

# Probabilistic evolution approach for the solution of explicit autonomous ordinary differential equations. Part 1: Arbitrariness and equipartition theorem in Kronecker power series

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**Abstract** Probabilistic evolution approach is a newly developed theory which may be utilized for the solution of ordinary differential equations. The approach may directly be applied for initial value problems of explicit first order autonomous ordinary differential equation sets with analytic right hand side functions. Analyticity plays an important role since it facilitates the expansion into direct power series which is the key element of the approach. Direct power series appear not only in all applications of probabilistic evolution but also show themselves as a promising tool for novel approximation methods. In this work, similarities and differences between Taylor series and direct power series are rigorously studied. Arbitrariness in transposed vector coefficients of direct power series is detailed. Equipartition theorem of direct power series is conjectured and proven in order to obtain unique transposed vector coefficients.

**Keywords** Dynamical systems · Probability · Expectation values · Ordinary differential equations · Linear algebra · Power series · Kronecker products

## 1 Introduction

Probabilistic evolution approach (PEA) is a relatively new approach for the solution of ordinary differential equations. Although the most promising application is its application to the solution of initial value problems, the approach has its roots in quantum mechanics. Currently initial value problems of ordinary differential equations and determination of quantum mechanical system motions by using expectation values

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are the two main areas of application of PEA. There are similarities and differences in these applications for the quantum world and the classical mechanical world. Direct power series is a series expansion that is crucial in PEA, and therefore in all applications involving PEA. “Direct product and power” statement has a broader meaning, what we have use here is peculiar to vectors and matrices of ordinary linear algebra and is widely known as Kronecker products and powers. The necessities of probabilistic evolution gave way to the introduction of direct power series. On the other hand, direct power series may be considered as a series expansion at its own right and it is an important tool for the formation of new approximation methods.

The method proposed in this paper is not a discretization method. The advantages and disadvantages of discretization are known. There are many novel discretization based methods in scientific literature for conserving certain properties of the system under consideration and obtaining results in high precision [1–9]. This paper builds on a method not based on discretization but on Taylor series and Taylor coefficients.

There is a range of papers having probabilistic evolution and/or direct power series as their focal points. The probabilistic evolution trilogy is the main source of information [10–12]. In this trilogy, quantum expectation value dynamics is detailed. Also, spectral properties of the evolution matrix, space extension, solution of the equations of Liouville mechanics are other key points. The works of Metin Demiralp, Emre Demiralp and Hernandez-Garcia are also milestone works of the theory [13, 14]. These were before the probabilistic evolution trilogy. The most recent papers are the two joint works of Metin Demiralp and Emre Demiralp. In these papers, probabilistic evolution and related approximants for unidimensional systems are detailed [15]. Novel definitions for multilinear algebra are given and the use of multilinear arrays for the solution of ordinary differential equation sets by way of probabilistic evolution is explained [16].

Also, there are many published conference proceedings on this subject and related subjects. The topics of these proceedings may be given in concise form as follows: The convergence related issues of probabilistic evolution [17], space extension as a tool for probabilistic evolution [18], application of mathematical fluctuation theory to probabilistic evolution [19–21], simplifications using the properties of system under consideration [22–25], study of the effects of singularities [26], quantum mechanics problems in view of probabilistic evolution [27], numerical solution of certain classical mechanics and statistical mechanics related problems [28, 29], preliminary steps for the numerical solution of celestial mechanics problems [30], studies for the applications to equation sets [31], numerical solution of certain quantum mechanical problems [32–36], high dimensional model representation and probabilistic evolution [37], initial value related inconsistencies and probabilistic evolution [38, 39], generalizations for the numerical solution of initial value problems [40, 41].

PEA is a powerful candidate for the solution of the initial value problems of ordinary differential equations which are basically used to investigate the dynamical system behaviors. The dynamical systems is a vast area to interpret many diverse phenomena including the events of chemistry also. This makes the content of this couple of papers important for also mathematical chemistry community members. We believe that these will have sufficient impact there.

