbb{C}^{6 \times 4}, \tilde{\mathbf{C}}_1 = \mathbf{C} \mathbf{M}^{(3)} \in \mathbb{C}^{4 \times 4},$$

$$\tilde{\mathcal{G}}_1 = \mathcal{G}_1 \cdot_1 \left(\mathbf{M}^{(1)}\right)^{-1} \cdot_2 \left(\mathbf{M}^{(2)}\right)^{-1} \cdot_3 \left(\mathbf{M}^{(3)}\right)^{-1}$$

¹³See also the next Example D.2.1.

and $\mathbf{M}^{(1)}, \mathbf{M}^{(2)}, \mathbf{M}^{(3)} \in \mathbb{C}^{4 \times 4}$ invertible transformation matrices. The constructed core tensor \mathcal{G}_1 has a particular structure:

$$\begin{aligned} \mathbf{G}_{1[1;3,2]} &= \left(\mathcal{G}_1(:, :, 1) \quad \mathcal{G}_1(:, :, 2) \quad \mathcal{G}_1(:, :, 3) \quad \mathcal{G}_1(:, :, 4) \right) \\ &= \left(\begin{array}{cccc|cccc|cccc|cccc} 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{array} \right). \end{aligned}$$

With a little thought, this means that the slices $\mathcal{G}_1(i_1, :, :)$ are upper-triangular:

$$\begin{aligned} \mathbf{G}_{1[2;1,3]} &= \left(\mathcal{G}_1(1, :, :) \quad \mathcal{G}_1(2, :, :) \quad \mathcal{G}_1(3, :, :) \quad \mathcal{G}_1(4, :, :) \right) \\ &= \left(\begin{array}{cccc|cccc|cccc|cccc} 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right). \end{aligned}$$

(D.16) is the desired result in Theorem 4.1.1.

Appendix E

Connection between the Null Space of the Macaulay Matrix and Systems Theory

Chapter 1 touched upon connections between univariate polynomial root-finding, linear algebra and systems theory. Section E.1 will formalize these connections. Much like in Appendix D, Section E.1 serves to create some insight in the reasoning on a well-known playground. Section E.2 will then extend the connections to the multivariate case. The results in [24] function as a starting point for this appendix.

E.1 Univariate Case

Consider the univariate polynomial root-finding problem

$$f(x) = x^d + a_{d-1}x^{d-1} + \dots + a_1x + a_0 = 0 \quad (\text{E.1})$$

where $f \in \mathcal{C}_d^1$. If $x^{(k)}, 1 \leq k \leq m_0 = m = d$ are the disjoint roots of f (with multiplicity $\mu_k = 1$), then the null space of the coefficient “matrix” \mathbf{f}^T of (E.1) contains m Vandermonde-structured vectors:

$$\mathbf{V} = \begin{pmatrix} \mathbf{v}_1 & \dots & \mathbf{v}_m \end{pmatrix} \in \mathbb{C}^{(d+1) \times m}$$

is a full Vandermonde basis for $\text{null}(\mathbf{f}^T)$ with

$$\mathbf{v}_k = (\mathbf{V})_k = \begin{pmatrix} 1 & x^{(k)} & \dots & x^{(k)d} \end{pmatrix}^T \in \mathbb{C}^{d+1}, \quad 1 \leq k \leq m.$$

Let $\mathbf{K} \in \mathbb{C}^{(d+1) \times m}$ be a numerical basis for $\text{null}(\mathbf{f}^T)$ related to \mathbf{V} by

$$\mathbf{K} = \mathbf{V}\mathbf{C}^T = \sum_{k=1}^m \mathbf{v}_k \otimes \mathbf{c}_k \quad (\text{E.2})$$

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where \mathbf{C}^T is an invertible transformation matrix. We give two (related) connections between (E.1)-(E.2) and one-dimensional systems theory.

First, an alternative view on (E.2) is the data model¹

$$\mathbf{Y} = \mathbf{C}\mathbf{S} \tag{E.3}$$

in which $\mathbf{Y} = \mathbf{K}^T \in \mathbb{C}^{m \times K_1}$ contains $K_1 = d + 1 = m + 1$ samples of m observed signals, $\mathbf{C} \in \mathbb{C}^{m \times m}$ is an unknown invertible mixing matrix and $\mathbf{S} = \mathbf{V}^T \in \mathbb{C}^{m \times K_1}$ is a matrix that contains m unknown source signals $s_k, 1 \leq k \leq m$. (E.3) is not unique, but can be made unique by imposing a Vandermonde structure on the sources:

$$s_k(k_1) \triangleq s_{k,k_1+1} = \left(x^{(k)}\right)^{k_1}, \quad 0 \leq k_1 \leq K_1 - 1 \text{ and } 1 \leq k \leq m.$$

$\left\{x^{(k)}\right\}_{k=1}^m$ are called the *poles* in (E.3), like in Example 1.1.2. Each row of \mathbf{Y} is a linear combination of the source signals:

$$y_i(k_1) \triangleq y_{i,k_1+1} = \sum_{k=1}^m c_{i,k} s_k(k_1) = \sum_{k=1}^m c_{i,k} \left(x^{(k)}\right)^{k_1}, \quad 0 \leq k_1 \leq K_1 - 1 \text{ and } 1 \leq i \leq m. \tag{E.4}$$

Compare (E.4) with (1.8). We can freely conclude that every possible vector in $\text{null}(\mathbf{f}^T)$ can be viewed as (a part of) the *output* of the linear time-invariant (LTI) discrete-time autonomous system, governed by the difference equation

$$w_{k_1+d} + a_{d-1}w_{k_1+d-1} + \dots + a_1w_{k_1+1} + a_0w_{k_1} = 0$$

that we may associate with f in (E.1). Herein, w_{k_1} is the output of the system at instant k_1 . In this respect, $y_i(k_1) = w_{k_1}$ and each row of \mathbf{C} contains coefficients to implicitly match some initial conditions.

More generally, if $\mu_k \geq 1, 1 \leq k \leq m_0$, such that the number of disjoint roots $m_0 \leq m$, we have that $f(x^{(k)}) = f'(x^{(k)}) = \dots = f^{(\mu_k-1)}(x^{(k)}) = 0$, which implies that both Vandermonde-structured vectors and their derivatives constitute a basis for $\text{null}(\mathbf{f}^T)$:

$$\mathbf{f}^T \begin{pmatrix} \partial_0[\mathbf{v}_k] & \partial_1[\mathbf{v}_k] & \dots & \partial_{\mu_k-1}[\mathbf{v}_k] \end{pmatrix} \triangleq \mathbf{f}^T \tilde{\mathbf{V}}_k = \mathbf{0}^T.$$

Let

$$\tilde{\mathbf{V}} = \begin{pmatrix} \tilde{\mathbf{V}}_1 & \dots & \tilde{\mathbf{V}}_{m_0} \end{pmatrix} \in \mathbb{C}^{(m+1) \times m}.$$

If $\mu_k \geq 1$, the source signals in the data model (E.3) change to $\mathbf{S} = \tilde{\mathbf{V}}^T \in \mathbb{C}^{m \times K_1}$, *i.e.*

$$s_k(k_1) \triangleq s_{k,k_1+1} = x_1^l \left(x^{(k)}\right)^{k_1}, \quad 0 \leq k_1 \leq K_1 - 1 \text{ and } 1 \leq k \leq m,$$

¹The data model (E.3) is a *transposed* variant of the 1D HR problem (2.10).

where $1 \leq k \leq m_0$ and $0 \leq l \leq \mu_k - 1$. Each row of \mathbf{Y} , that we may again view as an output of the system associated with f , can now be written as the linear combination²

$$y_i(k_1) \triangleq y_{i,k_1+1} = \sum_{k=1}^{m_0} \sum_{l=0}^{\mu_k-1} k_1^l \left(x^{(k)}\right)^{k_1}, \quad 0 \leq k_1 \leq K_1 - 1 \text{ and } 1 \leq i \leq m. \quad (\text{E.5})$$

Second, a connection between the third-order tensor decomposition (3.11) for f and the *system matrix* of the system that we may associate with f naturally follows³.

