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Exact expansions of arbitrary tensor functions $\mathbf{F}(\mathbf{A})$ and their derivatives

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Abstract

A general method is presented for determining the exact expansions of a tensor function $\mathbf{F}(\mathbf{A})$, where \mathbf{A} is a second order tensor in n -dimensional Euclidean space, and $\mathbf{F}(\mathbf{A})$ is defined by the power series. It is shown that $\mathbf{F}(\mathbf{A})$ can be obtained by differentiating a scalar function of the eigenvalues of \mathbf{A} . Using this method, closed-form, singularity-free expressions of arbitrary tensor functions and their first derivatives are deduced in two- and three-dimensional cases.

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1. Introduction

The aim of this paper is to establish a general method for determining finite term expansions for a tensor function $\mathbf{F}(\mathbf{A})$ defined by the power series

$$\mathbf{F}(\mathbf{A}) = a_0 \mathbf{I} + a_1 \mathbf{A} + \cdots + a_i \mathbf{A}^i + \cdots \quad (1)$$

Here \mathbf{A} is a second order tensor in n -dimensional Euclidean space. The scalar function

$$f(x) = a_0 + a_1 x + \cdots + a_i x^i + \cdots \quad (2)$$

is sometimes called the stem function for $\mathbf{F}(\mathbf{A})$. It is known that if the spectrum of \mathbf{A} lies within the radius of convergence of the series (2), then the tensor series (1) converges (Horn and Johnson, 1991). Tensor functions defined via power series are frequently used in continuum and computational mechanics. For instance, the exponential function is often employed in the numerical integrating of rate equation of the form $\dot{\mathbf{X}} = \mathbf{A}\mathbf{X}$. If the full Newton–Raphson algorithm is employed in computations, the derivative of function $\mathbf{F}(\mathbf{A})$ is required. Hence, it is always desirable to have closed-form, finite term expressions for $\mathbf{F}(\mathbf{A})$ and its derivative.

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There exist several methods for determining $\mathbf{F}(\mathbf{A})$ and its derivative for a *symmetric* tensor \mathbf{A} . Since a symmetric tensor possesses a full set of orthogonal eigenvectors, one can represent $\mathbf{F}(\mathbf{A})$ and its derivative in spectrum form, see Hill (1978) and Ogden (1984, Section 3.5) for a classical treatment in the context of generalized strains. In recent years, the spectrum representations have been widely used in computational mechanics (Simo and Taylor, 1991; Miehe, 1994; Miehe, 1998; Miehe and Lambrecht, 2001; Papadopoulos and Lu, 1998). Alternatively, exploiting the fact that $\mathbf{F}(\mathbf{A})$ is an isotropic function of \mathbf{A} , one can directly express $\mathbf{F}(\mathbf{A})$ in terms of polynomials of \mathbf{A} , and likewise for its derivative (Guo, 1984; Hoger and Carlson, 1984; Ting, 1985). In contrast, there does not appear to exist a well-developed algorithm in the literature for the general case, especially if the tensor \mathbf{A} is not diagonalizable. Algorithms based on truncated infinite series have been proposed (de Souza Neto, 2001). The accuracy and effectiveness of such algorithms is limited by round-off and choice of termination criterion.

In this paper, we develop a novel method for computing an arbitrary tensor function of a general unsymmetric tensor. We show that $\mathbf{F}(\mathbf{A})$ can be obtained by differentiating its *generating function*, a scalar function of the eigenvalues of \mathbf{A} . This approach is inspired by a recent paper of Kusnezov (1995) on the exponential map for $SU(n)$ group (i.e., group of tensors such that $\det \mathbf{A} = 1$), where author proposed the idea of obtaining the exponential map from differentiating a scalar function with respect to group parameters. In the present work, this approach has been systematically extended to *any* tensor function. In addition, having identified $\mathbf{F}(\mathbf{A})$ as the derivative of a scalar function, the derivative of $\mathbf{F}(\mathbf{A})$ can be readily computed as the second derivative. The method is then applied to two- and three-dimensional cases to establish closed-form representations for arbitrary tensor functions and the first derivatives. To the best of the author's knowledge, the main theorem established in this paper, as well as the representation formulae in two- and three-dimensional cases, have not been reported in the literature.

The paper is organized as follows: the main theorem is presented in Section 2, followed by a discussion of various representations of the general formula under different parameterizations. Closed-form, singularity-free representations for $\mathbf{F}(\mathbf{A})$ and its derivative in two- and three-dimensional cases are deduced in Sections 4 and 5.