Paper is organized as follows: The next section involves the definition of the direct power series in ordinary algebraic entities, vectors and matrices through subsections. The Sect. 2.1 emphasizes on the arbitrarinesses in the coefficient matrices of the direct power expansions. The ascendingly populated nature of the arbitrarinesses is investigated in a general look at the system vector direct powers and each arbitrariness coming from these terms is reflected to the relevant coefficient matrix via an arbitrary parameter. The second subsection focuses on the selection of these parameters to make the relevant matrix coefficients minimum normed. This leads us to the so-called “Equipartition Theorem”. The subsection covering the arbitrariness discussion in PEA perspective completes the Sect 2. The paper is finalized via conclusion section. Kernel separability, space extension and series solution via telescopic matrices to get the analytic solution for conical triangular cases of PEA is given in a companion (but somehow independent) paper [42].

## 2 Direct power series

There is a strong connection between direct power series and Taylor series. Therefore, the analyticity requirements for the function to be decomposed are the same for Taylor series and direct power series. Consider the point  $a$  on the real axis. Also consider a point on the real axis which has a distance  $x$  from  $a$ . Then,  $x$  may be considered as the independent variable and using Maclaurin expansion formed from there, it is possible to form the expansion

$$f(x + a) = \sum_{j=0}^{\infty} \frac{1}{j!} f^{(j)}(a) x^j = \sum_{j=0}^{\infty} \frac{1}{j!} x^j \frac{\partial^j}{\partial a^j} f(a). \quad (1)$$

where we have preferred to employ the partial derivative symbol for future generalizations even though just a single independent variable ( $a$ ) is considered here.

Using the operator definition

$$\mathcal{L}(x, a) \equiv x \frac{\partial}{\partial a} \quad (2)$$

(1) may be stated as

$$f(x + a) = \sum_{j=0}^{\infty} \frac{1}{j!} x^j \frac{\partial^j}{\partial a^j} f(a) = \left( \sum_{j=0}^{\infty} \frac{1}{j!} \mathcal{L}(x, a)^j \right) f(a) = \left( \sum_{j=0}^{\infty} \frac{1}{j!} x^j \frac{\partial^j}{\partial a^j} \right) f(a). \quad (3)$$

Here,  $x$  is considered to be independent of  $a$ . (3) may be rewritten in a more compact form using

$$e^{\mathcal{L}(x, a)} \equiv \sum_{j=0}^{\infty} \frac{1}{j!} \mathcal{L}(x, a)^j. \quad (4)$$

Then,

$$f(x + a) = e^{\mathcal{L}(x,a)} f(a) \tag{5}$$

appears. In order to further the analysis, a generalization in the form of

$$f(a + tx) \equiv \widehat{E}(t, a) f(a) \equiv e^{t\mathcal{L}(x,a)} f(a), \quad t \in [0, 1] \tag{6}$$

may be performed. Here, as  $t$  increases from 0 to 1, the left hand side, goes from  $f(a)$  to  $f(a + x)$ . Therefore, a propagation is under consideration on values of  $f$ . Although the end result is the values of  $f$ , they are formed by images of  $f(a)$  under an exponential operator. Therefore,  $\widehat{E}(t, a)$  is a propagator. Propagator is independent from  $f$ . It depends on  $t$  and the initial point  $a$ .  $t$  represents the dynamics of the system and therefore is named as “time”. Position is given by the operator  $\mathcal{L}(x, a)$ . Propagation connects the state of the system at any two different times. The operator on the exponent of the propagator,  $\mathcal{L}(x, a)$ , is the evolution operator.

The concept may be generalized to the two variable case as follows.

$$f(a_1 + x_1, a_2 + x_2) = \sum_{j_1=0}^{\infty} \frac{1}{j_1!} x_1^{j_1} \frac{\partial^{j_1}}{\partial a_1^{j_1}} f(a_1, a_2 + x_2). \tag{7}$$

Using the operator definition

$$\mathcal{L}_1(x_1, a_1) \equiv x_1 \frac{\partial}{\partial a_1} \tag{8}$$

in (7),

$$f(a_1 + x_1, a_2 + x_2) = \left( \sum_{j_1=0}^{\infty} \frac{1}{j_1!} \mathcal{L}_1(x_1, a_1)^{j_1} \right) f(a_1, a_2 + x_2) \tag{9}$$

may be obtained. The operator that performs the mapping from  $f(a_1, a_2 + x_2)$  to  $f(a_1 + x_1, a_2 + x_2)$  is again an exponential operator which has the evolution operator on the exponent. Using the series expansion

$$e^{\mathcal{L}_1(x_1, a_1)} \equiv \sum_{j_1=0}^{\infty} \frac{1}{j_1!} \mathcal{L}_1(x_1, a_1)^{j_1} \tag{10}$$

in (9), the compact form may be acquired.