Corollary E.1.1. *Let f be a univariate polynomial of degree $m = d$ and let $\mathbf{H}(d)$ denote the column echelon basis of $\text{null}(\mathbf{f}^T)$. Let*

$$\mathbf{w}_{k_1} \triangleq \begin{pmatrix} w_{k_1} \\ \vdots \\ w_{k_1+m-1} \end{pmatrix} \in \mathbb{C}^m$$

where w_{k_1} is the output at time instant k_1 of the autonomous system governed by the difference equation $f|_{x^\alpha=w_{k_1+\alpha}}$. Then the slice $\mathbf{A} \triangleq \mathcal{H}(2, :, :)$ of the third-order tensor

$$\mathbf{H}_{[1,2;3]} = \begin{pmatrix} \mathbf{H} \\ \mathbf{H} \end{pmatrix} \in \mathbb{C}^{(2 \cdot m) \times m}$$

is equal to the system matrix of the system, i.e.

$$\mathbf{w}_{k_1+1} \triangleq \begin{pmatrix} w_{k_1+1} \\ \vdots \\ w_{k_1+m} \end{pmatrix} = \mathbf{A} \mathbf{w}_{k_1} \in \mathbb{C}^m. \quad (\text{E.6})$$

Proof. By definition, $w_{k_1+\alpha} \cong x^\alpha$, such that (E.6) implicitly expresses the multiplication of the m standard monomials with x . On the other hand, from Corollary 4.1.1, we know that $\mathbf{A} \triangleq \mathcal{H}(2, :, :) = \mathbf{A}_x$ w.r.t. the normal set basis consisting of the m standard monomials. \square

E.2 Multivariate Case

Consider now the multivariate set of n polynomial equations

$$\begin{cases} f_1(x_1, x_2, \dots, x_n) = 0 \\ \vdots \\ f_n(x_1, x_2, \dots, x_n) = 0 \end{cases} \quad (\text{E.7})$$

²[12] implicitly establishes a relation between $\text{null}(\mathbf{f}^T)$ and the decomposition in rank- $(L_r, L_r, 1)$ terms (D.5) by starting from an expression that is similar to (E.5). There is one slight difference: in [12], each row of \mathbf{S} can contain more than one pole.

³See also Example 2.1.8, 3.1.2 and 4.1.4.

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where $f_i \in \mathcal{C}_{d_i}^n, 1 \leq i \leq n$. Let $\mathbf{x}^{(k)} = (x_1^{(k)} \ x_2^{(k)} \ \dots \ x_n^{(k)})^T, 1 \leq k \leq m_0 = m$, be its disjoint roots with multiplicity $\mu_k = 1$, with $m = \prod_{i=1}^n d_i$ the Bézout number of the system. The null space of the corresponding Macaulay matrix $\mathbf{M}(d)$ now contains m multivariate Vandermonde vectors, *e.g.*, in

$$\mathbf{V}(d) = (\mathbf{v}_1(d) \ \dots \ \mathbf{v}_m(d)) \in \mathbb{C}^{q(d) \times m}$$

in Chapter 3. From that same chapter, we know that $\text{null}(\mathbf{M}(d))$ has the structure of a CPD: define the genuine Vandermonde vectors

$$\mathbf{v}_k^{(j)}(d) = (1 \ x_j^{(k)} \ \dots \ x_j^{(k)d})^T \in \mathbb{C}^{d+1}, \quad 1 \leq k \leq m, \quad 1 \leq j \leq n,$$

and let a numerical basis for $\text{null}(\mathbf{M}(d))$ be given by $\mathbf{K}(d) = \mathbf{V}(d)\mathbf{C}^T$, then

$$\mathcal{K}(d) = \sum_{k=1}^m \mathbf{v}_k^{(1)}(d_1) \otimes \mathbf{v}_k^{(2)}(d_2) \otimes \dots \otimes \mathbf{v}_k^{(n)}(d_n) \otimes \mathbf{c}_k \in \mathbb{C}^{(d_1+1) \times (d_2+1) \times \dots \times (d_n+1) \times m} \quad (\text{E.8})$$

in which $\mathcal{K}(d)$ is an $(n+1)$ th-order tensor constructed from the entries of $\mathbf{K}(d)$ to match the CPD in the right-hand side⁴. The same remark as in Chapter 3 is in place: $d = \sum_{j=1}^n d_j$ is needed to reach *all* monomials in (E.8). We will now repeat the two related connections with systems theory in Section E.1.

First, (E.8) is clearly a higher-order generalization of (E.2) and the associated data model (E.3). An alternative view on the slices of \mathcal{K} is that they are a linear combination of multidimensional source signals:

$$y_i(k_1, k_2, \dots, k_n) \triangleq (\mathcal{K})_{k_1+1, k_2+1, \dots, k_n+1, i} = \sum_{k=1}^m c_{i,k} \left(x_1^{(k)}\right)^{k_1} \left(x_2^{(k)}\right)^{k_2} \dots \left(x_n^{(k)}\right)^{k_n},$$

$$0 \leq k_1 \leq d_1, 0 \leq k_2 \leq d_2, \dots, 0 \leq k_n \leq d_n \text{ and } 1 \leq i \leq m.$$

Now recall Definition 2.1.1 of \mathbf{x}^α and Definition 2.1.3 of $f(\mathbf{x})$ and let $\mathbf{x}^\alpha w$ be formally defined as in [24]:

$$(\mathbf{x}^\alpha w)_{k_1, k_2, \dots, k_n} \triangleq w_{k_1+\alpha_1, k_2+\alpha_2, \dots, k_n+\alpha_n}.$$

E.g., $(x^\alpha w)_{k_1} = w_{k_1+\alpha}$. Yet another view on the slices of \mathcal{K} is that they are the *output* of a multidimensional LTI discrete autonomous system, governed by the set of difference equations

$$\begin{cases} (f_1(\mathbf{x})w)_{k_1, k_2, \dots, k_n} = 0 \\ \vdots \\ (f_n(\mathbf{x})w)_{k_1, k_2, \dots, k_n} = 0 \end{cases}$$

that we may associate with the multivariate set of polynomial equations $\{f_i\}_{i=1}^n$ in (E.7). In this respect, $y_i(k_1, k_2, \dots, k_n) = w_{k_1, k_2, \dots, k_n}$ and each row of \mathbf{C} contains coefficients to implicitly match some initial conditions. The $\{x_j^{(k)}\}_{j=1, k=1}^{n, m}$ can be considered the multidimensional *poles* of the multidimensional system.

⁴(E.8) is the MHR model (2.14).

