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DECOUPLING MULTIVARIATE POLYNOMIALS USING FIRST-ORDER INFORMATION AND TENSOR DECOMPOSITIONS*

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Abstract. We present a method to decompose a set of multivariate real polynomials into linear combinations of univariate polynomials in linear forms of the input variables. The method proceeds by collecting the first-order information of the polynomials in a set of sampling points, which is captured by the Jacobian matrix evaluated at the sampling points. The canonical polyadic decomposition of the three-way tensor of Jacobian matrices directly returns the unknown linear relations as well as the necessary information to reconstruct the univariate polynomials. The conditions under which this decoupling procedure works are discussed, and the method is illustrated on several numerical examples.

Key words. polynomial, tensor decomposition, Waring problem, multilinear algebra, polynomial algebra

AMS subject classifications. 15A69, 11P05, 13P05

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1. Introduction.

1.1. Problem statement. The problem addressed in this paper is how to decouple a given set of multivariate real polynomials. Such a so-called decoupled representation expresses how the polynomials can be written as a linear combination of parallel univariate polynomials of linear forms of the input variables. Formally, the problem can be stated as follows: Consider a set of n multivariate real polynomials $f_i(u_1, \ldots, u_m)$ with $i = 1, \ldots, n$, of total degree[1] d in m variables. We wish to obtain a decomposition of the form

$$f_i(u_1, \ldots, u_m) = \sum_{j=1}^{r} w_{ij} \cdot g_j \left(\sum_{k=1}^{m} v_{kj} u_k \right) \quad \text{for } i = 1, \ldots, n,$$

where $g_j(x_j)$ are univariate polynomials of degree at most d. Generally, each $f_i(\mathbf{u})$ contains $\binom{m+d}{m}$ coefficients, of which many correspond to "coupled" monomials consisting of several variables u_i, e.g., u_1u_2, $u_1^2u_3$, $u_2u_3^3$, etc.

The decoupling task is visualized in Figure 1 and can be compactly represented using matrix-vector notation. Consider, therefore, the multivariate polynomial vector function $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^n$ that is defined as $\mathbf{f}(\mathbf{u}) := \begin{bmatrix} f_1(\mathbf{u}) & \ldots & f_n(\mathbf{u}) \end{bmatrix}^T$ in the variables $\mathbf{u} := (u_1, \ldots, u_m)$. A *decoupled representation* of $\mathbf{f}(\mathbf{u})$ is defined as

$$\mathbf{f}(\mathbf{u}) = \mathbf{W}\mathbf{g}(\mathbf{V}^T\mathbf{u}), \tag{1.1}$$

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[1]The total degree is defined as the maximal sum of the exponents of the variables in a term.

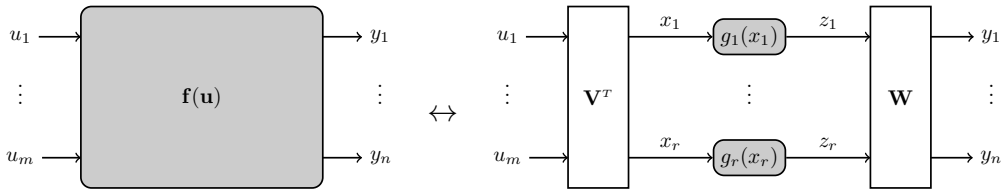

FIG. 1. *Decoupling problem. Find from the polynomial mapping* $\mathbf{y} = \mathbf{f}(\mathbf{u})$ *the transformations* $\mathbf{V}$ *and* $\mathbf{W}$ *and the mappings* $g_i(x_i)$ *that constitute the parallel structure* $\mathbf{f}(\mathbf{u}) = \mathbf{W}\mathbf{g}(\mathbf{V}^T\mathbf{u})$.

where $\mathbf{V} \in \mathbb{R}^{m\times r}$ and $\mathbf{W} \in \mathbb{R}^{n\times r}$ are linear transformation matrices that relate the input variables $\mathbf{u}$ and the output variables $\mathbf{y}$ to the internal variables $\mathbf{x}, \mathbf{z} \in \mathbb{R}^r$ by the relations $\mathbf{x} = \mathbf{V}^T\mathbf{u}$ and $\mathbf{y} = \mathbf{W}\mathbf{z}$, respectively. The function $\mathbf{g}\colon \mathbb{R}^r \to \mathbb{R}^r$ is defined as

$$\mathbf{g}(x_1, \ldots, x_r) = \begin{bmatrix} g_1(x_1) & \ldots & g_r(x_r) \end{bmatrix}^T$$

with $g_k : \mathbb{R} \to \mathbb{R}$. The number r corresponds to the number of internal univariate functions $g_i(x_i)$ and, as it will turn out, is closely related to the concept of *tensor rank*, as will be discussed in section 2.

The question may be studied in an exact or an approximate setting. For the exact case, the goal is to obtain an identical representation of a given set of polynomials, whereas in the nonexact case, an approximate representation (up to some degree of accuracy) is desired. The relevance of the question at hand is twofold: first, both in the exact and the nonexact setting, a decoupled representation may reveal new insights into a problem or may reduce the number of variables; second, in an approximate context, a decoupling may be useful to simplify a complex system.

In this paper, we will study the decoupling task in the exact sense: we seek a decoupled representation that *identically* matches a given set of multivariate polynomials, and we assume that it exists. In order to clearly convey the ideas, in Example 1 we show a simple instance of two polynomials that have a decoupled representation. Throughout the remainder of the paper, this simple example will be revisited to illustrate the results of the presented decoupling procedure.

Example 1. Consider the polynomials $f_1(u_1, u_2)$ and $f_2(u_1, u_2)$ of total degree $d = 3$, given as

$$\begin{aligned} y_1 &= f_1(u_1, u_2) \\ &= 54u_1^3 - 54u_1^2u_2 + 8u_1^2 + 18u_1u_2^2 + 16u_1u_2 - 2u_2^3 + 8u_2^2 + 8u_2 + 1, \qquad (1.2) \\ y_2 &= f_2(u_1, u_2) \\ &= -27u_1^3 + 27u_1^2u_2 - 24u_1^2 - 9u_1u_2^2 - 48u_1u_2 - 15u_1 + u_2^3 - 24u_2^2 - 19u_2 - 3. \qquad (1.3) \end{aligned}$$

Equations (1.2)–(1.3) were obtained from the decoupled structure

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ -3 & -1 \end{bmatrix} \begin{bmatrix} 2x_1^2 - 3x_1 + 1 \\ 2x_2^3 - x_2 \end{bmatrix} \quad \text{with} \quad \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -2 & -2 \\ -3 & -1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix},$$

revealing the internal univariate polynomials and the linear transformations at the input and output of the structure.