2. General formula

In this section, we show that an arbitrary tensor function $\mathbf{F}(\mathbf{A})$ can be obtained by differentiating a scalar-valued function of \mathbf{A} , referred to as the generating function. To this end, first introduce an auxiliary function

$$g(x) = \int f(x) dx = g_0 + a_0 x + \frac{1}{2} a_1 x^2 + \dots, \quad (3)$$

where g_0 is an arbitrary constant. It is known that the power series in (3) has the radius of convergence no less than that of (2). Let $\{\lambda_i, i = 1, \dots, n\}$ be the eigenvalues of \mathbf{A} . Given $\mathbf{F}(\mathbf{A})$, the associated *generating function* is defined by

$$G(\mathbf{A}) = g(\lambda_1) + g(\lambda_2) + \dots + g(\lambda_n). \quad (4)$$

Next, define the derivative of a scalar-valued function $\phi(\mathbf{A})$ by the standard formula (assuming all the requisite smoothness conditions are satisfied)

$$\frac{\partial \phi(\mathbf{A})}{\partial \mathbf{A}} \cdot \mathbf{H} = \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \phi(\mathbf{A} + \epsilon \mathbf{H}) \quad \forall \mathbf{H}, \quad (5)$$

where the operation (\cdot) means the inner product $\mathbf{U} \cdot \mathbf{V} = \text{tr}(\mathbf{U}^T \mathbf{V})$, and the superscript T stands for tensor transpose.

The main result of this paper is as follows:

Theorem. Let $f(x)$ be an analytical function and $\mathbf{F}(\mathbf{A})$ be the associated tensor function defined by (1), and let $G(\mathbf{A})$ be the generating function given in (4). Then

$$\mathbf{F}(\mathbf{A}) = \frac{\partial G}{\partial \mathbf{A}^T} \quad (6)$$

for any second order tensor \mathbf{A} .

Proof. First, it is well-known that, if $|\lambda_i| < R$ ($i = 1, \dots, n$) where R is radius of convergence of power series (3)₂, then $\{g(\lambda_i), i = 1, \dots, n\}$ are the eigenvalues of the tensor $\mathbf{G}(\mathbf{A})$ defined by

$$\mathbf{G}(\mathbf{A}) = g_0 \mathbf{I} + a_0 \mathbf{A} + \dots + \frac{1}{i+1} a_i \mathbf{A}^{i+1} + \dots \quad (7)$$

See, e.g. Ting (1985). Hence, we identify $G(\mathbf{A}) = \text{tr} \mathbf{G}(\mathbf{A})$. It follows then

$$G(\mathbf{A} + \varepsilon \mathbf{H}) = \text{tr} \left[g_0 \mathbf{I} + a_0 (\mathbf{A} + \varepsilon \mathbf{H}) + \dots + \frac{1}{(i+1)!} a_i (\mathbf{A} + \varepsilon \mathbf{H})^{i+1} + \dots \right]. \quad (8)$$

Notice

$$\frac{d}{d\varepsilon} \Big|_{\varepsilon=0} \text{tr} \left[(\mathbf{A} + \varepsilon \mathbf{H})^{i+1} \right] = (i+1) \text{tr} [\mathbf{A}^i \mathbf{H}] = (i+1) (\mathbf{A}^T)^i \cdot \mathbf{H}, \quad (9)$$

where used is made of the cyclic property $\text{tr}[\mathbf{A}_1 \mathbf{A}_2 \dots \mathbf{A}_m] = \text{tr}[\mathbf{A}_2 \dots \mathbf{A}_m \mathbf{A}_1]$. Differentiating both sides of (8) with respect to ε at $\varepsilon = 0$ leads to

$$\frac{\partial G(\mathbf{A})}{\partial \mathbf{A}} \cdot \mathbf{H} = [a_0 \mathbf{I} + a_1 \mathbf{A}^T + \dots + a_i (\mathbf{A}^T)^i + \dots] \cdot \mathbf{H} = \mathbf{F}(\mathbf{A}^T) \cdot \mathbf{H}. \quad (10)$$

Therefore,

$$\mathbf{F}(\mathbf{A}^T) = \frac{\partial G}{\partial \mathbf{A}}. \quad (11)$$