Example E.2.1. [24, Example 7] Consider the set of $n = 2$ polynomial equations in $n = 2$ variables

$$\begin{cases} f_1(x_1, x_2) = 4x_1^2 - 16x_1 + x_2^2 - 2x_2 + 13 = 0 \\ f_2(x_1, x_2) = 2x_1 + x_2 - 7 = 0 \end{cases}$$

in which $m_0 = m = 2 \cdot 1 = 2$. Fig. E.1b shows the zero level curves of f_1 and f_2 . The intersections at $\begin{pmatrix} x_1^{(1)} & x_2^{(1)} \end{pmatrix}^T = \begin{pmatrix} 2 & 3 \end{pmatrix}$ and $\begin{pmatrix} x_1^{(2)} & x_2^{(2)} \end{pmatrix}^T = \begin{pmatrix} 3 & 1 \end{pmatrix}$ are the sought for common roots of f_1 and f_2 . A full multivariate Vandermonde basis for $\text{null}(\mathbf{M}(2))$ is given by $\mathbf{V}(2)$:

$$\begin{aligned} \mathbf{M}(2)\mathbf{V}(2) &= \mathbf{M}(2) \begin{pmatrix} 1 & 1 \\ x_1^{(1)} & x_1^{(2)} \\ x_2^{(1)} & x_2^{(2)} \\ x_1^{(1)2} & x_1^{(2)2} \\ x_1^{(1)}x_2^{(1)} & x_1^{(2)}x_2^{(2)} \\ x_1^{(1)2} & x_2^{(2)2} \end{pmatrix} \\ &= \left(\begin{array}{cc|cc|cc} 13 & -16 & -2 & 4 & 0 & 1 \\ -7 & 2 & 1 & 0 & 0 & 0 \\ 0 & -7 & 0 & 2 & 1 & 0 \\ 0 & 0 & -7 & 0 & 2 & 1 \end{array} \right) \begin{pmatrix} 1 & 1 \\ 2 & 3 \\ 3 & 1 \\ 4 & 9 \\ 6 & 3 \\ 9 & 1 \end{pmatrix} = \mathbf{0}. \end{aligned}$$

Take $d = 4$ and let $\mathbf{K}(4) = \mathbf{V}(4)\mathbf{C}^T$ be another (possibly numerical) basis for $\text{null}(\mathbf{M}(4))$, then

$$\begin{aligned} \mathcal{K}(4) &= \sum_{k=1}^2 \mathbf{v}_k^{(1)}(2) \otimes \mathbf{v}_k^{(2)}(2) \otimes \mathbf{c}_k = \begin{pmatrix} 1 \\ x_1^{(1)} \\ x_1^{(1)2} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ x_2^{(1)} \\ x_2^{(1)2} \end{pmatrix} \otimes \mathbf{c}_1 + \begin{pmatrix} 1 \\ x_1^{(2)} \\ x_1^{(2)2} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ x_2^{(2)} \\ x_2^{(2)2} \end{pmatrix} \otimes \mathbf{c}_2 \\ &= \begin{pmatrix} 1 \\ 2 \\ 4 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 3 \\ 9 \end{pmatrix} \otimes \mathbf{c}_1 + \begin{pmatrix} 1 \\ 3 \\ 9 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \otimes \mathbf{c}_2 \in \mathbb{C}^{3 \times 3 \times 2}. \end{aligned}$$

Remark that $d = 4$ is needed, e.g., to reach the monomial $x_1^{(1)2}x_2^{(1)2} = 4 \cdot 9 = 36$. Assume that $\mathbf{C}(1, :) = \begin{pmatrix} 1 & -1 \end{pmatrix}$. Fig. E.1a shows the first slice

$$(\mathcal{K}(4))_{k_1, k_2, 1} = 1 \cdot 2^{k_1} \cdot 3^{k_2} + (-1) \cdot 3^{k_1} \cdot 1^{k_2}, \quad 0 \leq k_1 \leq 2, \quad 0 \leq k_2 \leq 2,$$

which we may as well view as the output w_{k_1, k_2} of the two-dimensional discrete autonomous system governed by the set of difference equations

$$\begin{cases} 4w_{k_1+2, k_2} - 16w_{k_1+1, k_2} + w_{k_1, k_2+2} - 2w_{k_1, k_2+1} + 13w_{k_1, k_2} = 0 \\ 2w_{k_1+1, k_2} + w_{k_1, k_2+1} - w_{k_1, k_2} = 0 \end{cases} \quad (\text{E.9})$$

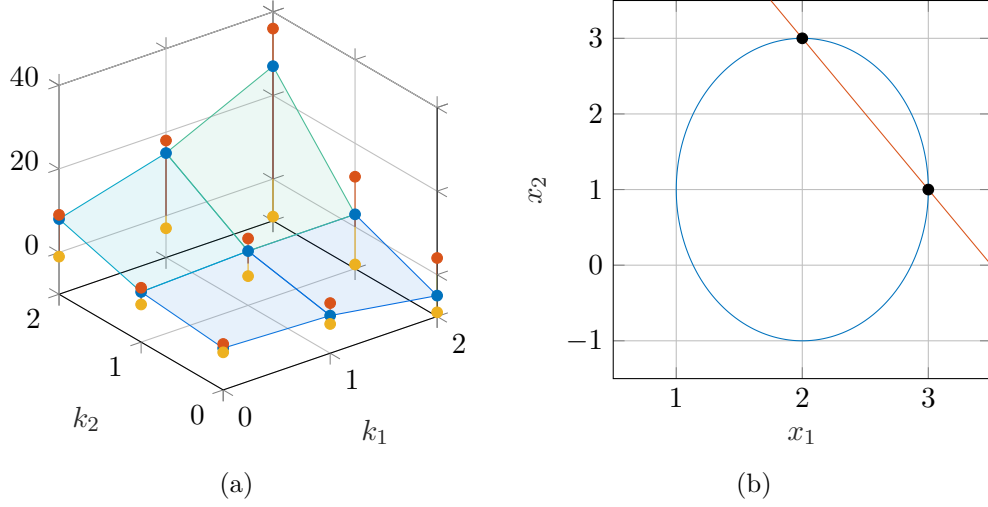


Figure E.1: (a) Output w_{k_1, k_2} (—) of the system (E.9), $2^{k_1} \cdot 3^{k_2}$ (—) and -3^{k_1} (—). (b) The zero level curves of f_1 (—) and f_2 (—) with the “two-dimensional poles” of the system.

that matches the initial condition $\begin{pmatrix} w_{0,0} & w_{1,0} \end{pmatrix}^T = \begin{pmatrix} 0 & -1 \end{pmatrix}^T$ ⁵.

More generally, if $\mu_k \geq 1, 1 \leq k \leq m_0$, such that the number of disjoint roots $m_0 \leq m$, both multivariate Vandermonde vectors and their derivatives $\left\{ \partial_{\mathbf{j}_{k,l}}[\mathbf{v}_k] \right\}_{l=0}^{\mu_k-1}$ with $\mathbf{j}_{k,l} \in \mathbb{N}^n$ constitute a basis for the null space of the Macaulay matrix:

$$\mathbf{M}(d) \begin{pmatrix} \partial_{\mathbf{j}_{k,0}}[\mathbf{v}_k] & \partial_{\mathbf{j}_{k,1}}[\mathbf{v}_k] & \dots & \partial_{\mathbf{j}_{k,\mu_k-1}}[\mathbf{v}_k] \end{pmatrix} \triangleq \mathbf{M}(d) \tilde{\mathbf{V}}_k = \mathbf{0}.$$

Following a reasoning that is completely analogous to the one outlined in Section E.1, each slice of \mathcal{K} can now be written as the linear combination

$$\begin{aligned} y_i(k_1, k_2, \dots, k_n) &\triangleq (\mathcal{K})_{k_1+1, k_2+1, \dots, k_n+1, i} \\ &= \sum_{k=1}^{m_0} \sum_{l=1}^{\mu_k-1} c_{i,k} k_1^{\mathbf{j}_{k,l}(1)} k_2^{\mathbf{j}_{k,l}(2)} \dots k_n^{\mathbf{j}_{k,l}(n)} \left(x_1^{(k)} \right)^{k_1} \left(x_2^{(k)} \right)^{k_2} \dots \left(x_n^{(k)} \right)^{k_n}, \\ &0 \leq k_1 \leq d_1, 0 \leq k_2 \leq d_2, \dots, 0 \leq k_n \leq d_n \text{ and } 1 \leq i \leq m. \end{aligned}$$

Second, Corollary E.2.1 introduces a *system tensor* instead of the system matrix in Corollary E.1.1.