It will turn out that a decoupled representation $\mathbf{f}(\mathbf{u}) = \mathbf{W}\mathbf{g}(\mathbf{V}^T\mathbf{u})$ is not unique. To clearly make the distinction, the underlying representation (when it exists) will

henceforth be denoted by barred symbols, i.e., $\overline{\mathbf{f}}(\mathbf{u}) = \overline{\mathbf{W}}\overline{\mathbf{g}}(\overline{\mathbf{V}}^T\mathbf{u})$, whereas the result of the decoupling procedure will be denoted by nonbarred symbols, i.e., $\mathbf{f}(\mathbf{u}) = \mathbf{W}\mathbf{g}(\mathbf{V}^T\mathbf{u})$. Hence, for (1.2)–(1.3), we have

$$\overline{\mathbf{V}} = \begin{bmatrix} -2 & -3 \\ -2 & -1 \end{bmatrix},$$
$$\overline{\mathbf{W}} = \begin{bmatrix} 1 & 2 \\ -3 & 1 \end{bmatrix},$$
$$\overline{\mathbf{g}}(\overline{\mathbf{x}}) = \begin{bmatrix} \overline{g}_1(\overline{x}_1) \\ \overline{g}_2(\overline{x}_2) \end{bmatrix} = \begin{bmatrix} 2\overline{x}_1^2 - 3\overline{x}_1 + 1 \\ 2\overline{x}_2^3 - \overline{x}_2 \end{bmatrix}.$$

1.2. Related work and applications. The problem at hand is related to the Waring problem for polynomials [1, 21, 25, 28] which concerns the decomposition of a single homogeneous multivariate polynomial $f(u_1, \ldots, u_m)$ of degree d as

$$f(u_1, \ldots, u_m) = \sum_{i=1}^{r} w_i(v_1u_1 + \cdots + v_mu_m)^d,$$

in which r denotes the so-called Waring rank. Research on obtaining upper bounds on r, as well as developing algorithms for computing this decomposition, dates back to Sylvester, who solved the case $m = 2$ in 1886 [33]. The Waring decomposition for $m > 2$ and several extensions of the problem have attracted research activity ever since (see [1, 11, 21, 26] and references therein). Today, the problem still receives a lot of research attention, especially due to the bijective relation between the homogeneous Waring decomposition and the symmetric tensor decomposition [4, 10, 11, 22, 25, 26, 30, 36], of which the latter—and tensor methods in general—have become an important research domain in the last decades [22].

The problem we study is very reminiscent of the classical Waring problem, but we consider the *nonhomogeneous case* of *several polynomials*. The nonhomogeneous Waring problem is studied in [3, 29]. The simultaneous Waring problem for several homogeneous polynomials is studied in [5, 35]. In this paper, we will restrict our attention to the case in which the Waring rank is low, and we focus on the computation of the decomposition.

The decoupling task is of interest in nonlinear block-oriented system identification [18] and nonlinear state-space identification [27], where it is often desired to recover the internal structure of an identified static nonlinear mapping [30, 35, 37]. More generally, the task has connections with applications of tensor algebra methods in signal processing; see recent surveys [8, 9] and references therein.

1.3. Notation. Scalars are denoted by lowercase or uppercase letters. Vectors are denoted by lowercase boldface letters, e.g., $\mathbf{x} \in \mathbb{R}^r$. Elements of a vector are denoted by lowercase letters with an index as subscript, e.g., $\mathbf{x} = \begin{bmatrix} x_1 & \ldots & x_r \end{bmatrix}^T$. The Euclidean norm of a vector $\mathbf{x}$ is denoted as $\|\mathbf{x}\|$. When a vector is passed to a function as an argument, the notation $\mathbf{x} := (x_1, \ldots, x_r)$ is often used, e.g., $y_1 = f_1(u_1, u_2)$ (see also below). Matrices are denoted by uppercase boldface letters, e.g., $\mathbf{V} \in \mathbb{R}^{m\times r}$. The entry in the ith row and jth column of the matrix $\mathbf{V}$ is v_{ij}, and we may represent a matrix $\mathbf{V}$ as $\mathbf{V} = [v_{ij}]$. A matrix $\mathbf{V} \in \mathbb{R}^{m\times r}$ can be represented by its columns as $\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \ldots & \mathbf{v}_r \end{bmatrix}$. The transpose and pseudoinverse of a matrix $\mathbf{W}$ are denoted by $\mathbf{W}^T$ and $\mathbf{W}^\dagger$, respectively. A diagonal matrix with diagonal elements a_1, a_2, a_3 is denoted by $\mathrm{diag}(a_1, a_2, a_3)$ or $\mathrm{diag}(a_i)$. The rank of a matrix $\mathbf{A}$ is

denoted as rank($\mathbf{A}$). The dimension of the (right) null space of a matrix $\mathbf{A}$ is denoted by dim null $\mathbf{A}$. Higher-order tensors are N-way arrays and are denoted by boldface uppercase caligraphical letters, e.g., $\boldsymbol{\mathcal{J}} \in \mathbb{R}^{n \times m \times N}$. The outer product is denoted by $\circ$ and defined as follows: For $\boldsymbol{\mathcal{X}} = \mathbf{u} \circ \mathbf{v} \circ \mathbf{w}$, the entry in position (i, j, k) is $u_i v_j w_k$. The Frobenius norm of a tensor $\boldsymbol{\mathcal{X}}$ is denoted as $\|\boldsymbol{\mathcal{X}}\|_F$. For functions, we employ the same convention as above. Scalar functions are denoted by lowercase symbols, e.g., $f\colon \mathbb{R}^n \to \mathbb{R}$. Vector functions are denoted by lowercase bold symbols, e.g., $\mathbf{f}\colon \mathbb{R}^m \to \mathbb{R}^n$ with $\mathbf{f}(\mathbf{u}) := \begin{bmatrix} f_1(u_1, \ldots, u_m) & \ldots & f_n(u_1, \ldots, u_m) \end{bmatrix}^T$. Matrix functions are denoted by uppercase boldface symbols, e.g., the Jacobian of $\mathbf{f}$ is denoted by $\mathbf{J}\colon \mathbb{R}^m \to \mathbb{R}^{n \times m}$ and is defined as $\mathbf{J}(\mathbf{u}) := [\partial f_i / \partial u_j(\mathbf{u})]$. The derivative of a univariate function $g(x)$ is often denoted using the simplified representation $g'(x) := \mathrm{d}g(x)/\,\mathrm{d}x$. The ceiling function of a real number x is denoted by $\lceil x \rceil$ and defined as the smallest integer not less than x.

1.4. Outline of the paper. The remainder of this paper is organized as follows. Section 2 contains the description of the proposed approach that leads to a simultaneous matrix diagonalization problem, which is solved by a tensor decomposition. The method is presented and its properties are discussed. In section 3 we point out open problems for future work. Section 4 is devoted to the conclusions.

2. Method.

2.1. A simultaneous matrix diagonalization problem. The rationale behind the proposed method is to capture the behavior of $\mathbf{f}(\mathbf{u})$ by means of its first-order information collected in a set of sampling points. The first-order information of a nonlinear function $\mathbf{f}$ is contained in the Jacobian matrix of $\mathbf{f}(\mathbf{u})$, denoted by $\mathbf{J}(\mathbf{u})$ and defined as

$$\mathbf{J}(\mathbf{u}) := \begin{bmatrix} \dfrac{\partial f_1}{\partial u_1}(\mathbf{u}) & \ldots & \dfrac{\partial f_1}{\partial u_m}(\mathbf{u}) \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_n}{\partial u_1}(\mathbf{u}) & \ldots & \dfrac{\partial f_n}{\partial u_m}(\mathbf{u}) \end{bmatrix}. \tag{2.1}$$

By evaluating the Jacobian matrix in the sampling points $\mathbf{u}^{(k)}$, $k = 1, \ldots, N$, we will find that the decoupling task is solved by a simultaneous diagonalization of the set of Jacobian matrices $\mathbf{J}(\mathbf{u}^{(k)})$, obtained in this way.[2] After the transformations $\mathbf{V}$ and $\mathbf{W}$ are determined, the internal univariate $g_i(x_i)$ can also be reconstructed.