$$f(a_1 + x_1, a_2 + x_2) = e^{\mathcal{L}_1(x_1, a_1)} f(a_1, a_2 + x_2). \tag{11}$$

The  $f(a_1, a_2 + x_2)$  term on the right hand side may be analyzed in the same manner using the expansion

$$f(a_1, a_2 + x_2) = \sum_{j_2=0}^{\infty} \frac{1}{j_2!} x_2^{j_2} \frac{\partial^{j_2}}{\partial a_2^{j_2}} f(a_1, a_2) \quad (12)$$

and the operator definition

$$\mathcal{L}_2(x_2, a_2) \equiv x_2 \frac{\partial}{\partial a_2}. \quad (13)$$

Avoiding the intermediate steps,

$$f(a_1 + x_1, a_2 + x_2) = e^{\mathcal{L}_1(x_1, a_1)} e^{\mathcal{L}_2(x_2, a_2)} f(a_1, a_2) \quad (14)$$

may be formed. Since the operands of the two evolution operators are assumed to be analytic,  $\mathcal{L}_1$  and  $\mathcal{L}_2$  are commutative operators. By using the commutativity property, the product of two propagators may be written as

$$e^{\mathcal{L}_1(x_1, a_1)} e^{\mathcal{L}_2(x_2, a_2)} = e^{\mathcal{L}_1(x_1, a_1) + \mathcal{L}_2(x_2, a_2)}. \quad (15)$$

Here, multivariability may be shown in a compact form by using vectors and matrices. Under the definitions

$$\mathbf{x} \equiv \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad \mathbf{a} \equiv \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \quad (16)$$

a new evolution operator

$$\mathcal{L}(\mathbf{x}, \mathbf{a}) \equiv \mathcal{L}_1(x_1, a_1) + \mathcal{L}_2(x_2, a_2) \quad (17)$$

may be defined. Differentiation with respect to  $a_1$  and  $a_2$  is given by the gradient operator

$$\nabla_{\mathbf{a}} \equiv \begin{bmatrix} \frac{\partial}{\partial a_1} \\ \frac{\partial}{\partial a_2} \end{bmatrix} \quad (18)$$

to form the compact expression

$$\mathcal{L}(\mathbf{x}, \mathbf{a}) = \mathbf{x}^T \nabla_{\mathbf{a}} \quad (19)$$

for the evolution operator. This operator is the two variable counterpart of the aforementioned  $\mathcal{L}(x, a)$ . The two variable counterpart of (6) is then

$$f(\mathbf{a} + t\mathbf{x}) \equiv \widehat{E}(t, \mathbf{a}) f(\mathbf{a}) \equiv e^{t\mathcal{L}(\mathbf{x}, \mathbf{a})} f(\mathbf{a}), \quad t \in [0, 1]. \quad (20)$$

The number of variables, which is also the number of elements of  $\mathbf{x}$  and  $\mathbf{a}$ , is not explicit in (20). Utilizing the definitions

$$\mathbf{x} \equiv \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix}, \quad \mathbf{a} \equiv \begin{bmatrix} a_1 \\ \vdots \\ a_N \end{bmatrix}, \quad \nabla_{\mathbf{a}} \equiv \begin{bmatrix} \frac{\partial}{\partial a_1} \\ \vdots \\ \frac{\partial}{\partial a_N} \end{bmatrix} \tag{21}$$

it is possible to say that (20) is valid for all positive integer  $N$  values. Here,  $\widehat{E}(t, \mathbf{a})$  is the propagation operator and  $\mathcal{L}(\mathbf{x}, \mathbf{a})$  is the evolution operator.  $\mathbf{x}$  is the system vector and  $N$  denotes the system’s degree of freedom or, in other words, dimensionality. The case where  $t = 1$  is of importance. A vector with  $N$  elements depicts a point in  $N$  dimensional Euclidean space. Going from one point to another is thus given by