Corollary E.2.1. Let $\{f_i\}_{i=1}^n$ be a system of n multivariate polynomial equations in n variables with Bézout number m and let $\mathbf{H}(d)$ denote the column echelon basis of $\text{null}(\mathbf{M}(d))$. Let $\mathbf{w}_{\mathbf{k}} \in \mathbb{C}^m$ be defined as

$$(\mathbf{w}_{\mathbf{k}})_k \triangleq (\mathbf{x}^{\alpha_k} w)_{k_1, k_2, \dots, k_n}, \quad 1 \leq k \leq m,$$

⁵Example E.2.1 is merely an illustrative example; because the poles have magnitudes > 1 , the discrete system is called *unstable*.

where $\{\mathbf{x}^{\alpha_k}\}_{k=1}^m$ are the standard monomials and w_{k_1, k_2, \dots, k_n} is the output of the multidimensional autonomous system governed by the difference equations $\{f_i(\mathbf{x})w\}_{i=1}^n$. Similarly, let $\mathbf{W}_{\mathbf{k}+1} \in \mathbb{C}^{m \times n}$ be defined as

$$\begin{aligned} (\mathbf{W}_{\mathbf{k}+1})_{k,j} &\triangleq (x_j \mathbf{x}^{\alpha_k} w)_{k_1, k_2, \dots, k_n} \\ &= (\mathbf{x}^{\alpha_k} w)_{k_1, k_2, \dots, k_{j-1}, k_j+1, k_{j+1}, \dots, k_n}, \quad 1 \leq k \leq m, \quad 1 \leq j \leq n. \end{aligned}$$

Then the third-order tensor

$$\mathbf{A}_{[1,2,3]} \triangleq \begin{pmatrix} \hat{\mathbf{S}}_2^{(1)} \mathbf{H}(d) \\ \vdots \\ \hat{\mathbf{S}}_2^{(n)} \mathbf{H}(d) \end{pmatrix} \in \mathbb{C}^{(n \cdot m) \times m}$$

in Corollary 4.1.1 is equal to the system tensor of the multidimensional system, i.e.

$$\mathbf{W}_{\mathbf{k}+1}^T = \mathcal{A} \cdot_3 \mathbf{w}_{\mathbf{k}}^T \in \mathbb{C}^{n \times m}. \quad (\text{E.10})$$

Proof. (E.10) can be rewritten as

$$\text{vec}(\mathbf{W}_{\mathbf{k}+1}) = \mathbf{A}_{[1,2,3]} \mathbf{w}_{\mathbf{k}} = \begin{pmatrix} \mathcal{A}(1, :, :) \\ \vdots \\ \mathcal{A}(n, :, :) \end{pmatrix} \mathbf{w}_{\mathbf{k}} \in \mathbb{C}^{n \cdot m}.$$

By definition, $w_{k_1+\alpha_1, k_2+\alpha_2, \dots, k_n+\alpha_n} \cong \mathbf{x}^\alpha$, such that (E.10) actually expresses the multiplication of the m standard monomials with $\{x_j\}_{j=1}^n$. On the other hand, from Corollary 4.1.1, we know that the slices $\{\mathcal{A}(j, :, :)\}_{j=1}^n \triangleq \{\hat{\mathbf{S}}_2^{(j)} \mathbf{H}\}_{j=1}^n$ are indeed equal to the multiplication tables $\{\mathbf{A}_{x_j}\}_{j=1}^n$ w.r.t. the normal set basis. \square

Example E.2.2. Consider the system in Example E.2.1 again. The column echelon basis for $(\text{null } \mathbf{M}(2))$ is given by $\mathbf{H}(2)$:

$$\mathbf{H}(2) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 7 & -2 \\ -6 & 5 \\ 12 & -3 \\ 25 & -8 \end{pmatrix}$$

The third-order tensor \mathcal{A} in (E.10) is given by

$$\mathbf{A}_{[1,2,3]} = \begin{pmatrix} \hat{\mathbf{S}}_2^{(1)} \mathbf{H} \\ \hat{\mathbf{S}}_2^{(1)} \mathbf{H} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -6 & 5 \\ 7 & -2 \\ 12 & -3 \end{pmatrix} \in \mathbb{C}^{(2 \cdot 2) \times 2}.$$

We have that

$$\mathbf{W}_1^T = \begin{pmatrix} w_{1,0} & w_{2,0} \\ w_{0,1} & w_{1,1} \end{pmatrix} = \mathcal{A} \cdot_3 \begin{pmatrix} 0 & -1 \end{pmatrix} = \begin{pmatrix} -1 & -5 \\ 2 & 3 \end{pmatrix},$$

as can be seen in Fig. [E.1a](#).

Appendix F

Rank-1 Vandermonde Detection Procedure

Chapter 3 showed that the null space of the Macaulay matrix of a set of polynomial equations that has only simple roots, admits a CPD. Section F.1 will outline the so-called SD method or rank-1 detection procedure [10, Algorithm 2.1] that can be used to compute that CPD. If the set has also got multiple roots, Chapter 4 showed that the null space of its Macaulay matrix admits a BTD. As an alternative to the BTD, [17, Algorithm 1] is a promising extension of the rank-1 detection procedure that could possibly detect the $m_0 < m$ disjoint roots in the null space of the Macaulay matrix. Unfortunately, Section F.2 will show that one cannot expect this.

F.1 Rank-1 Detection Procedure

Recall from Chapter 3 that if the conditions in Theorem 3.2.1 (or Theorem 3.2.2) are satisfied, (3.12) can be computed by means of the rank-1 detection procedure in Algorithm F.1. A few remarks are in order.

Step 2-3. [10, Theorem 2.1] shows that $\Phi(\mathbf{X}, \mathbf{X}) \equiv \mathcal{O}$ iff $r_{\mathbf{X}} = 1$, from which the *rank-1 detection* ability of the procedure stems.

Output. Once the output \mathbf{W} is known, the R vectorized rank-1 matrices in the column space of the input \mathbf{E} follow from a best rank-1 approximation of the R columns of $\mathbf{E}\mathbf{W}^1$.

In (3.12) in the polynomial root-finding context, we have that $\mathbf{E} = \mathbf{Y}_{[1,2;3]}$, $\mathbf{G} = \mathbf{C}$ and the $R = m$ multivariate Vandermonde vectors follow from a best rank-1 approximation of the m columns of $\mathbf{Y}_{[1,2;3]}\mathbf{W}$.

¹See also Example ??.

Algorithm F.1 Rank-1 Detection Procedure [10, Algorithm 2.1]

Input: The matrix $\mathbf{E} \in \mathbb{C}^{IJ \times R}$ that is the matricization of a CPD $\mathbf{E} = (\mathbf{A} \odot \mathbf{B}) \mathbf{G}^T$.

Output: The matrix $\mathbf{W} \triangleq (\mathbf{G}^T)^\dagger \in \mathbb{C}^{R \times R}$ such that $\mathbf{E}\mathbf{W} = \mathbf{A} \odot \mathbf{B} \in \mathbb{C}^{IJ \times R}$.