LEMMA 2.1. *The first-order derivatives of the parameterization* (1.1) *are given by*

$$\mathbf{J}(\mathbf{u}) = \mathbf{W}\, \mathrm{diag}\left(g_i'(\mathbf{v}_i^T \mathbf{u})\right) \mathbf{V}^T, \tag{2.2}$$

where $g_i'(x_i) := \mathrm{d}g_i(x_i)/\,\mathrm{d}x_i$.

Proof. The parameterization (1.1) is written more conveniently as

$$\mathbf{f}(\mathbf{u}) = \mathbf{W} \begin{bmatrix} g_1(\mathbf{v}_1^T \mathbf{u}) & \ldots & g_r(\mathbf{v}_r^T \mathbf{u}) \end{bmatrix}^T,$$

from which the lemma immediately follows by applying the chain rule. ∎

[2] In the classical literature, the simultaneous (or joint) diagonalization refers to the simultaneous congruence transformation $\mathbf{A}_k = \mathbf{V}\mathbf{D}_k\mathbf{V}^T$, where the $\mathbf{A}_k$ are square matrices. (See [7] for a recent survey paper.) In this paper, simultaneous diagonalization concerns the nonsymmetrical problem $\mathbf{A}_k = \mathbf{W}\mathbf{D}_k\mathbf{V}^T$, where, in addition to having different linear transformations on the left and on the right, the matrices $\mathbf{A}_k$ are not necessarily square.

Lemma 2.1 implies that the first-order derivatives of the parameterization (1.1), evaluated at the points $\mathbf{u}^{(k)}$, lead to the simultaneous diagonalization of a set of matrices

$$\mathbf{J}(\mathbf{u}^{(k)}) = \mathbf{W}\,\mathrm{diag}(g_i'(\mathbf{v}_i^T\mathbf{u}^{(k)}))\mathbf{V}^T,$$

in which the matrix factors $\mathbf{W}$ and $\mathbf{V}$ do not depend on the choice of the sampling point $\mathbf{u}^{(k)}$. Simultaneous matrix diagonalization can be computed by tensor methods. Let us illustrate this for the simultaneous matrix diagonalizaton problem that we encounter in the decoupling task. Consider the factorizations of the Jacobian matrices $\mathbf{J}(\mathbf{u}^{(k)})$ and their rank-one expansions

$$\mathbf{J}(\mathbf{u}^{(1)}) = \mathbf{W}\mathbf{D}^{(1)}\mathbf{V}^T = \mathbf{w}_1 d_1^{(1)}\mathbf{v}_1^T + \cdots + \mathbf{w}_r d_r^{(1)}\mathbf{v}_r^T, \tag{2.3}$$

$$\mathbf{J}(\mathbf{u}^{(2)}) = \mathbf{W}\mathbf{D}^{(2)}\mathbf{V}^T = \mathbf{w}_1 d_1^{(2)}\mathbf{v}_1^T + \cdots + \mathbf{w}_r d_r^{(2)}\mathbf{v}_r^T, \tag{2.4}$$

$$\vdots \qquad\qquad \vdots$$

$$\mathbf{J}(\mathbf{u}^{(N)}) = \mathbf{W}\mathbf{D}^{(N)}\mathbf{V}^T = \mathbf{w}_1 d_1^{(N)}\mathbf{v}_1^T + \cdots + \mathbf{w}_r d_r^{(N)}\mathbf{v}_r^T, \tag{2.5}$$

where $\mathbf{W} := [\ \mathbf{w}_1 \quad \ldots \quad \mathbf{w}_r\ ]$ and $\mathbf{V} := [\ \mathbf{v}_1 \quad \ldots \quad \mathbf{v}_r\ ]$ are common factors to all Jacobian matrices and $\mathbf{D}^{(k)} := \mathrm{diag}(d_1^{(k)}, \ldots, d_r^{(k)})$ with $d_i^{(k)} = g_i'(\mathbf{v}^T\mathbf{u}^{(k)})$ by Lemma 2.1.

We stack the Jacobian evaluations $\mathbf{J}(\mathbf{u}^{(k)})$ behind each other into a three-way tensor $\boldsymbol{\mathcal{J}}$ of dimensions $n \times m \times N$. From the rank-one expansions in (2.3)–(2.5), we see that the simultaneous matrix diagonalization problem is equivalent to expressing tensor $\boldsymbol{\mathcal{J}}$ as a (minimal) sum of rank-one tensor terms, which is called the *canonical polyadic decomposition* (CP decomposition) [6, 20, 22]

$$\boldsymbol{\mathcal{J}} = \sum_{i=1}^{r} \mathbf{w}_i \circ \mathbf{v}_i \circ \mathbf{h}_i, \tag{2.6}$$

where $\circ$ denotes the outer product and $\mathbf{h}_i$ contains the evaluations of the $g_i'(\mathbf{v}_i^T\mathbf{u})$ in the N sampling points as

$$\mathbf{h}_i = \left[\ g_i'(\mathbf{v}_i^T\mathbf{u}^{(1)}) \quad \ldots \quad g_i'(\mathbf{v}_i^T\mathbf{u}^{(N)})\ \right]^T. \tag{2.7}$$

In the remainder of this paper, we will often refer to the CP decomposition of $\boldsymbol{\mathcal{J}}$ into the factors $\mathbf{W}$, $\mathbf{V}$, and $\mathbf{H} := [\ \mathbf{h}_1 \quad \ldots \quad \mathbf{h}_r\ ]$, by which we mean (2.6). Figure 2 gives an overview of the simultaneous matrix diagonalization question and the CP decomposition.

2.2. Uniqueness and computation of the canonical polyadic decomposition.

2.2.1. Kruskal-like uniqueness conditions. Two aspects can easily be observed in the CP decomposition (2.6) that prohibit the unique retrieval of the factors $\mathbf{V}$, $\mathbf{W}$, and $\mathbf{H}$. By rewriting (2.6) as $\boldsymbol{\mathcal{J}} = \sum_{i=1}^{r}(\alpha_i\mathbf{w}_i) \circ (\beta_i\mathbf{v}_i) \circ (\gamma_i\mathbf{h}_i)$ with $\alpha_i\beta_i\gamma_i = 1$, a columnwise scaling invariance becomes clear. Additionally, the specific order in which the r terms are collected into the factor matrices $\mathbf{V}$, $\mathbf{W}$, and $\mathbf{H}$ gives rise to an admissible permutation of the columns of the factors.