$$f(\mathbf{x} + \mathbf{a}) = e^{\mathcal{L}(\mathbf{x}, \mathbf{a})} f(\mathbf{a}) \tag{22}$$

using the propagation operator. In order to figure out the explicit structure of (22), consider the Taylor expansion of its right hand side. That expansion includes  $\mathcal{L}(\mathbf{x}, \mathbf{a})^2$ . That is

$$\begin{aligned} \mathcal{L}(\mathbf{x}, \mathbf{a})^2 &= (\mathbf{x}^T \nabla_{\mathbf{a}}) (\mathbf{x}^T \nabla_{\mathbf{a}}) = (\mathbf{x}^T \nabla_{\mathbf{a}}) \otimes (\mathbf{x}^T \nabla_{\mathbf{a}}) = (\mathbf{x}^T \otimes \mathbf{x}^T) (\nabla_{\mathbf{a}} \otimes \nabla_{\mathbf{a}}) \\ &= (\mathbf{x}^{\otimes 2})^T (\nabla_{\mathbf{a}}^{\otimes 2}) \end{aligned} \tag{23}$$

since the product of two scalars is also the direct product of the same two scalars and direct product is distributive over product. Here and in the rest of the paper  $\otimes$  symbol is used to denote direct product and direct power in superscripts. For matrices and vectors, direct product is exactly same as Kronecker product and power even though they are defined on a broader set of elements and have more abstractness than Kronecker product and power. This may be generalized to obtain the result

$$\mathcal{L}(\mathbf{x}, \mathbf{a})^k = (\mathbf{x}^{\otimes k})^T (\nabla_{\mathbf{a}}^{\otimes k}), \quad k = 0, 1, 2, \dots \tag{24}$$

Using (24) in (22) and utilizing the Taylor expansion of the exponential term, the explicit structure may be obtained in the form of

$$\begin{aligned} f(\mathbf{a}, \mathbf{x}) &= \sum_{j=0}^{\infty} \frac{1}{j!} \mathcal{L}(\mathbf{x}, \mathbf{a})^j f(\mathbf{a}) \\ &= \sum_{j=0}^{\infty} \frac{1}{j!} (\mathbf{x}^{\otimes j})^T (\nabla_{\mathbf{a}}^{\otimes j}) f(\mathbf{a}) \\ &= \sum_{j=0}^{\infty} \frac{1}{j!} (\nabla_{\mathbf{a}}^{\otimes j} f(\mathbf{a}))^T \mathbf{x}^{\otimes j}. \end{aligned} \tag{25}$$

If the coefficient vector definition

$$\mathbf{F}_j \equiv \frac{1}{j!} \nabla_{\mathbf{a}}^{\otimes j} f(\mathbf{a}), \quad j = 0, 1, 2, \dots \tag{26}$$

is utilized, direct power series is then

$$f(\mathbf{a} + \mathbf{x}) = \sum_{j=0}^{\infty} \mathbf{F}_j^T \mathbf{x}^{\otimes j}. \quad (27)$$

The function is decomposed as infinite number of inner products. Each term of the infinite sum involves vectors of different number of elements compared to the other terms. If the trivial case where  $N$  is chosen as 1 is under consideration, each term of the infinite sum involves scalars. That case is just a rewriting of Taylor expansion of a univariate function.

### 2.1 Arbitrariness in coefficient vectors

Direct power series is a rearrangement of Taylor series. The only subtlety between direct power series and Taylor series is the arbitrariness in coefficient vectors of direct power series. Although direct power series coefficients may be calculated by (26), there are infinitely many choices for the coefficient vectors in the expansion. This arbitrariness appears in all the coefficient vectors except for the constant term and the terms having only the first derivatives. This is a consequence of the nature of direct powers.

Consider the term of the expansion where  $j$  is 0. This term has a one element coefficient vector multiplied by a scalar. The next term has  $j$  as 1. This term is the inner product of a coefficient vector with the system vector which is an  $N$ -element vector containing the variables of the system. The term with  $j$  as 2 contains  $\mathbf{x}^{\otimes 2}$ . This vector has  $N^2$  elements. For each  $x_i x_j$  in this vector where  $j$  is different from  $i$ , there is an  $x_j x_i$  element. Therefore, there are linear dependences between these elements of  $\mathbf{x}^{\otimes 2}$ .