1: Construct $\mathcal{E} \in \mathbb{C}^{I \times J \times R}$:

$$(\mathcal{E})_{ijr} = (\mathbf{E})_{(i-1)J+j,r}.$$

2: Construct $\{\mathcal{P}_{rs} \triangleq \Phi(\mathbf{E}_r, \mathbf{E}_s)\}_{r=1,s=1}^{R,R}$ with $\mathbf{E}_r \triangleq \mathcal{E}(:, :, r)$,

$$\Phi : \mathbb{C}^{I \times J} \times \mathbb{C}^{I \times J} \rightarrow \mathbb{C}^{I \times I \times J \times J} : (\mathbf{X}, \mathbf{Y}) \mapsto \mathcal{P}$$

and

$$(\mathcal{P})_{ijkl} = x_{ik}y_{jl} + y_{ik}x_{jl} - x_{il}y_{jk} - y_{il}x_{jk}.$$

3: Construct the symmetric $\{\mathbf{M}_k \in \mathbb{C}^{R \times R}\}_{k=1}^R$ as the R solutions of

$$\sum_{r,s=1}^R m_{rs} \mathcal{P}_{rs} = \mathcal{O} \quad \text{s.t.} \quad m_{rs} = m_{sr}.$$

4: Find \mathbf{W} that *simultaneously diagonalizes* (SD) the \mathbf{M}_k from the CPD of $\mathcal{M} \in \mathbb{C}^{R \times R \times R}$ with $\mathcal{M}(:, :, k) \triangleq \mathbf{M}_k$:

$$\mathcal{M} = \llbracket \mathbf{M}, \mathbf{M}, \mathbf{\Lambda} \rrbracket.$$

5: **return** \mathbf{W}

F.2 Extension to Multiple Roots

If a set of polynomial equations has only got $m_0 < m$ disjoint roots $\mathbf{x}^{(k)}$ with multiplicity $\mu_k \geq 1, 1 \leq k \leq m_0$, and $\exists k' : \mu_{k'} > 1$, then multivariate Vandermonde vectors and their derivatives constitute a basis for the null space of its Macaulay matrix, *i.e.*

$$\tilde{\mathbf{V}}(d) = \begin{pmatrix} \tilde{\mathbf{V}}_1 & \dots & \tilde{\mathbf{V}}_{m_0} \end{pmatrix} \in \mathbb{C}^{q(d) \times m}$$

is a full basis and

$$\tilde{\mathbf{V}}_k = \begin{pmatrix} \partial_{\mathbf{j}_{k,0}}[\mathbf{v}_k] & \partial_{\mathbf{j}_{k,1}}[\mathbf{v}_k] & \dots & \partial_{\mathbf{j}_{k,\mu_k-1}}[\mathbf{v}_k] \end{pmatrix} \in \mathbb{C}^{q(d) \times \mu_k}$$

with both $\mathbf{j}_{k,l} = \mathbf{0}$ and $\mathbf{j}_{k,l} \neq \mathbf{0}$. Remember from Section 4.1 that the newly introduced columns in $\tilde{\mathbf{V}}(d)$ do *not* exhibit the multiplicative shift structure exploited in (3.12). Therefore, $\mathbf{Y}_{[1,2;3]}$ does not admit a CPD and we cannot use Algorithm F.1 anymore.

It is shown in [17] though that Algorithm F.1 can be *extended* to detect $R < R_{\text{tot}}$

vectorized rank-1 matrices in a more general $\mathbf{E} \in \mathbb{C}^{IJ \times R_{\text{tot}}}$ of the form:

$$\mathbf{E} = \mathbf{U} \begin{pmatrix} \mathbf{G} & \mathbf{H} \end{pmatrix}^T = \begin{pmatrix} \mathbf{A} \odot \mathbf{B} & \mathbf{F} \end{pmatrix} \begin{pmatrix} \mathbf{G} & \mathbf{H} \end{pmatrix}^T = (\mathbf{A} \odot \mathbf{B}) \mathbf{G}^T + \mathbf{F} \mathbf{H}^T \quad (\text{F.1})$$

where $\mathbf{G} \in \mathbb{C}^{R_{\text{tot}} \times R}$, $\mathbf{H} \in \mathbb{C}^{R_{\text{tot}} \times R_{\text{add}}}$, $\mathbf{F} \in \mathbb{C}^{IJ \times R_{\text{add}}}$ and $R_{\text{add}} = R_{\text{tot}} - R$ now. As Example F.2.1 shows, (F.1) is a convincing extension of (3.12) to the case where $R = m_0 < R_{\text{tot}} = m$.

Example F.2.1. Consider the system of $s = 2$ polynomial equations in $n = 2$ variables with $m_0 = 1 < m = 4$ in Example 4.1.1 again. A possible basis for $\text{null}(\mathbf{M}(d^*)) = \text{null}(\mathbf{M}(2))$ is defined by:

$$\tilde{\mathbf{V}}_1 = \begin{pmatrix} \partial_{00}[\mathbf{v}_1] & \partial_{10}[\mathbf{v}_1] & \partial_{01}[\mathbf{v}_1] & (\partial_{20} + \partial_{11})[\mathbf{v}_1] \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ x_1^{(1)} & 1 & 0 & 0 \\ x_2^{(1)} & 0 & 1 & 0 \\ x_1^{(1)2} & 2x_1^{(1)} & 0 & 2 \\ x_1^{(1)}x_2^{(1)} & x_2^{(1)} & x_1^{(1)} & 1 \\ x_2^{(1)2} & 0 & 2x_2^{(1)} & 0 \end{pmatrix}.$$

(3.12) changes to

$$\begin{aligned} \mathbf{Y}_{[1,2;3]} &= \begin{pmatrix} \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(0)} \mathbf{K} \\ \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(1)} \mathbf{K} \\ \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(2)} \mathbf{K} \end{pmatrix} = \begin{pmatrix} \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(0)} \tilde{\mathbf{V}}_1 \\ \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(1)} \tilde{\mathbf{V}}_1 \\ \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(2)} \tilde{\mathbf{V}}_1 \end{pmatrix} \mathbf{C}^T = \mathbf{U} \mathbf{C}^T = \mathbf{U} \begin{pmatrix} \mathbf{G} & \mathbf{H} \end{pmatrix}^T \\ &= \begin{pmatrix} \mathbf{A} \odot \mathbf{B} & \mathbf{F} \end{pmatrix} \begin{pmatrix} \mathbf{G} & \mathbf{H} \end{pmatrix}^T = \left(\begin{pmatrix} 1 \\ x_1^{(1)} \\ x_2^{(1)} \end{pmatrix} \odot \begin{pmatrix} 1 \\ x_1^{(1)} \\ x_2^{(1)} \end{pmatrix} \mathbf{F} \right) \begin{pmatrix} \mathbf{G} & \mathbf{H} \end{pmatrix}^T. \quad (\text{F.2}) \end{aligned}$$

We have that $\mathbf{E} = \mathbf{Y}_{[1,2;3]}$ and that $\mathbf{A} \odot \mathbf{B}$ and \mathbf{F} correspond to $\partial_{\mathbf{j}}[\mathbf{v}_1]$ with $\mathbf{j} = \mathbf{0}$ and $\partial_{\mathbf{j}}[\mathbf{v}_1]$ with $\mathbf{j} \neq \mathbf{0}$, respectively. $R_{\text{tot}} = m = 4$, $R = m_0 = 1$ and $R_{\text{add}} = m - m_0 = 3$.

The extension has thus the potential to detect in a very elegant way the $m_0 < m$ multivariate Vandermonde vectors corresponding to the m_0 disjoint roots in the more general $\mathbf{E} = \mathbf{Y}_{[1,2;3]}$ — be it without their associated multiplicities.

However, an essential assumption to be met for the extended procedure to work, is that the tensors $\mathcal{P} = \Phi(\mathbf{X}, \mathbf{Y})$ as defined in Step 2 in Algorithm F.1 are a *linearly independent* set when one takes $\text{vec}(\mathbf{X}) = \mathbf{u}_r$ and $\text{vec}(\mathbf{Y}) = \mathbf{u}_s$ equal to all

$$\frac{R_{\text{tot}}(R_{\text{tot}} + 1)}{2} - R$$

possible pairwise combinations of the columns in \mathbf{U} in (F.1) — not including the R combinations $\mathbf{u}_s = \mathbf{u}_r = \mathbf{a}_r \odot \mathbf{b}_r$, because then we know from the above that $\mathcal{P} \equiv \mathcal{O}^2$.