The term *essential uniqueness* is used to denote the uniqueness of the CP decomposition up to the columnwise scaling and permutation of the columns. Henceforth, we will use the term uniqueness when we refer to essential uniqueness. Kruskal [23, 24] has derived a condition that guarantees uniqueness of the CP decomposition. Essentially it provides an upper bound on the rank of a tensor in order to have a unique CP decomposition. We denote by $k_{\mathbf{X}}$ the *Kruskal rank of a matrix* $\mathbf{X}$, which is defined

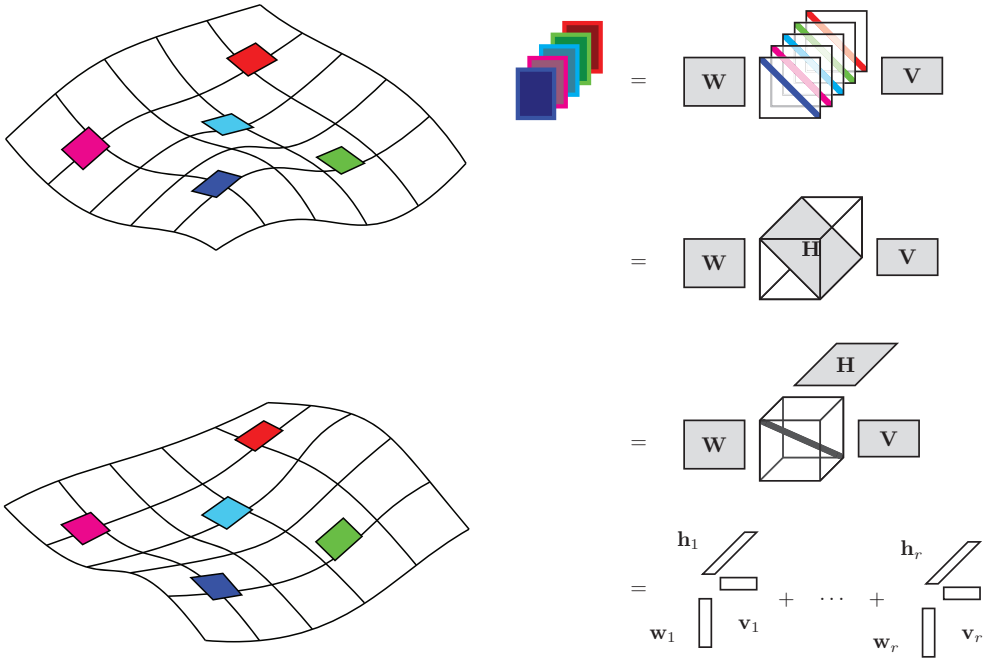

FIG. 2. *The first-order information of* $\mathbf{f}(\mathbf{u})$ *is collected in a set of sampling points* $\mathbf{u}^{(k)}$ *with* $k = 1, \ldots, N$ *(indicated by the colored patches on the surfaces shown in* (a)*). The corresponding Jacobian matrices* $\mathbf{J}(\mathbf{u}^{(k)})$ *are placed in a three-way tensor* (b). *Lemma* 2.1 *states that each Jacobian matrix* $\mathbf{J}(\mathbf{u}^{(k)})$ *can be written as* $\mathbf{J}(\mathbf{u}^{(k)}) = \mathbf{W}\,\mathrm{diag}(g_i'(\mathbf{v}_i^T\mathbf{u}^{(k)}))\mathbf{V}^T$. *This results in a simultaneous matrix diagonalization problem, which is computed by the CP decomposition.*

as the largest number k for which any set of k columns of $\mathbf{X}$ is linearly independent. We will state two results regarding the uniqueness of the CP decomposition of an $I \times J \times K$ tensor $\boldsymbol{\mathcal{T}}$ satisfying

$$\boldsymbol{\mathcal{T}} = \sum_{i=1}^{r} \mathbf{a}_i \circ \mathbf{b}_i \circ \mathbf{c}_i$$

with factor matrices $\mathbf{A} := [\ \mathbf{a}_1\ \ldots\ \mathbf{a}_R\ ]$, $\mathbf{B} := [\ \mathbf{b}_1\ \ldots\ \mathbf{b}_R\ ]$ and $\mathbf{C} := [\ \mathbf{c}_1\ \ldots\ \mathbf{c}_R\ ]$ of compatible dimensions.

THEOREM 2.2 (Kruskal [23, 24]). *The CP decomposition of* $\boldsymbol{\mathcal{T}}$ *is unique, provided that*

$$k_{\mathbf{A}} + k_{\mathbf{B}} + k_{\mathbf{C}} \geq 2R + 2. \tag{2.8}$$

The following theorem provides a stronger condition than Theorem 2.2 but starts from more restrictive assumptions.

THEOREM 2.3 (De Lathauwer [12]). *The CP decomposition of* $\boldsymbol{\mathcal{T}}$ *is generically*[3] *unique for* $R \leq K$ *if*

$$I(I-1)J(J-1) \geq 2R(R-1).$$

[3] A property is called to hold *generically* if it holds everywhere, except for a set of Lebesgue measure zero [12]. An instance in which the genericity condition holds is when the factor matrices are sampled randomly from a continuous distrubution [15].

For the decoupling task, it is more practical to think of the uniqueness conditions in terms of the number of inputs m and outputs n of the nonlinear function $\mathbf{f}(\mathbf{u})$. In generic conditions and with $N \geq r$, we find from Theorem 2.3 the condition

$$m(m-1)n(n-1) \geq 2r(r-1). \tag{2.9}$$

One has to keep in mind that the above uniqueness conditions cannot be assessed prior to the decoupling task. The rank conditions on the factors $\mathbf{V}$ and $\mathbf{W}$ depend on the structure underlying the function $\mathbf{f}(\mathbf{u})$, and the user only has control over the choice of the sampling points $\mathbf{u}^{(k)}$, which influence factor $\mathbf{H}$ through (2.7). Nevertheless, the uniqueness conditions provide us with an intuition regarding the admissible number of inputs m, outputs n, and internal functions r. The condition (2.9) is useful as the number of sampling points N can be chosen sufficiently large, and genericity is a common assumption. Theorem 2.2 is mentioned for completeness; it is a rather weak condition but does not require further assumptions on $\boldsymbol{\mathcal{T}}$. Finally, it should be noted that these conditions are quite reasonable in terms of number of inputs, outputs, and number of internal $g_i(x_i)$.

2.2.2. Computing the canonical polyadic decomposition. If the CP decomposition holds in the exact sense (exact equality in (2.6)), algebraic algorithms can be employed to compute the CP decomposition [12, 16]. These algorithms are called "algebraic" since they compute the CP decomposition by means of linear algebra tools such as (generalized) eigendecompositions. The exposition of this paper could be set into a purely linear algebraic framework. However, we have deliberately not opted for such an algebraic approach to solving the decoupling task, but rather phrase the problem in the language of tensor decompositions and propose to solve the latter using optimization-based tools.

The optimization-based tensor decompositions point-of-view was chosen for the following reasons. The algebraic approach is known to be sensitive to perturbations on tensor entries but is in practice used to initialize optimization-based algorithms [16]. We, therefore, suggest the tensor-based framework as the proper starting point for the more general approximate or noisy instance of the decoupling task, as explored briefly in [17]. Even though optimization-based algorithms do not formally guarantee to retrieve the (globally optimal) solution, the recent interest in tensor decomposition algorithms has spawned a host of fast and reliable methods [2, 31, 32]. Numerical results reported in the remainder of this article were obtained using Tensorlab [32], using the default settings. Computation times of the CP decompositions were negligible (under one hundredth of a second on a common laptop computer).

Remark 1. The uniqueness conditions do not imply that an optimization routine computing the CP decomposition is not harmed by the problem of local minima: The result states that if the approximation error of the CP decomposition is zero, the retrieved factors are (essentially) identical to the underlying factors.

2.3. Tensor rank. The integer r has occurred in the above as the number of internal mappings $g_i(x_i)$ in the decoupled structure and as the number of terms in the CP decomposition. In the latter sense, the smallest integer r for which (2.6) holds exactly is the definition of the rank of the tensor $\boldsymbol{\mathcal{J}}$. As opposed to the matrix rank, which is smaller than the smallest dimension, it is possible that $\operatorname{rank} \boldsymbol{\mathcal{J}} > \max(m, n, N)$. This also means that the number of internal mappings $g_i(x_i)$ may exceed the number of inputs and/or outputs.