Effects of these linear dependences may be seen in the expansion of a function with two variables. Direct power expansion of a function with two variables is

$$f(a_1 + x_1, a_2 + x_2) = \sum_{j=0}^{\infty} \mathbf{F}_j^T \mathbf{x}^{\otimes j}. \quad (28)$$

Taylor expansion of the same function is

$$f(a_1 + x_1, a_2 + x_2) = \sum_{j_1=0}^{\infty} \sum_{j_2=0}^{\infty} f_{j_1, j_2} x_1^{j_1} x_2^{j_2} \quad (29)$$

with Taylor coefficients

$$f_{j_1, j_2} = \frac{1}{j_1! j_2!} \left( \frac{\partial^{j_1+j_2} f}{\partial x_1^{j_1} \partial x_2^{j_2}} \right)_{\mathbf{x}=\mathbf{0}}. \quad (30)$$

Since the decompositions are exact equalities, right hand sides of (28) and (29) should be equal, thus satisfying

$$\sum_{j=0}^{\infty} \mathbf{F}_j^T \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^{\otimes j} = \sum_{j_1=0}^{\infty} \sum_{j_2=0}^{\infty} f_{j_1, j_2} x_1^{j_1} x_2^{j_2}. \tag{31}$$

The only unknowns in (31) are the transposed vector coefficients  $\mathbf{F}_j^T$ s. For the equality to hold, all coefficients corresponding to the same powers of the variable  $x_1$  and  $x_2$  should be equal. The constant term corresponds to the case where  $j, j_1$  and  $j_2$  are all 0. Then, it is possible to conclude that

$$\mathbf{F}_0^T = f_{0,0} = f(0, 0). \tag{32}$$

Therefore,  $\mathbf{F}_0^T$  is a scalar. A similar analysis for the terms containing only the first powers of the system variables by themselves yield

$$\mathbf{F}_1^T = [f_{1,0} \ f_{0,1}]. \tag{33}$$

$\mathbf{F}_1^T$  is a transposed vector with two elements. The next step is to observe the coefficients for the terms where  $(j_1 + j_2)$  is 2. The second and the third terms of  $\mathbf{x}^{\otimes 2}$  are equal. Therefore, they correspond to the same Taylor term. Equating both sides of (31) for the terms and solving the  $\mathbf{F}_2^T$ ,

$$\mathbf{F}_2^T \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^{\otimes 2} = f_{2,0} x_1^2 + f_{1,1} x_1 x_2 + f_{0,2} x_2^2 \tag{34}$$

may be acquired. Making the definition

$$\mathbf{F}_2^T \equiv [F_1^{(2)} \ F_2^{(2)} \ F_3^{(2)} \ F_4^{(2)}] \tag{35}$$

the solution for the elements of the transposed vector coefficient is

$$\begin{aligned} F_1^{(2)} &= f_{2,0} \\ F_4^{(2)} &= f_{0,2} \\ (F_2^{(2)} + F_3^{(2)}) &= f_{1,1}. \end{aligned} \tag{36}$$

Although first and last elements of the vector may be determined uniquely, there is arbitrariness for second and third elements.

These results show that it is possible to determine  $\mathbf{F}_0^T$  and  $\mathbf{F}_1^T$  uniquely.  $\mathbf{F}_2^T$  may not be determined uniquely. There is arbitrariness for all the coefficients of direct power series except for  $\mathbf{F}_0^T$  and  $\mathbf{F}_1^T$ . This is valid for all  $N$ -variate functions which may be expanded into Taylor series.