Observing that

$$\mathbf{F}(\mathbf{A}^T) = (\mathbf{F}(\mathbf{A}))^T \quad \text{and} \quad \left(\frac{\partial G}{\partial \mathbf{A}} \right)^T = \frac{\partial G}{\partial \mathbf{A}^T}, \quad (12)$$

and taking the transpose of both sides of (11) yields the stated result. \square

Having established (6), it follows that the first derivative of $\mathbf{F}(\mathbf{A})$ is then given by

$$\frac{\partial \mathbf{F}(\mathbf{A})}{\partial \mathbf{A}} = \frac{\partial^2 G}{\partial \mathbf{A} \partial \mathbf{A}^T} \quad (13)$$

or, using components,

$$\frac{\partial [\mathbf{F}(\mathbf{A})]_{ij}}{\partial A_{kl}} = \frac{\partial^2 G}{\partial A_{kl} \partial A_{ji}}. \quad (14)$$

In particular, if \mathbf{A} is symmetric, we obtain

$$\mathbf{F}(\mathbf{A}) = \frac{\partial G}{\partial \mathbf{A}}, \quad \frac{\partial \mathbf{F}(\mathbf{A})}{\partial \mathbf{A}} = \frac{\partial^2 G}{\partial \mathbf{A} \partial \mathbf{A}}. \quad (15)$$

As a useful corollary, Eq. (15) shows that if \mathbf{A} is symmetric, then $\frac{\partial \mathbf{F}(\mathbf{A})}{\partial \mathbf{A}}$ possesses major symmetry, in the sense that

$$\frac{\partial [\mathbf{F}(\mathbf{A})]_{ij}}{\partial A_{kl}} = \frac{\partial [\mathbf{F}(\mathbf{A})]_{kl}}{\partial A_{ij}}. \quad (16)$$

The generating function depends on the eigenvalues of \mathbf{A} . Once the eigenvalues of \mathbf{A} are obtained, the formulae (6) and (13) can be directly applied. The method is completely general, as it applies to any tensor function and arbitrary tensor, diagonalizable or not. The method is particularly effective in lower dimension cases where closed-form eigenvalues are available. As will become evident later, the major advantages of this approach relate to the facts that: (1) the generating functions can be judiciously parameterized, thus allowing for optimal representations most suitable for a given problem; and (2) no knowledge of the eigenspace is required. This largely alleviates the difficulty in dealing with tensors which do not possess a full set of eigenvectors.

3. Selected representations

In this section we provide some representations for the general formula (6) in n -dimensional case.

3.1. Component form

Let $\{\mathbf{e}_i, i = 1, \dots, n\}$ be an orthonormal basis in \mathbb{R}^n . Consider the component expression

$$\mathbf{A} = A_{ij} \mathbf{e}_i \otimes \mathbf{e}_j \quad \text{where } A_{ij} = \mathbf{A} \cdot \mathbf{e}_i \otimes \mathbf{e}_j. \quad (17)$$

Here, summation convention applies to repeated indexes. We have

$$\frac{\partial A_{ij}}{\partial \mathbf{A}} = \mathbf{e}_i \otimes \mathbf{e}_j \Rightarrow \frac{\partial A_{ij}}{\partial \mathbf{A}^T} = \mathbf{e}_j \otimes \mathbf{e}_i. \quad (18)$$

Regarding $G(\mathbf{A})$ as a function of the components A_{ij} , and assuming A_{ij} are independent, it follows by use of chain rule that

$$\mathbf{F}(\mathbf{A}) = \frac{\partial G}{\partial A_{ji}} \frac{\partial A_{ji}}{\partial \mathbf{A}^T} = \frac{\partial G}{\partial A_{ji}} \mathbf{e}_i \otimes \mathbf{e}_j. \quad (19)$$

Hence, we arrive at a remarkable component formula

$$[\mathbf{F}(\mathbf{A})]_{ij} = \frac{\partial G}{\partial A_{ji}}. \quad (20)$$

Note that for the cases where some of the components are related (e.g., symmetric or skew symmetric), Eq. (20) has to be evaluated in the space of general matrices.