Determining the value for r is a part of the decoupling procedure. As opposed to the matrix case, where the (numerical) rank can be determined using the singular value

decomposition [19], there are currently no easy ways to determine the (numerical) rank of a given tensor. In practice, the tensor rank r is determined by assessing the approximation error of the rank-r approximation of a tensor for consecutive values of r by computing its CP decomposition. For the exact decoupling task, the CP decomposition will indeed reach an approximation error that is sufficiently close to machine precision when the correct r is checked.

Remark 2. There exists notions of typical and generic rank of a tensor, as well as upper bounds on the rank, that are known for specific cases [34]. Furthermore, it can be shown that $\operatorname{rank} \boldsymbol{\mathcal{J}} \leq \min(mn, mN, nN)$ [22]. Since the number of sampling points N is typically chosen (much) larger than m and n, we have $\operatorname{rank} \boldsymbol{\mathcal{J}} \leq mn$.

Example 2. We revisit (1.2)–(1.3) from Example 1. We choose $N = 2$ sampling points $\mathbf{u}^{(k)}$ and their corresponding Jacobians $\overline{\mathbf{J}}(\mathbf{u}^{(k)})$, as

$$\mathbf{u}^{(1)} = \begin{bmatrix} -1 \\ 0 \end{bmatrix}, \qquad \overline{\mathbf{J}}(\mathbf{u}^{(1)}) = \begin{bmatrix} 146 & -62 \\ -48 & 56 \end{bmatrix},$$
$$\mathbf{u}^{(2)} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}, \qquad \overline{\mathbf{J}}(\mathbf{u}^{(2)}) = \begin{bmatrix} 434 & -158 \\ -192 & 104 \end{bmatrix},$$

giving rise to a $2 \times 2 \times 2$ tensor $\overline{\boldsymbol{\mathcal{J}}}$. Since we know that $\overline{r} = 2$ and Kruskal's uniqueness condition (2.8) guarantees uniqueness if $r \leq 2$, the choice $N = 2$ is justified. It can be verified that the tensor can be decomposed using a rank-two CP decomposition up to a relative error of 1.64×10^{-16}, which confirms $r = 2$ as expected.

The internal $\overline{\mathbf{x}}^{(k)}$ can be computed using the expression $\overline{\mathbf{x}} = \overline{\mathbf{V}}^T \mathbf{u}$, leading to

$$\overline{\mathbf{x}}^{(1)} = \begin{bmatrix} 2 \\ -3 \end{bmatrix} \quad \text{and} \quad \overline{\mathbf{x}}^{(2)} = \begin{bmatrix} 2 \\ 5 \end{bmatrix},$$

from which we can also compute the entries of $\overline{\mathbf{H}}$ using $\overline{h}_{ki} = \overline{g}_i'(\overline{x}_i^{(k)})$:

$$\overline{\mathbf{H}} = \begin{bmatrix} 5 & 26 \\ 5 & 74 \end{bmatrix}.$$

The CP decomposition is computed using Tensorlab [32] and returns three factors, $\mathbf{V}$, $\mathbf{W}$, and $\mathbf{H}$, equal to the true factors up to a scaling and permutation of the columns as[4]

$$\mathbf{V} = \begin{bmatrix} -512.1246 & -31.6350 \\ 170.7082 & -31.6350 \end{bmatrix} = \begin{bmatrix} -2 & 3 \\ -2 & -1 \end{bmatrix} \begin{bmatrix} 0 & 15.8175 \\ -170.7082 & 0 \end{bmatrix},$$

$$\mathbf{W} = \begin{bmatrix} -0.9189 & -0.4470 \\ 0.4595 & 1.3411 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ -3 & 1 \end{bmatrix} \begin{bmatrix} 0 & -0.4470 \\ -0.4595 & 0 \end{bmatrix},$$

$$\mathbf{H} = \begin{bmatrix} 0.3315 & -0.7071 \\ 0.9435 & -0.7071 \end{bmatrix} = \begin{bmatrix} 5 & 26 \\ 5 & 74 \end{bmatrix} \begin{bmatrix} 0 & -0.1414 \\ 0.0127 & 0 \end{bmatrix}.$$

It can easily be verified that the product of the scaling factors for the three factors yields unity for both columns.

[4]Due to the lack of *global* uniqueness, the numerical result of the CP decomposition may differ between executions, as well as when using a different routine for computing the CP decomposition.

2.4. Reconstructing the internal functions $g_i(x_i)$. In this section we will describe how the coefficients of $g_i(x_i)$ are obtained from the retrieved $\mathbf{V}$ and $\mathbf{W}$, using input-output pairs $(\mathbf{u}^{(k)}, \mathbf{y}^{(k)})$.[5] We can write each output $\mathbf{y}^{(k)}$ as a linear function of the coefficients $c_{i,j}$ and combine them into a block-equation system from which the coefficients can be determined.

2.4.1. Block-Vandermonde-like linear system. Recall that we have $\mathbf{y} = \mathbf{W}\mathbf{g}(\mathbf{x})$, which we write more conveniently as

$$\mathbf{y} = \mathbf{W} \begin{bmatrix} c_{1,0} + c_{1,1}x_1 + \cdots + c_{1,d}x_1^d \\ \cdots \\ c_{r,0} + c_{r,1}x_r + \cdots + c_{r,d}x_r^d \end{bmatrix},$$

where $c_{i,j}$ denote the coefficients of the ith polynomial $g_i(x_i)$. The coefficients $c_{i,j}$ can then be combined into a single coefficient vector, leading to

$$\mathbf{y} = \mathbf{W} \left[\begin{array}{cccc|c|cccc} 1 & x_1 & \dots & x_1^d & & & & & \\ & & & & \ddots & & & & \\ & & & & & 1 & x_r & \dots & x_r^d \end{array}\right] \begin{bmatrix} c_{1,0} \\ c_{1,1} \\ \vdots \\ \underline{c_{1,d}} \\ \vdots \\ \overline{c_{r,0}} \\ c_{r,1} \\ \vdots \\ c_{r,d} \end{bmatrix}, \tag{2.10}$$

where the empty entries correspond to zeros. Since $\mathbf{V}$ and $\mathbf{W}$ have been derived from the CP decomposition, we can compute $\mathbf{x}^{(k)} = \mathbf{V}^T\mathbf{u}^{(k)}$ for a given sampling point $\mathbf{u}^{(k)}$. By combining several instances of (2.10) in this way for $k = 1, \dots, K$, the coefficients can be estimated using the linear system

(2.11)

$$\begin{bmatrix} \mathbf{y}^{(1)} \\ \vdots \\ \mathbf{y}^{(K)} \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{W} & & \\ & \ddots & \\ & & \mathbf{W} \end{bmatrix} \underbrace{\left[\begin{array}{cccc|c|cccc} 1 & x_1^{(1)} & \dots & (x_1^{(1)})^d & & & & & \\ & & & & \ddots & & & & \\ & & & & & 1 & x_r^{(1)} & \dots & (x_r^{(1)})^d \\ \hline & & \dots & & & & & & \\ \hline 1 & x_1^{(K)} & \dots & (x_1^{(K)})^d & & & & & \\ & & & & \ddots & & & & \\ & & & & & 1 & x_r^{(K)} & \dots & (x_r^{(K)})^d \end{array}\right]}_{\mathbf{X}_K} \begin{bmatrix} c_{1,0} \\ c_{1,1} \\ \vdots \\ \underline{c_{1,d}} \\ \vdots \\ \overline{c_{r,0}} \\ c_{r,1} \\ \vdots \\ c_{r,d} \end{bmatrix}}_{\mathbf{R}_K},$$

where the empty entries represent (block) zeros. The block-diagonal matrix with $\mathbf{W}$