For the decomposition of an  $N$ -variate function, it is important to determine the number of linearly dependent elements for each transposed vector coefficient. For an element to be linearly dependent to other elements, it should contain at least two different  $x_i$  factors. The elements that are linearly dependent to each other have the



same number of occurrences of  $x_i$  considering that all powers are given as products of terms. If in a set of linearly dependent terms, the power of  $x_k$  is given by  $m_k$ , then  $m_1 + \dots + m_N = j$ . The number of elements for each set of linearly dependent elements may be calculated. This question may be restated as follows for all  $\mathbf{F}_j$ : “Consider the letters  $x_1, x_2, \dots, x_N$ . How many distinct  $j$ -letter words may be formed where  $x_k$  appears  $m_k$  times and  $k = 1, \dots, N$ ?” The answer to this question is

$$\bar{n} = \frac{j!}{m_1! \dots m_N!}. \quad (37)$$

This answer states that the number of terms having  $j$  factors with  $x_k$  having multiplicity  $m_k$  where  $k = 1, 2, \dots, N$  is  $j! / (m_1! \dots m_N!)$ . These terms create the arbitrariness in transposed vector coefficient  $\mathbf{F}_j^T$ .

In order to continue this analysis, it is necessary to define a permutation operator  $\widehat{\pi}$ . Let

$$u_k(x_1, \dots, x_N) \equiv \widehat{\pi}_k(x_1^{m_1} \dots x_N^{m_N}), \quad k = 1, 2, \dots, \bar{n}. \quad (38)$$

$\widehat{\pi}_k$  permutes the factors of its operand.  $k$  parameter uniquely defines a permutation and it takes an integer value from 1 to  $\bar{n}$ . If a linear combination in the form of

$$u \equiv \alpha_1 u_1 + \dots + \alpha_{\bar{n}} u_{\bar{n}} \quad (39)$$

is defined, then

$$u \equiv (\alpha_1 + \dots + \alpha_{\bar{n}}) x_1^{m_1} \dots x_N^{m_N}. \quad (40)$$

This is due to the fact that all  $u_k$  function values are equal.  $u$  has 0 value as long as

$$\alpha_1 + \dots + \alpha_{\bar{n}} = 0 \quad (41)$$

is satisfied. Therefore any  $\bar{n}$  coefficients which add up to 0 cause the term to vanish. Using such coefficients,

$$\sum_{k=1}^{\bar{n}} \alpha_k u_k(x_1, \dots, x_N) = 0 \quad (42)$$

may be formed. Direct product of direct powers of Cartesian unit vectors may be utilized to form the operands of the permutation operator. By a careful investigation, it is possible to form  $u_k$  as

$$u_k(x_1, \dots, x_N) = \widehat{\pi}_k \left( \left( \mathbf{e}_1^{\otimes m_1} \otimes \dots \otimes \mathbf{e}_N^{\otimes m_N} \right)^T \mathbf{x}^{\otimes j} \right), \quad k = 1, \dots, \bar{n} \quad (43)$$

and using (43) in (42), the linear combination is

$$\sum_{k=1}^{\bar{n}} \alpha_k \widehat{\pi}_k \left( \left( \mathbf{e}_1^{\otimes m_1} \otimes \dots \otimes \mathbf{e}_N^{\otimes m_N} \right)^T \mathbf{x}^{\otimes j} \right) = 0. \tag{44}$$

Then each term of (27) may equivalently be stated as

$$\mathbf{F}_j^T \mathbf{x}^j = \left( \mathbf{F}_j^T - \sum_{k=1}^{\bar{n}} \alpha_k \widehat{\pi}_k \left( \mathbf{e}_1^{\otimes m_1} \otimes \dots \otimes \mathbf{e}_N^{\otimes m_N} \right)^T \right) \mathbf{x}^{\otimes j}. \tag{45}$$

The transposed vector coefficient on the right hand side is dependent on  $\alpha_k$ ,  $k = 1, \dots, \bar{n}$ . Transpose of this vector is

$$\bar{\mathbf{F}}_j(\boldsymbol{\alpha}) \equiv \mathbf{F}_j - \sum_{k=1}^{\bar{n}} \alpha_k \widehat{\pi}_k \left( \mathbf{e}_1^{\otimes m_1} \otimes \dots \otimes \mathbf{e}_N^{\otimes m_N} \right) \tag{46}$$

where  $\mathbf{e}_k^T \boldsymbol{\alpha} = \alpha_k$ . In (27),  $\bar{\mathbf{F}}_j(\boldsymbol{\alpha})$  may be used instead of  $\mathbf{F}_j$ . The  $\alpha$  parameters are arbitrary parameters which should add up to 0. These steps may be recursively performed for all sets of linearly dependent terms for a certain  $j$  value. By making certain choices for these newly introduced parameters, it is possible to force the transposed vector coefficient to have the desired characteristics under some limitations.