²For the initial \mathbf{E} in Algorithm F.1, this essential assumption is equivalent to Theorem C.1.4 stating that condition (C2) holds for \mathbf{A} and \mathbf{B} .

To see why this assumption is essential, we refer the reader to [10]. As Example F.2.2 shows now, the essential assumption is *not* met for (F.2).

Example F.2.2. Let $\mathbf{U}^r \triangleq \text{vec}^{-1}(\mathbf{u}_r)$ in (F.2) and let $\mathcal{P}_{rs} \triangleq \Phi(\mathbf{U}^r, \mathbf{U}^s)$. Then

$$\begin{aligned}
 (\mathcal{P}_{12})_{ijkl} &= u_{ik}^1 u_{jl}^2 + u_{ik}^2 u_{jl}^1 - u_{il}^1 u_{jk}^2 - u_{il}^2 u_{jk}^1 \\
 &= u_{ik}^1 \partial_{10} u_{jl}^1 + \partial_{10} u_{ik}^1 u_{jl}^1 - u_{il}^1 \partial_{10} u_{jk}^1 - \partial_{10} u_{il}^1 u_{jk}^1 \\
 &= \partial_{10} (u_{ik}^1 u_{jl}^1) - \partial_{10} (u_{il}^1 u_{jk}^1) = 1/2 \partial_{10} (2u_{ik}^1 u_{jl}^1 - 2u_{il}^1 u_{jk}^1) \\
 &= 1/2 \partial_{10} ((\mathcal{P}_{11})_{ijkl}) \equiv 1/2 \partial_{10}(0) = 0.
 \end{aligned}$$

Likewise, $\mathcal{P}_{13} = \mathcal{O}$ and it can be shown that $\mathcal{P}_{34} \in \text{span}(\mathcal{P}_{23}, \mathcal{P}_{24})$, such that the \mathcal{P}_{rs} are not a linearly independent set.

More generally, Example F.2.2 makes it clear that the assumption of linear independence of the \mathcal{P}_{rs} is not met if $m_0 < m$. Put in other words: one cannot expect that the extension of Algorithm F.1 proposed in [17] will successfully detect the m_0 multivariate Vandermonde vectors corresponding to the disjoint roots of the set of polynomial equations if $m_0 < m$.

Appendix G

SVD Compression in Algorithm 3.1

In this appendix, we show that the compression in Step 7 in Algorithm 3.1 has no effect on the uniqueness properties of (3.12) established in Chapter 3.

Let $\mathbf{Y}_{[2;1,3]} = \mathbf{U}^{(2)}\mathbf{S}^{(2)}\mathbf{U}^{(1,3)H} = \hat{\mathbf{U}}^{(2)}\hat{\mathbf{S}}^{(2)}\hat{\mathbf{U}}^{(1,3)H} \in \mathbb{C}^{q(d-1) \times (n+1) \cdot m}$ be the SVD of the mode-2 matricization of \mathcal{Y} in (3.12). $\hat{\mathbf{U}}^{(2)} = \mathbf{U}^{(2)}(:, 1 : R_2)$ contains the first R_2 columns of the unitary matrix $\mathbf{U}^{(2)}$, where $R_2 = \text{rank}_2(\mathcal{Y})$, *i.e.* R_2 equals the number of nonzero entries in $\mathbf{S}^{(2)}$. Then

$$\hat{\mathcal{Y}} \triangleq \mathcal{Y} \cdot_2 \hat{\mathbf{U}}^{(2)H} = \llbracket \mathbf{A}, \hat{\mathbf{U}}^{(2)H} \mathbf{B}(d-1), \mathbf{C} \rrbracket \triangleq \llbracket \mathbf{A}, \hat{\mathbf{B}}(d-1), \mathbf{C} \rrbracket$$

is “compressed” CPD in Algorithm 3.1 with matricization

$$\hat{\mathbf{Y}}_{[1,2;3]} = \begin{pmatrix} \hat{\mathbf{U}}^{(2)H} \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(0)} \mathbf{K} \\ \hat{\mathbf{U}}^{(2)H} \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(1)} \mathbf{K} \\ \vdots \\ \hat{\mathbf{U}}^{(2)H} \bar{\mathbf{S}}_{\mathbf{B}(d-1)}^{(n)} \mathbf{K} \end{pmatrix} = (\mathbf{A} \odot \hat{\mathbf{B}}(d-1)) \mathbf{C}^T \in \mathbb{C}^{((n+1) \cdot R_2) \times m}. \quad (\text{G.1})$$

We need to show that if decomposition (3.12) is unique, also (G.1) is unique. Indeed, let $\hat{\mathcal{Y}} = \llbracket \tilde{\mathbf{A}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}} \rrbracket$ be another CPD of $\hat{\mathcal{Y}}$. Note that $\hat{\mathbf{Y}}_{[2;1,3]} = \hat{\mathbf{S}}^{(2)}\hat{\mathbf{U}}^{(1,3)H}$. Then

$$\mathbf{Y}_{[2;1,3]} = \hat{\mathbf{U}}^{(2)}\hat{\mathbf{Y}}_{[2;1,3]} = \hat{\mathbf{U}}^{(2)}\tilde{\mathbf{B}} \left(\tilde{\mathbf{A}} \odot \tilde{\mathbf{C}} \right)^T.$$

If the CPD of \mathcal{Y} is essentially unique, then it follows that there should exist a permutation matrix $\mathbf{\Pi} \in \mathbb{C}^{m \times m}$ and a nonsingular diagonal matrix $\mathbf{\Lambda} \in \mathbb{C}^{m \times m}$ such that

$$\mathbf{B}(d-1) = \hat{\mathbf{U}}^{(2)}\tilde{\mathbf{B}}\mathbf{\Pi}\mathbf{\Lambda} \Leftrightarrow \hat{\mathbf{U}}^{(2)H}\mathbf{B}(d-1) = \hat{\mathbf{B}}(d-1) = \tilde{\mathbf{B}}\mathbf{\Pi}\mathbf{\Lambda}$$

and therefore also the CPD of $\hat{\mathcal{Y}}^h$ is essentially unique. For completeness, the same procedure could be applied with $\mathbf{U}^{(1)} = \mathbf{I}_{n+1}$ and $\mathbf{U}^{(3)} = \mathbf{I}_m$.

Appendix H

Algorithms in Matlab

A Matlab implementation of the algorithms presented in Chapter 3 and 4 accompanies this text. The algorithms are mostly wrappers in Matlab 9.1 (R2016b) that construct the third-order tensor \mathcal{Y} and forward the computation of its decomposition to Tensorlab, version 3.0 [45]. PNLA [1] is used to construct the Macaulay matrix. This appendix highlights the use of the algorithms. Section H.1 and H.2 will first cover some prerequisites and Section H.3 will describe the use of the algorithms.

H.1 Installation

Once you have fetched P2Tlab containing the programs, Tensorlab, version 3.0 and PNLA to the current directory, add them to the Matlab search path.

```
>> addpath('p2tlab', 'tensorlab', 'PNLA_MATLAB_OCTAVE')
```

H.2 Representation of a Set of Polynomial Equations

For the representation of a set of polynomial equations, we have adopted the convention in PNLA. A set $\{f_i\}_{i=1}^s$ of s polynomial equations in n affine¹ variables is represented as an s -by-2 cell array \mathbf{c} where

- $\mathbf{c}\{\mathbf{i},1\}$ is the coefficient vector \mathbf{f}_i of length p_i ;
- $\mathbf{c}\{\mathbf{i},2\}$ is a matrix of size $p_i \times n$ which contains at position (l, j) the exponent of x_j in the monomial that corresponds with the l th coefficient in \mathbf{f}_i .