[5] Other methods exist to retrieve the coefficients of $g_i(x_i)$, for instance, by using the fact that the factor $\mathbf{H}$ contains information about the differentiated $g_i(x_i)$ as in (2.7). Such *fitting and integration* methods may be of interest in the nonexact case, where the additional information can be helpful to obtain a better approximation, but they are not discussed in the current paper.

blocks has size $Kn \times Kr$, the block-Vandermonde-like matrix $\mathbf{X}_K$ has size $Kr \times r(d+1)$, and their product $\mathbf{R}_K$ has size $Kn \times r(d+1)$. We introduce the short-hand notation $\mathbf{y}_K = \mathbf{R}_K \mathbf{c}$ as a compact way to represent (2.11).

2.4.2. Existence and uniqueness of solutions. Let us investigate the existence and uniqueness aspects of (2.11), where we assume that K is sufficiently large for the time being (i.e., $K \gg d+1$). Since the outputs $\mathbf{y}^{(k)}$ are constructed using $\mathbf{y} = \mathbf{W}\mathbf{g}(\mathbf{V}^T\mathbf{u})$, it can be understood immediately that a solution of (2.11) always exists (in the exact sense).

Understanding whether (2.11) has a *unique* solution requires investigating the rank of $\mathbf{R}_K$. The system $\mathbf{y}_K = \mathbf{R}_K\mathbf{c}$ has a unique solution if $\mathbf{R}_K$ has full rank. We immediately see that the rank of $\mathbf{R}_K$ will depend on whether $\mathbf{W}$ has full rank and on the choice of sampling points $\mathbf{u}^{(k)}$, which determine $x_i^{(k)}$ through the relation $\mathbf{x}^{(k)} = \mathbf{V}^T\mathbf{u}^{(k)}$.

Recall that $\mathbf{X}_K$ contains in its rows Vandermonde vectors constructed from the x_i-variables evaluated at K sampling points. Furthermore, the rank of $\mathbf{X}_K$ can be assessed for each of the x_i-blocks seperately, since a single row of $\mathbf{X}_K$ contains powers of $x_i^{(k)}$ for one specific i only. Due to the Vandermonde-like structure and the assumption that $K \gg d+1$, the matrix $\mathbf{X}_K$ will only drop rank in the pathological case that $x_i^{(1)} = x_i^{(2)} = \cdots = x_i^{(K)}$ for one or more $i = 1, \ldots, r$. Tracing this back to the choice of the operating points $\mathbf{u}^{(k)}$, we find that this happens if (and only if) $\mathbf{u}^{(k)} = \mathbf{v}_i^T(\tilde{\mathbf{u}} + \mathbf{u}_0^{(k)})$, where $\tilde{\mathbf{u}}$ may assume any value and $\mathbf{v}_i^T\mathbf{u}_0^{(k)} = 0$. In practice, the sampling points $\mathbf{u}^{(k)}$ are typically drawn from some random distribution, for which the above pathological cases do not occur.

To assess the influence of $\mathbf{W}$, we make use of the fact that certain columns of the Vandermonde-like matrix $\mathbf{X}_K$ consist of ones only. By reordering the columns of $\mathbf{X}_K$ such that the columns containing the ones (corresponding to the constant terms $c_{i,0}$) are placed on the left-hand side, the system $\mathbf{y}_K = \mathbf{R}_K\mathbf{c}$ becomes $\mathbf{y}_K = \overline{\mathbf{R}}_K\overline{\mathbf{c}}$, where

$$\overline{\mathbf{R}}_K = \left[\begin{array}{c|ccc} \mathbf{W} & \times_1 & \ldots & \times_r \\ \vdots & \vdots & & \vdots \\ \mathbf{W} & \times_1 & \ldots & \times_r \end{array}\right]$$

is the column-reordered version of $\mathbf{R}_K$ and $\overline{\mathbf{c}}$ represents the corresponding reordered coefficient vector. An immediate consequence is that the matrices $\mathbf{W}$ and $\overline{\mathbf{R}}_K$ (and hence $\mathbf{R}_K$) share the same column rank-deficiency: the block-column containing the matrices $\mathbf{W}$ has the same column rank as $\mathbf{W}$, whereas the right-hand side part of $\overline{\mathbf{R}}_K$ (represented using the entries $\times_i$) contains the powers of the $x_i^{(k)}$ and has full column rank if the sampling points $\mathbf{u}^{(k)}$ are taken sufficiently general (that is, discarding the pathological cases described in the previous paragraph).

Rank-deficiency of $\mathbf{W}$ occurs for example when there are fewer outputs n than internal functions r, so that $r - \operatorname{rank}\mathbf{W}$ coefficients $c_{i,0}$ can be chosen freely, while $\mathbf{y}_K = \mathbf{R}_K\mathbf{c}$ remains exactly solvable. Remark that the "free parameters" are the constant terms $c_{i,0}$ only, as they correspond to the columns that form the $\mathbf{W}$ block in $\overline{\mathbf{R}}_K$.

The above considerations give rise to a straightforward way to determine the minimal number of sampling points K that is required to obtain an exactly solvable

system. The system (2.11) should become sufficiently overdetermined, meaning that the number of rows of $\mathbf{R}_K$ should be at least equal to the rank of $\mathbf{R}_K$. We have thus $Kn \geq \operatorname{rank} \mathbf{R}_K$, which directly leads to the condition

$$K \geq \left\lceil \frac{r(d+1) - \dim \operatorname{null} \mathbf{W}}{n} \right\rceil. \tag{2.12}$$

Example 3. We revisit once again (1.2)–(1.3) and show how the $g_i(x_i)$ are reconstructed. We compute the minimal value for $K \geq 4$ using the formula (2.12) and choose $K = 4$ sampling points $\mathbf{u}^{(k)}$, the corresponding outputs $\mathbf{y}^{(k)}$, and the internal variables $\mathbf{x}^{(k)} = \mathbf{V}^T \mathbf{u}^{(k)}$ as

$$\mathbf{u}^{(1)} = \begin{bmatrix} -0.20 \\ 0 \end{bmatrix}, \quad \mathbf{y}^{(1)} = \begin{bmatrix} 0.8880 \\ -0.7440 \end{bmatrix}, \quad \mathbf{x}^{(1)} = \begin{bmatrix} 102.4249 \\ 6.3270 \end{bmatrix},$$

$$\mathbf{u}^{(2)} = \begin{bmatrix} 0.25 \\ -2.00 \end{bmatrix}, \quad \mathbf{y}^{(2)} = \begin{bmatrix} 51.0938 \\ -63.0469 \end{bmatrix}, \quad \mathbf{x}^{(2)} = \begin{bmatrix} -469.4476 \\ 55.3612 \end{bmatrix},$$

$$\mathbf{u}^{(3)} = \begin{bmatrix} 0.50 \\ 0.25 \end{bmatrix}, \quad \mathbf{y}^{(3)} = \begin{bmatrix} 11.4063 \\ -30.7032 \end{bmatrix}, \quad \mathbf{x}^{(3)} = \begin{bmatrix} -213.3853 \\ -23.7262 \end{bmatrix},$$

$$\mathbf{u}^{(4)} = \begin{bmatrix} 0 \\ 0.50 \end{bmatrix}, \quad \mathbf{y}^{(4)} = \begin{bmatrix} 6.7500 \\ -18.3750 \end{bmatrix}, \quad \mathbf{x}^{(4)} = \begin{bmatrix} 85.3541 \\ -15.8175 \end{bmatrix}.$$