The component formula (20) may be applied to symbolic operations in lower dimension spaces where the generating function is readily available. To demonstrate this point, consider an example where

$$[\mathbf{A}] = \begin{bmatrix} a & d \\ c & b \end{bmatrix}, \quad (21)$$

and

$$f(x) = x^{-1} \quad \text{that is } \mathbf{F}(\mathbf{A}) = \mathbf{A}^{-1}. \quad (22)$$

Note that $f(x)$ is analytical everywhere except at $x = 0$. By construction,

$$g = \int x^{-1} dx = \log x. \quad (23)$$

It follows that

$$G(\mathbf{A}) = \log \lambda_1 + \log \lambda_2 = \log \lambda_1 \lambda_2 = \log(\det \mathbf{A}) = \log(ab - cd). \quad (24)$$

Using Eq. (20),

$$[\mathbf{F}(\mathbf{A})] = \begin{bmatrix} \frac{\partial G}{\partial a} & \frac{\partial G}{\partial c} \\ \frac{\partial G}{\partial d} & \frac{\partial G}{\partial b} \end{bmatrix} = \frac{1}{ab - cd} \begin{bmatrix} b & -d \\ -c & a \end{bmatrix}. \quad (25)$$

As is seen, we recover the inverse formula for a 2×2 matrix.

3.2. Invariant form

The generating function can be regarded as a function of the invariants of \mathbf{A} . Consider for example the following invariants:

$$J_1 = \text{tr } \mathbf{A}, \quad J_2 = \frac{1}{2} \text{tr } \mathbf{A}^2, \dots \quad J_n = \frac{1}{n} \text{tr } \mathbf{A}^n. \quad (26)$$

Using formula (5), we find

$$\frac{\partial J_1}{\partial \mathbf{A}^T} = \mathbf{I}, \quad \frac{\partial J_2}{\partial \mathbf{A}^T} = \mathbf{A}, \dots \quad \frac{\partial J_n}{\partial \mathbf{A}^T} = \mathbf{A}^{n-1}. \quad (27)$$

Then, applying the chain rule to (6) yields

$$\mathbf{F}(\mathbf{A}) = \frac{\partial G}{\partial J_i} \frac{\partial J_i}{\partial \mathbf{A}^T} = \frac{\partial G}{\partial J_1} \mathbf{I} + \frac{\partial G}{\partial J_2} \mathbf{A} + \dots + \frac{\partial G}{\partial J_n} \mathbf{A}^{n-1}. \quad (28)$$

Note that the powers of \mathbf{A} serves as the basis for $\mathbf{F}(\mathbf{A})$. If the tensors $\mathbf{I}, \mathbf{A}, \mathbf{A}^2, \dots, \mathbf{A}^{n-1}$ are linearly independent, the above equation uniquely identifies the coefficients for the general representation

$$\mathbf{F}(\mathbf{A}) = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{A} + \dots + \alpha_{n-1} \mathbf{A}^{n-1}.$$

Further, with the invariant form (28), the second derivative of $G(\mathbf{A})$ can be readily computed. Indeed, we have

$$\frac{\partial \mathbf{F}(\mathbf{A})}{\partial \mathbf{A}} = \frac{\partial^2 G}{\partial J_i \partial J_j} \frac{\partial J_i}{\partial \mathbf{A}^T} \otimes \frac{\partial J_j}{\partial \mathbf{A}} + \frac{\partial G}{\partial J_k} \frac{\partial^2 J_k}{\partial \mathbf{A} \partial \mathbf{A}^T}. \quad (29)$$

Here \otimes stands for the tensor product of two second order tensors defined by

$$(\mathbf{A} \otimes \mathbf{B}) \mathbf{H} = \mathbf{A} \text{tr}(\mathbf{B}^T \mathbf{H}) \quad (30)$$

or, in components,

$$[\mathbf{A} \otimes \mathbf{B}]_{ijkl} = A_{ij} B_{kl}. \quad (31)$$

Starting from (27), the second derivative of the invariants are computed as

$$\begin{aligned} \frac{\partial^2 J_1}{\partial \mathbf{A} \partial \mathbf{A}^T} &= \mathbb{O}, \\ \frac{\partial^2 J_2}{\partial \mathbf{A} \partial \mathbf{A}^T} &= \mathbb{I}, \\ &\vdots \\ \frac{\partial^2 J_n}{\partial \mathbf{A} \partial \mathbf{A}^T} &= \mathbf{A}^{n-2} \boxtimes \mathbf{I} + \mathbf{A}^{n-3} \boxtimes \mathbf{A}^T + \cdots + \mathbf{A} \boxtimes (\mathbf{A}^{n-3})^T + \mathbf{I} \boxtimes (\mathbf{A}^{n-2})^T. \end{aligned} \quad (32)$$

Here, \mathbb{O} and \mathbb{I} are the fourth order zero and identity tensors, and \boxtimes stands for the Kronecker product of two tensors defined by

$$(\mathbf{A} \boxtimes \mathbf{B})\mathbf{H} = \mathbf{A}\mathbf{H}\mathbf{B}^T \quad (33)$$

or, in components,

$$[\mathbf{A} \boxtimes \mathbf{B}]_{ijkl} = A_{ik}B_{jl}. \quad (34)$$

In the remainder of this paper, we will use a set of slightly different invariants to deduce closed-form representations for $\mathbf{F}(\mathbf{A})$ and its first derivative in lower dimension cases.