Consider for instance the system of $s = 2$ polynomial equations in $n = 2$ variables

$$\begin{cases} f_1(x_1, x_2) = x_1x_2 - x_1 = 0 \\ f_2(x_1, x_2) = x_1x_2 - x_2 = 0 \end{cases} \quad (\text{H.1})$$

¹There is a 1-to-1 correspondence between a system and its homogenization, so the convention in this section holds for homogeneous systems in $n + 1$ variables as well.

where $\mathbf{f}_1 = \mathbf{f}_2 = \begin{pmatrix} 1 & -1 \end{pmatrix}^T$. Define the set of polynomial equations as follows:

```
>> polysys = cell(2,2); % an n-by-2 cell array
>> polysys{1,1} = [1; -1];
>> polysys{1,2} = [1 1; 1 0];
>> polysys{2,1} = [1; -1];
>> polysys{2,2} = [1 1; 0 1];
```

H.3 Multivariate Polynomial Root-Finding and Subspace-Finding Algorithms

H.3.1 Algorithms

Algorithm 3.1 and 4.1 are root- or subspace-finding algorithms for 0-dimensional systems of polynomial equations. We briefly recap (the differences between) their Matlab implementations here.

- `poly_cpd` is Algorithm 3.1 where the CPD of $\hat{\mathcal{Y}}$ in Step 8 is computed directly using one of the many CPD algorithms in Tensorlab.
- `poly_sd` is Algorithm 3.1 where the CPD of $\hat{\mathcal{Y}}$ in Step 8 is computed at by means of (an adaptation of) the SD method in Algorithm F.1. The CPD in Step 4 in Algorithm F.1 should still be computed using one of the CPD algorithms in Tensorlab.
- `poly_btd` is Algorithm 4.1 where the BTD of $\hat{\mathcal{Y}}$ in Step 8 is computed using one of the BTD algorithms in Tensorlab.
- `mergesolve` is the recursive polynomial root-finding scheme in Fig. 4.3.

After homogenization, it is easy to verify that (H.1) has $m = 4$ roots in the projective space: $\begin{pmatrix} x_0 & x_1 & x_2 \end{pmatrix}^T = \begin{pmatrix} 1 & 1 & 1 \end{pmatrix}^T, \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}^T, \begin{pmatrix} 0 & 1 & 0 \end{pmatrix}^T$ and $\begin{pmatrix} 0 & 0 & 1 \end{pmatrix}^T$. `poly_cpd` can be used to find the roots. By default, the algorithm constructs the Macaulay matrix at $d = d^* + 1$ and computes $m = \prod_{i=1}^s d_i$ roots using the high-level algorithm `cpd` in Tensorlab. If $d = d^* + 1$, the computation of the CPD reduces to a GEVD. `cpd` will therefore automatically choose `cpd_gevd` to initialize the CPD. Afterwards, `cpd` refines the solution, *e.g.*, using the NLS type algorithm `cpd_nls`. An extra output structure contains this information.

```
>> [X, output] = poly_cpd(polysys)

X =

    1.0000    1.0000    0.0000    0.0000
    1.0000    0.0000    1.0000    0.0000
    1.0000    0.0000    0.0000    1.0000
```

```

output =

    struct with fields:

        AlgorithmOutput: [1x1 struct]
        Options: [1x1 struct]

>> output.AlgorithmOutput.Initialization.Name

ans =

cpd_gevd

```

Note that `poly_cpd` returns the m roots as the factor matrix \mathbf{A} in the CPD (3.12), *i.e.* as a matrix which contains as columns the $(n+1)$ -dimensional (normalized) solution vectors in the projective space.

Recall that if there are multiple roots, \mathcal{Y} in (4.6) admits a BTD in which the core tensors \mathcal{G}_k have size $\mu_k \times \mu_k \times \mu_k$ with μ_k the multiplicity of the root $\mathbf{x}^{(k)}$, $1 \leq k \leq m_0$ ². Therefore, `poly_btd` requires a second input argument. It is either

- `size_core`: a numerical array of size $1 \times m_0$ containing the μ_k , $1 \leq k \leq m_0$, or
- a cell array `G = {G{1}, G{2}, ...}` containing m_0 fixed core tensors \mathcal{G}_k , $1 \leq k \leq m_0$, *e.g.*, to try to recover the canonical BTB in Theorem 4.1.1. In this case, the BTB is computed using the structured data fusion framework in Tensorlab.

H.3.2 Options

Like in Tensorlab, the above algorithms can be tuned using options provided in a structure, passed as an extra argument. Options for different algorithms are often very alike. Here, we show the options for `poly_cpd`.

- `degree`: If specified, it forces `poly_cpd` to construct $\mathbf{M}(d)$ at this degree.
- `Nsol`: The number of solutions returned, *i.e.* the rank of the computed CPD. This (and the previous) option is particularly useful when you solve an over-constrained set ($s = Nn$)³. You don't want to compute the default $\prod_{i=1}^n d_i^N$ roots blindly, but only an approximation of the original $m = \prod_{i=1}^n d_i$ roots of the underlying square system.

²See Example 4.3.1.

³See Section 3.3.2.

- `sparse`: If you have SuiteSparseQR [8] installed, setting this option to `true` ensures that \mathbf{K} in Step 3 in Algorithm 3.1 gets computed using a sparse QR algorithm.
- `RecursiveOrthogonalization`: If `true`, if `Nsol` is not specified and if `sparse` is not set, use the recursive orthogonalization scheme [2, Algorithm 4.2] to compute \mathbf{K} .
- `Compression`: If `'svd'`, do SVD compression. This is the default. If `'none'`, don't compress \mathcal{Y} , *i.e.* skip Step 6 and 7 in Algorithm 3.1.
- `Algorithm`: The algorithm from Tensorlab to compute the CPD.

If specifying an option creates additional output information, it is added to `output`. For more information about the options, use `help`. The explanation should be comprehensible. Below is an example that instructs `poly_cpd` to compute the CPD at $d = d^*$ using (a random initialization for) NLS.

```
>> options = struct;  
>> options.degree = dbound(polysys); % dbound is a P2Tlab ...  
    function that calculates the degree of regularity  
>> options.Compression = 'svd'; % does nothing; 'svd' is ...  
    the default  
>> options.Algorithm = @cpd_nls;  
>> [X, output] = poly_cpd(polysys, options);
```

H.3.3 Other programs

P2Tlab further includes some other useful programs, such as `polysys2tens`, to go from a system of polynomial equations to \mathcal{Y} ⁴, or `reset`, to repeat a square set as an over-constrained set of noisy polynomial equations.

⁴The algorithms above all call `polysys2tens`.

Appendix I

Poster



KATHOLIEKE UNIVERSITEIT
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INGENIEURSWETENSCHAPPEN

Master
Wiskundige
ingenieurstechnieken

Masterproef
Jeroen
Vanderstukken

Promotor
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De Lathauwer

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Stegeman

Academiejaar
2016-2017

Sets of polynomial equations, decompositions of higher-order tensors and multidimensional harmonic retrieval: connections and algorithms

Higher-order tensors

- A **canonical polyadic decomposition (CPD)** of an N th-order tensor $\mathcal{A} \in \mathbb{C}^{I_1 \times I_2 \times \dots \times I_N}$ expresses \mathcal{A} as a minimal sum of $r_{\mathcal{A}}$ rank-1 terms

- Striking differences with matrix rank:
 - Border rank:** $r_{\mathcal{A}} > R$ but approximated arbitrarily well by a rank- R CPD.
 - Typical rank:** $r_{\mathcal{A}}$ can take more than one value, depending on \mathbb{F} .