We construct the 8×8 matrix $\mathbf{R}_K$, having rank 8. Solving (2.11) returns the coefficients $c_{i,j}$, and we find

$$\begin{aligned} g_1(x_1) &= -0.0127 x_1^3 - 4.3751 \times 10^{-7} x_1, \\ g_2(x_2) &= -0.0179 x_2^2 + 0.4243 x_2 - 2.2369. \end{aligned}$$

We verify that $\overline{\mathbf{f}}(\mathbf{u})$ corresponds to $\mathbf{f}(\mathbf{u})$ up to a relative error on the coefficients (i.e., $\|\mathbf{c} - \overline{\mathbf{c}}\|/\|\overline{\mathbf{c}}\|$) of 0.0925×10^{-14} for f_1 and 0.1302×10^{-14} for f_2. We notice that $g_i(x_i) \neq \overline{g}_i(\overline{x}_i)$; in section 2.4.3 we will discuss the exact relation between the coefficients of $g_i(x_i)$ and $\overline{g}_i(\overline{x}_i)$.

Example 4. We present an example for which $m = n = 3$ and $r = 4$, in which the matrix $\mathbf{W}$ is column rank-deficient. It can be verified that uniqueness conditon (2.8) holds. Consider the equations

$$\begin{aligned} \overline{f}_1(u_1, u_2, u_3) &= -4u_1^2 + 8u_1u_3 + 6u_1 - 3u_3^2 - 8u_3 - 6, \\ \overline{f}_2(u_2, u_2, u_3) &= 2u_1^2 - 4u_1u_3 - 3u_1 + u_2^3 + 6u_2^2u_3 \\ &\quad + 12u_2u_3^2 - u_2 + 8u_3^3 + 2u_3^2 + u_3 + 3, \\ \overline{f}_3(u_1, u_2, u_3) &= -2u_1^2 + 4u_1u_3 + 4u_1 - 2u_3^2 - 3u_3 - u_2 - 8, \end{aligned}$$

which were obtained as $\overline{f}(\mathbf{u}) = \overline{\mathbf{W}}\overline{\mathbf{g}}(\overline{\mathbf{V}}^T\mathbf{u})$ with

$$\overline{\mathbf{V}} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & -1 \\ -1 & 2 & 1 & 0 \end{bmatrix},$$

$$\overline{\mathbf{W}} = \begin{bmatrix} -2 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}, \quad \text{and}$$

$$\overline{\mathbf{g}}(\overline{\mathbf{x}}) = \begin{bmatrix} 2x_1^2 - 3x_1 + 3 \\ x_2^3 - x_2 \\ x_3^2 - 2x_3 \\ x_4 - 5 \end{bmatrix}.$$

We evaluate the Jacobian of $\overline{\mathbf{f}}(\mathbf{u})$ in the $N = 4$ points (N is chosen such that $N \geq r$)

$$\mathbf{u}^{(1)} = \begin{bmatrix} -0.2500 \\ 0 \\ 0.3333 \end{bmatrix}, \quad \mathbf{u}^{(2)} = \begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix}, \quad \mathbf{u}^{(3)} = \begin{bmatrix} 1 \\ 0.5000 \\ 0.3333 \end{bmatrix}, \quad \mathbf{u}^{(4)} = \begin{bmatrix} 0.3333 \\ 0 \\ -0.6667 \end{bmatrix},$$

which leads to a $3 \times 3 \times 4$ tensor $\boldsymbol{\mathcal{J}}$. The CP decomposition is computed with Tensorlab [32] and returns a rank-four representation with a relative error $\|\boldsymbol{\mathcal{J}} - \hat{\boldsymbol{\mathcal{J}}}\|_F / \|\boldsymbol{\mathcal{J}}\|_F$ of 6.40×10^{-14} and returns the factors

$$\mathbf{V} = \begin{bmatrix} 0.0000 & -0.3464 & 0.0000 & 1.6749 \\ 1.0821 & 0.3464 & 0.0000 & 0.0000 \\ 2.1641 & 0.0000 & -1.6455 & -1.6749 \end{bmatrix},$$

$$\mathbf{W} = \begin{bmatrix} 0.0000 & 0.0000 & -1.5072 & -1.9387 \\ 2.2561 & 0.0000 & 0.0000 & 0.9693 \\ 0.0000 & 0.4803 & 0.0000 & -0.9693 \end{bmatrix},$$

$$\mathbf{H} = \begin{bmatrix} 0.1365 & -6.0104 & -0.5376 & -3.2850 \\ 0.8193 & -6.0104 & -0.8064 & -1.8478 \\ 1.2630 & -6.0104 & -0.5376 & -0.2053 \\ 1.7751 & -6.0104 & -1.3440 & 0.6159 \end{bmatrix},$$

which can be related to the underlying factors $\overline{\mathbf{V}}$, $\overline{\mathbf{W}}$ and $\overline{\mathbf{H}}$.

Formula (2.12) tells us that we need $K \geq 5$ points to reconstruct the internal mappings $g_i(x_i)$ so we add

$$\mathbf{u}^{(5)} = \begin{bmatrix} 0.3750 \\ -0.6667 \\ 1.0000 \end{bmatrix}$$

to have available $K = 5$ points $\mathbf{u}^{(k)}$ and the corresponding $\mathbf{y}^{(k)}$. We construct the matrix $\mathbf{R}_K$ of size 15×16 and verify that its rank equals 15. From the solution of the system (2.11) we retrieve the internal functions as

$$\begin{aligned} g_1(x_1) &= 0.3499x_1^3 - 0.4096x_1 - 2.2163, \\ g_2(x_2) &= -6.0104x_2, \\ g_3(x_3) &= -0.2450x_3^2 - 0.8064x_3 - 6.6347, \\ g_4(x_4) &= 0.7355x_4^2 - 1.8478x_4 + 8.2530. \end{aligned}$$

Ultimately the complete input-output mapping $\mathbf{f}(\mathbf{u}) = \mathbf{W}\mathbf{g}(\mathbf{V}^T\mathbf{u})$ is reconstructed with a relative error on the coefficients (i.e., $\|\mathbf{c} - \overline{\mathbf{c}}\|/\|\overline{\mathbf{c}}\|$) of 1.3807×10^{-12} for f_1, 1.7105×10^{-12} for f_2, and 1.8102×10^{-11} for f_3.

2.4.3. Relation $g_i(x_i)$ to $\overline{g}_i(\overline{x}_i)$. Since the factors $\mathbf{V}$, $\mathbf{W}$, and $\mathbf{H}$ are only identifiable up to scaling and permutation of the columns, the reconstruction of the $g_i(x_i)$ will differ from one representation to the other. As it turns out, nonlinear relations between the coefficients of $g_i(x_i)$ in the the different (equivalent) representations will show up.