4. Two-dimensional case

In this section, we specialize the invariant representations to two-dimensional space to deduce closed-form expressions for $\mathbf{F}(\mathbf{A})$ and its first derivative.

4.1. Preliminaries

Consider a 2×2 tensor \mathbf{A} , and denoted by $\bar{\mathbf{A}}$ its deviatoric part

$$\bar{\mathbf{A}} = \mathbf{A} - \frac{1}{2}(\text{tr } \mathbf{A})\mathbf{I}. \quad (35)$$

Let

$$I_1 = \text{tr } \mathbf{A}, \quad \bar{J}_2 = \frac{1}{2} \text{tr } \bar{\mathbf{A}}^2. \quad (36)$$

A straight forward manipulation shows that the characteristic equation of \mathbf{A} can be written as

$$\left(\lambda - \frac{I_1}{2} \right)^2 - \bar{J}_2 = 0. \quad (37)$$

Therefore the eigenvalues of \mathbf{A} , that is, the roots of (37), are given as

$$\lambda_1 = \frac{I_1}{2} + \sqrt{\bar{J}_2}, \quad \lambda_2 = \frac{I_1}{2} - \sqrt{\bar{J}_2}. \quad (38)$$

Assume temporarily that $\lambda_1 \neq \lambda_2$. From (38), we readily conclude

$$\frac{\partial \lambda_\alpha}{\partial I_1} = \frac{1}{2}, \quad \frac{\partial \lambda_\alpha}{\partial \bar{J}_2} = \frac{(-1)^{\alpha-1}}{2\sqrt{\bar{J}_2}}, \quad \alpha = 1, 2, \quad (39)$$

and

$$2\sqrt{\bar{J}_2} = \lambda_1 - \lambda_2. \quad (40)$$

Further, we have the standard results

$$\frac{\partial \bar{I}_1}{\partial \mathbf{A}^T} = \mathbf{I}, \quad \frac{\partial \bar{J}_2}{\partial \bar{\mathbf{A}}^T} = \bar{\mathbf{A}}. \quad (41)$$

Here \mathbf{I} is the 2D second order identity tensor. We need to evaluate the derivative of \bar{J}_2 relative to \mathbf{A} . To this end, first record a formula

$$\frac{\partial \bar{\mathbf{A}}}{\partial \mathbf{A}} = \frac{\partial \bar{\mathbf{A}}^T}{\partial \mathbf{A}^T} = \mathbb{I} - \frac{1}{2} \mathbf{I} \otimes \mathbf{I}, \quad (42)$$

which can be directly verified from the definition of $\bar{\mathbf{A}}$. Here, \mathbb{I} is the fourth order identity tensors in 2D. It follows then

$$\frac{\partial \bar{J}_2}{\partial \mathbf{A}^T} = \left[\mathbb{I} - \frac{1}{2} \mathbf{I} \otimes \mathbf{I} \right] \bar{\mathbf{A}} = \bar{\mathbf{A}}. \quad (43)$$

4.2. Invariant representation for $\mathbf{F}(\mathbf{A})$

From (6), and regarding $G(\mathbf{A})$ as a function of I_1, \bar{J}_2 , we can write,

$$\mathbf{F}(\mathbf{A}) = \frac{\partial G}{\partial I_1} \mathbf{I} + \frac{\partial G}{\partial \bar{J}_2} \bar{\mathbf{A}}. \quad (44)$$