Univariate polynomial root-finding problem

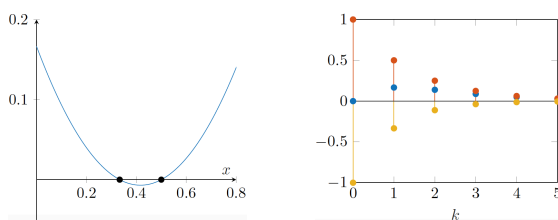
$$f(x) = 0$$

- A solution $x^{(k)}$ generates a Vandermonde vector $\mathbf{v}_k = \begin{pmatrix} 1 & x^{(k)} & \dots & x^{(k)d} \end{pmatrix}^T$ in null (\mathbf{f}^T)
- The (1D) **harmonic retrieval (HR)** problem

$$\mathbf{Y}_{[1,2,3]} = \begin{pmatrix} \mathbf{K} \\ \mathbf{K} \end{pmatrix} = \begin{pmatrix} \mathbf{V} \\ \mathbf{V} \end{pmatrix} \mathbf{C}^T = \begin{pmatrix} \mathbf{c}_1 \\ \begin{pmatrix} 1 \\ x^{(1)} \end{pmatrix} \end{pmatrix} + \dots$$

is a third-order tensor CPD that can be linked (ESPRIT) to the EVD of the **Frobenius companion matrix**

$$\mathbf{Y}_{[1,2,3]} = \begin{pmatrix} \mathbf{I}_d \\ \mathbf{A} \end{pmatrix} \tilde{\mathbf{C}}^T$$

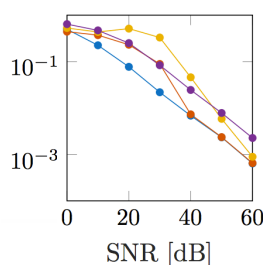


The zeros (poles) of $f(x)$ (left) determine the output y_k of an LTI autonomous system (right).

- $\mathbf{A} = \mathbf{PJP}^{-1}$ is a Jordan form instead of an EVD

Algorithms

- Existing methods: computer algebra, **homotopy continuation** [1], NPA [2] and **PNLA** [3], ...
- Tensorlab [4]: **cpd3_sd**, **cpd_gevd**, **cpd_nls**, ...



Error on the solution of an over-constrained set ($N = 10$) of noisy polynomial equations ($n = 2; d_0 = 3$) as a function of the signal-to-noise ratio.

Set of multivariate polynomial equations

- $$\begin{cases} f_1(x_1, x_2, \dots, x_n) = 0 \\ \vdots \\ f_n(x_1, x_2, \dots, x_n) = 0 \end{cases}$$
- A solution $\mathbf{x}^{(k)} = \begin{pmatrix} x_1^{(k)} & \dots & x_n^{(k)} \end{pmatrix}^T$ generates a Vandermonde-like $\mathbf{v}_k = \begin{pmatrix} 1 & x_1^{(k)} & \dots & x_n^{(k)d} \end{pmatrix}^T$ in the null space of the **Macaulay matrix**

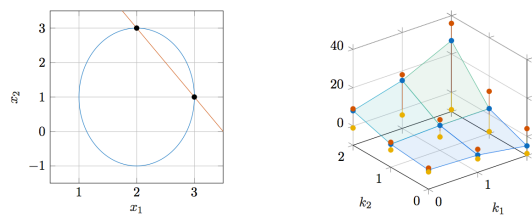
$$\mathbf{M}(d) = \begin{pmatrix} f_1 \\ x_1 f_1 \\ \vdots \\ x_n^{d-d_n} f_n \end{pmatrix}$$

- The **multidimensional harmonic retrieval (MHR)** problems

$$\mathbf{Y}^{(j)} = \begin{pmatrix} \mathbf{S}^{(j)} \mathbf{K} \\ \mathbf{S}^{(j)} \mathbf{K} \end{pmatrix} = \begin{pmatrix} \mathbf{c}_1 \\ \begin{pmatrix} 1 \\ x_j^{(1)} \end{pmatrix} \end{pmatrix} + \dots + \begin{pmatrix} \mathbf{c}_m \\ \begin{pmatrix} 1 \\ x_j^{(m)} \end{pmatrix} \end{pmatrix}$$

yield a third-order tensor CPD that can be linked to the **joint EVD** of the **multiplication tables** $\{\mathbf{A}_{x_j}\}_{j=1}^n$

- Natural **homogeneous** ($x_0 \neq 1$) interpretation
- Relaxed (generic) **uniqueness** conditions



The zeros (poles) of $f_1(x_1, x_2)$ and $f_2(x_1, x_2)$ (left) determine the output y_{k_1, k_2} of a multidimensional LTI autonomous system (right).

- \mathcal{Y} admits a **block term decomposition (BTD)** involving confluent Vandermonde matrices

- If $\exists k : \mu_k > 1$, \mathcal{G}_k has **border rank** μ_k and \mathcal{Y} has **border rank** $m = \sum_{k=1}^{m_0} \mu_k$
- If there are complex conjugated roots, \mathcal{Y} admits a BTD with blocks $\mathcal{G}_k \in \mathbb{R}^{2 \times 2 \times 2}$ with the (only) **typical rank** $r_{\mathcal{G}} = 2$ over \mathbb{C} , but with the **typical rank** $r_{\mathcal{G}} = 3$ over \mathbb{R}

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Fiche masterproef

Student: Jeroen Vanderstukken

Titel: Sets of polynomial equations, decompositions of higher-order tensors and multidimensional harmonic retrieval: connections and algorithms

Nederlandse titel: Stelsels veeltermvergelijkingen, hogere orde tensorontbindingen en multidimensionale *harmonic retrieval*: verbanden en algoritmes

UDC: 621.3

Korte inhoud:

Sets of multivariate polynomial equations arise frequently as the result of modeling in science and engineering. To solve such a system means finding all common roots of the polynomials. In his NPA, Stetter (2004) linked the problem to eigenvalue computations and brought it to the field of numerical linear algebra. Recently, Batselier and Dreesen (2013) built on NPA in their PNLA. Applying an ESPRIT-like reasoning that expresses the shift-invariance property of the multivariate monomials to a numerical basis for the null space of the system's Macaulay matrix, gives an EVD that reveals the common roots. This thesis brings the problem to the field of multilinear algebra: the algebra of higher-order tensors. In this thesis, a tensor is viewed as a higher-order generalization of a vector and a matrix, *i.e.* an array indexed by three or more indexes. A connection between symmetric higher-order tensors and homogeneous polynomials is long known in algebraic geometry. Yet, we take the well-known connections between univariate polynomial root-finding, linear algebra and HR and translate them into connections between their higher-order generalizations: 0-dimensional sets of polynomial equations, multilinear algebra and MHR. We rely on the shift-invariance properties in each mode in MHR to jointly exploit the shift-invariance in each variable present in the null space of the Macaulay matrix. The result is in an easily unique third-order tensor CPD that reveals the roots of the system. No difference between affine and projective roots exists in multilinear algebra. The CPD is exactly the joint EVD of the multiplication tables in NPA — opposed to only one EVD in PNLA. Taking roots with multiplicities into account, a third-order tensor BTD arises as a generalization of the CPD. The BTD is exactly the joint triangularization of the multiplication tables in NPA. It sheds a new light on the border rank, the problem of diverging rank-1 terms and the typical rank of a higher-order tensor. The established connections in this thesis can serve as a firm basis for future tensor computation-based and complex optimization-based multivariate polynomial root-finding algorithms.

Thesis voorgedragen tot het behalen van de graad van Master of Science in de ingenieurswetenschappen: wiskundige ingenieurstechnieken

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Assessoren: Prof. dr. ir. Marc Van Barel

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