Let us denote by $\mathbf{V} = \overline{\mathbf{V}}\mathbf{D}_\beta$ and $\mathbf{W} = \overline{\mathbf{W}}\mathbf{D}_\alpha$ the relationship between the representations of the factors $\overline{\mathbf{V}}$ and $\mathbf{V}$, and $\overline{\mathbf{W}}$ and $\mathbf{W}$, respectively, which is caused by the columnwise scaling and permutation invariance of the CP decomposition. Without loss of generality, we will discard the case of a column permutation in the exposition, implying that $\mathbf{D}_\alpha$ and $\mathbf{D}_\beta$ are diagonal $r \times r$ matrices containing the columnwise scaling factors α_i and β_i for $\mathbf{V}$ and $\mathbf{W}$, respectively. This implies that the ith scaling factors α_i and β_i are associated with the ith columns of $\mathbf{V}$ and $\overline{\mathbf{V}}$, $\mathbf{W}$ and $\overline{\mathbf{W}}$, and the ith univariate functions $g_i(x_i)$ and $\overline{g}_i(\overline{x}_i)$.

We have now that $\overline{\mathbf{f}}(\mathbf{u}) = \mathbf{f}(\mathbf{u})$ and $\mathbf{V} = \overline{\mathbf{V}}\mathbf{D}_\alpha$ and $\mathbf{W} = \overline{\mathbf{W}}\mathbf{D}_\beta$, leading to

$$\overline{\mathbf{W}}\overline{\mathbf{g}}(\overline{\mathbf{V}}^T\mathbf{u}) = \mathbf{W}\mathbf{g}(\mathbf{V}^T\mathbf{u}) \quad \text{and}$$
$$\overline{\mathbf{W}} \begin{bmatrix} \overline{g}_1(\overline{x}_1) \\ \vdots \\ \overline{g}_r(\overline{x}_r) \end{bmatrix} = \overline{\mathbf{W}} \begin{bmatrix} \beta_1 g_1(\alpha_1 \overline{x}_1) \\ \vdots \\ \beta_r g_r(\alpha_r \overline{x}_r) \end{bmatrix}.$$

From the expressions $g_i(x_i) = c_{i,0} + c_{i,1}x_i + \cdots + c_{i,d}x_i^d$ and $\overline{g}_i(\overline{x}_i) = \overline{c}_{i,0} + \overline{c}_{i,1}\overline{x}_i + \cdots + \overline{c}_{i,d}\overline{x}_i^d$, we then find the relation between the coefficients of $g_i(x_i)$ and $\overline{g}_i(\overline{x}_i)$ as

$$\overline{c}_{i,\delta} = \beta_i \, \alpha_i^\delta \, c_{i,\delta}. \tag{2.13}$$

Remark 3. When $\mathbf{W}$ is column rank-deficient, the constant terms of the $g_i(x_i)$ cannot be reconstructed uniquely, and the relation (2.13) will only hold for $\delta \geq 1$ (see section 2.4.2).

Example 5. For the reconstruction obtained in Example 3, we can verify that the coefficients of the $g_i(x_i)$ indeed relate to the coefficients of the $\overline{g}_i(\overline{x}_i)$ through (2.13). Notice that a permutation took place between the columns of the factors, which requires an additional permutation of the scaling factors. We have $\overline{g}_1(\overline{x}_1) = 2\overline{x}_1^2 - 3\overline{x}_1 + 1$ and $g_2(x_2) = -0.0179x_2^2 + 4.2426x_2 - 2.2369$. We verify that

$$1 = -0.4470 \times -2.2369 \quad \Longrightarrow \quad \overline{c}_{2,0} = \beta_2 c_{1,0},$$
$$-3 = -0.4470 \times 15.8175 \times -0.4243 \quad \Longrightarrow \quad \overline{c}_{2,1} = \beta_2 \alpha_2 c_{1,1}, \quad \text{and}$$
$$2 = -0.4470 \times 15.8175^2 \times -0.0179 \quad \Longrightarrow \quad \overline{c}_{2,2} = \beta_2 \alpha_2^2 c_{1,2}.$$

A similar analysis can be performed for the relationship between $\overline{g}_2(\overline{x}_2)$ and $g_1(x_1)$.

2.5. Algorithm summary. The complete algorithm can be summarized as follows:

1. Evaluate the Jacobian matrix $\mathbf{J}(\mathbf{u})$ (see (2.1)) in N sampling points $\mathbf{u}^{(k)}$ (section 2.1).

2. Stack the Jacobian matrices into a three-way tensor $\mathcal{J}$ of dimensions $n \times m \times N$ (section 2.1).
3. Find an appropriate value for r by computing the CP decomposition of $\mathcal{J}$ (section 2.3).
4. Retrieve $\mathbf{V}$, $\mathbf{W}$, and $\mathbf{H}$ from the CP decomposition $\mathcal{J} = \sum_{i=1}^{r} \mathbf{w}_i \circ \mathbf{v}_i \circ \mathbf{h}_i$ (see (2.6)).
5. Reconstruct the internal univariate $g_i(x_i)$ by solving (2.11).
6. Check the approximation error of the decoupling procedure, e.g., by checking the coefficientwise errors on the reconstructed $\mathbf{f}(\mathbf{u})$.

3. Open questions. Several aspects remain to be investigated, such as generalizing the decoupling method to the nonexact case. How the approximation error can be quantified in a noisy setting should be studied: how does noise enter the problem, and how are the estimated polynomial coefficients affected by noise? This poses the question of how this knowledge can be employed in an *(elementwise) weighted CP decomposition* and to what extent the decoupling can be improved.

Another interesting question is whether the *uniqueness conditions* can be relaxed by using the knowledge that $\mathbf{H}$ contains evaluations in $g_i'(x_i)$ (as in (2.7)). A tailored CP decomposition, in which such additional information is employed, may guarantee uniqueness up to a greater number of internal functions $g_i(x_i)$.

Although this paper focuses on the polynomial case, the presented method does not require that the nonlinear function $\mathbf{f}(\mathbf{u})$ is polynomial or that the reconstructed univariate $g_i(x_i)$ are polynomial. The method can be easily generalized to the *nonpolynomial case*, as explored in [17].

Although it is known that a CP decomposition always exists (given a sufficiently large r), a *partial decoupling* that allows cross-linking among a smaller number of variables may be more appropriate. One can imagine the case where only some groups of variables can be decoupled from one another, but where an inherent structural (e.g., physical) coupling among the variables in a group exists. The partial decoupling question suggests the use of the block-term decomposition [14, 13] instead of the CP decomposition.

4. Conclusions. A method is developed that decomposes a set of multivariate polynomials into linear combinations of univariate polynomials in linear forms of the input variables. The paper covers the exact case where a decoupled representation exists and derives a method to retrieve it. The method proceeds by collecting the first-order information of the given functions in a set of Jacobian matrices. A simultaneous diagonalization of the Jacobian matrices reveals the linear transformations in the decoupled representation. The coefficients of the univariate internal mappings are obtained from the solution of a block-Vandermonde-like linear system of equations that is constructed using the transformation matrices and a set of input-output samples.

An important advantage of the method is that the curse-of-dimensionality is avoided in the sense that only a third-order tensor is constructed, regardless of the degree of the input polynomials. The simultaneous diagonalization of the set of Jacobian matrices is computed by means of the tensor canonical polyadic decomposition, which is known to be unique (up to certain scaling and permutation invariances) under mild conditions. It was shown how different (equivalent) decoupled representations are related to each other. The different parts of the method were illustrated by means of numerical examples.

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