### 2.2 Equipartition theorem

One desired characteristic for transposed vector coefficients can be minimal norm. For ease of computation, norm square minimization may be used as objective functional. Also, the restriction shown by (41) should show itself as a Lagrange multiplier. Therefore the functional is

$$J(\boldsymbol{\alpha}, \lambda) \equiv \|\bar{\mathbf{F}}_j(\boldsymbol{\alpha})\|^2 + \lambda \left( \sum_{k=1}^{\bar{n}} \alpha_k \right). \tag{47}$$

Differentiating with respect to  $\lambda$  and equating to 0, gives

$$\sum_{k=1}^{\bar{n}} \alpha_k = 0 \tag{48}$$

which is the desired restriction. On the other hand, differentiation with respect to  $\alpha_k$  yields

$$\frac{\partial \|\bar{\mathbf{F}}_j(\boldsymbol{\alpha})\|^2}{\alpha_k} + \lambda = 0, \quad k = 1, 2, \dots, \bar{n}. \tag{49}$$

Using (46) in (49)

$$2\alpha_k - 2\hat{\pi} \left( \mathbf{e}_1^{\otimes m_1} \otimes \cdots \otimes \mathbf{e}_N^{\otimes m_N} \right) \mathbf{F}_j + \lambda = 0, \quad k = 1, 2, \dots, \bar{n} \quad (50)$$

is obtained. Summing both sides over all the possible subindices of  $\alpha$

$$2 \sum_{k=1}^{\bar{n}} \alpha_k - 2 \sum_{k=1}^{\bar{n}} \hat{\pi} \left( \mathbf{e}_1^{\otimes m_1} \otimes \cdots \otimes \mathbf{e}_N^{\otimes m_N} \right)^T \mathbf{F}_j + \bar{n}\lambda = 0 \quad (51)$$

and using (48),

$$-2 \sum_{k=1}^{\bar{n}} \hat{\pi} \left( \mathbf{e}_1^{\otimes m_1} \otimes \cdots \otimes \mathbf{e}_N^{\otimes m_N} \right)^T \mathbf{F}_j + \bar{n}\lambda = 0 \quad (52)$$

may be acquired. The terms of the finite sum in (52) are

$$\hat{\pi} \left( \mathbf{e}_1^{\otimes m_1} \otimes \cdots \otimes \mathbf{e}_N^{\otimes m_N} \right)^T \mathbf{F}_j = \frac{1}{j!} \frac{\partial^j f(\mathbf{a})}{\partial a_1^{m_1} \cdots \partial a_N^{m_N}} \quad (53)$$

since the order of differentiation may be changed for a continuous multivariate function. Using (53) in (52) and solving for  $\lambda$ , it is possible to deduce

$$\lambda = \frac{2}{j!} \frac{\partial^j f(\mathbf{a})}{\partial a_1^{m_1} \cdots \partial a_N^{m_N}}. \quad (54)$$

This result may be used in (50) to form

$$\alpha_k = 0, \quad k = 1, 2, \dots, \bar{n}. \quad (55)$$

Therefore,  $\mathbf{F}_j$  is norm minimized  $\bar{\mathbf{F}}_j(\alpha)$ . Norm minimization creates uniqueness and carries us to the expansion given in (26) and (27). This result may be stated in the framework of a theorem named as equipartition theorem of direct power series.

Equipartition theorem of direct power series says that the coefficients of the expansion in (27) may be calculated by (26). Since some of the elements of  $\mathbf{x}^{\otimes j}$  linearly dependent, it is possible to form a vector  $\bar{\mathbf{F}}_j(\alpha)$  dependent on arbitrary parameters instead of  $\mathbf{F}_j$ .  $\mathbf{F}_j$  is the vector with minimum norm of all possible  $\bar{\mathbf{F}}_j(\alpha)$ . Minimum norm implies equal distribution amongst the equivalent elements of direct powers of  $\mathbf{x}$ . Therefore, the total coefficient value is divided equally amongst all terms of the equivalency set for all equivalency sets.

The cause of the arbitrariness in direct power squared term may be seen in (23).  $(\mathbf{x}^T \nabla_{\mathbf{a}}) \otimes (\mathbf{x}^T \nabla_{\mathbf{a}}) = (\mathbf{x}^T \otimes \mathbf{x}^T) (\nabla_{\mathbf{a}} \otimes \nabla_{\mathbf{a}})$  says that direct product of two inner products is equal to inner product of two direct products. However, inner product of two direct products is really working in a high dimensional space and creating a projection at the end. On the other hand, direct product of two inner products is the

product of two projected entities. Therefore, inner product of two direct products is more general. Possible arbitrariness vanishes at the last step. For the case where  $N$  is 2, an arbitrary value may be added to second element of  $(\nabla_{\mathbf{a}} \otimes \nabla_{\mathbf{a}})$  and the same arbitrary value may be subtracted from third element of  $(\nabla_{\mathbf{a}} \otimes \nabla_{\mathbf{a}})$  without changing the result. This is the cause of arbitrariness for the direct power squared term. Similar analysis may be performed for higher direct powered terms.

Equipartition theorem is not the only way to go for uniqueness. It is necessary to find out which impositions produce the desired result for different kinds of applications.

### 2.3 Arbitrariness from probabilistic evolution perspective

PEA for the solution of the initial value problem of a set of explicit first order ordinary differential equations with analytic right hand side functions involves the determination of the exponential of evolution matrix. In this case, direct power series expansion is performed for all the right hand side functions and transposed vector coefficients are stacked in the given order to form matrix coefficients. The resulting matrices are direct multiplied by unit matrices to form the evolution matrix. Due to the nature of differentiation, the solution of the initial value problem is related to the exponential of this matrix. In order to obtain a unique numerical approximation, this matrix should not contain any arbitrary parameters. Equipartition theorem creates a unique evolution matrix, consequently a unique approximate solution of the initial value problem.

It is also important to point out that evolution matrix is an infinite matrix. Therefore, the truncation of this matrix creates the numerical approximation. Convergence issues due to this truncation are related to the eigenpairs of evolution matrix. Therefore, arbitrary parameters may be utilized in such a way that evolution matrix exhibits the desired structure especially in eigenvectors for the case of triangularity. The case of nontriangular but upper Hessenberg block form can be facilitated by not only eigenvectors but eigenvalues also.

It is known from previous works of the authors that block triangularity of evolution matrix plays an important role in convergence. In the most general case, evolution matrix is an upper Hessenberg block form. Upper Hessenberg block form should be avoided when possible. Block triangularity facilitates the calculation of the exponential matrix thus reducing the computational burden. Therefore, if possible, the arbitrary parameters should be chosen in such a way that block triangularity is observed. This is an optimization problem the solution of which may or may not exist depending on the structure of the right hand side functions and the order of truncation.

## 3 Conclusion

In this paper, we have investigated the formation and utilization of direct power series. The formation of arbitrariness of transposed vector coefficients of direct power series is shown. Equipartition theorem is conjectured as a natural way to form unique transposed vector coefficients. The logic for the proof is explained in detail. We enumerate what we have obtained as original findings below.

1. Although the relation between Taylor series and direct power series was already known, it was not investigated extensively. Some important points were given by words in the previous papers involving direct power series. This paper shows the similarities and differences between Taylor series and direct power series.
2. The arbitrariness in transposed vector coefficients is shown. Using the approach given in this paper, it is possible to calculate the number of arbitrary elements for each term of direct power series.
3. Equipartition theorem is proposed for forming unique transposed vector coefficients. It is shown that minimum norm restriction on vectors with the arbitrariness creates uniqueness in which total coefficient value is equally divided amongst all terms of the equivalency set for all equivalency sets.

Direct power series is a tool for probabilistic evolution. Therefore, these findings are expected to promote the use of probabilistic evolution in the study of dynamical systems.

On the other hand, direct power series is an infinite series expansion which may be used in the formation of novel approximation methods. Since Taylor series and direct power series are strongly related, the application of direct power series in situations where Taylor series methods are traditionally applied may facilitate the formation of fast converging numerical approximation methods. This is one of the new horizons for science of computation.

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