The derivative of G relative to the invariants can be computed as follows. Assume $\lambda_1 \neq \lambda_2$. Recalling that $G(\mathbf{A}) = g(\lambda_1) + g(\lambda_2)$, observing $g'(x) = f(x)$, and making use of the relations (39), (40), we obtain

$$\begin{aligned} c_1 &:= \frac{\partial G}{\partial I_1} = \frac{\partial G}{\partial \lambda_1} \frac{\partial \lambda_1}{\partial I_1} + \frac{\partial G}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial I_1} = \frac{f_1 + f_2}{2}, \\ c_2 &:= \frac{\partial G}{\partial \bar{J}_2} = \frac{\partial G}{\partial \lambda_1} \frac{\partial \lambda_1}{\partial \bar{J}_2} + \frac{\partial G}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial \bar{J}_2} = \frac{f_1 - f_2}{\lambda_1 - \lambda_2}, \end{aligned} \quad (45)$$

where we have used the short-hand notations $f_a = f(\lambda_a)$ and $f'_a = f'(\lambda_a)$ for $a = 1, 2$.

In the limiting case where $\lambda_1 = \lambda_2$, the quotient $\frac{f(\lambda_1) - f(\lambda_2)}{\lambda_1 - \lambda_2}$ is replaced by the derivative of f , and we have

$$c_1 = f_1, \quad c_2 = f'_1. \quad (46)$$

We therefore conclude that, in two-dimensional case,

$$\mathbf{F}(\mathbf{A}) = \begin{cases} \frac{f_1 + f_2}{2} \mathbf{I} + \frac{f_1 - f_2}{\lambda_1 - \lambda_2} \bar{\mathbf{A}} & \text{if } \lambda_1 \neq \lambda_2, \\ f_1 \mathbf{I} + f'_1 \bar{\mathbf{A}} & \text{if } \lambda_1 = \lambda_2. \end{cases} \quad (47)$$

4.3. Derivative of $\mathbf{F}(\mathbf{A})$

Starting from (44), using the chain rule leads to

$$\frac{\partial \mathbf{F}(\mathbf{A})}{\partial \mathbf{A}} = \frac{\partial^2 G}{\partial I_1 \partial I_1} \mathbf{I} \otimes \mathbf{I} + \frac{\partial^2 G}{\partial I_1 \partial \bar{J}_2} \left[\mathbf{I} \otimes \bar{\mathbf{A}}^T + \bar{\mathbf{A}} \otimes \mathbf{I} \right] + \frac{\partial^2 G}{\partial \bar{J}_2 \partial \bar{J}_2} \bar{\mathbf{A}} \otimes \bar{\mathbf{A}}^T + \frac{\partial G}{\partial \bar{J}_2} \left[\mathbb{I} - \frac{1}{2} \mathbf{I} \otimes \mathbf{I} \right]. \quad (48)$$

For the case of distinct eigenvalues, the coefficients are derived to be

$$\begin{aligned} d_{11} &:= \frac{\partial^2 G}{\partial I_1 \partial I_1} = \frac{1}{4}(f'_1 + f'_2), \\ d_{12} &:= \frac{\partial^2 G}{\partial I_1 \partial \bar{J}_2} = \frac{f'_1 - f'_2}{2(\lambda_1 - \lambda_2)}, \\ d_{22} &:= \frac{\partial^2 G}{\partial \bar{J}_2 \partial \bar{J}_2} = \frac{f'_1 + f'_2}{(\lambda_1 - \lambda_2)^2} - \frac{2(f_1 - f_2)}{(\lambda_1 - \lambda_2)^3}. \end{aligned} \quad (49)$$

When $\lambda_1 = \lambda_2$, the coefficients assume the limiting values

$$d_{11} = \frac{1}{2}f'_1, \quad d_{12} = \frac{1}{2}f''_1, \quad d_{22} = \frac{1}{6}f'''_1. \quad (50)$$

In this case we obtain a remarkable formula

$$\frac{\partial \mathbf{F}(\mathbf{A})}{\partial \mathbf{A}} = f'_1 \mathbb{I} + \frac{1}{2}f''_1 [\mathbf{I} \otimes \bar{\mathbf{A}}^T + \bar{\mathbf{A}} \otimes \mathbf{I}] + \frac{1}{6}f'''_1 \bar{\mathbf{A}} \otimes \bar{\mathbf{A}}^T. \quad (51)$$

5. Three-dimensional case

Parallel to the two-dimensional case, here we derive the representations for $\mathbf{F}(\mathbf{A})$ and its derivative in three-dimensional space.

5.1. Preliminaries

Consider a second order tensor \mathbf{A} in \mathbb{R}^3 , and let

$$\bar{\mathbf{A}} = \mathbf{A} - \frac{1}{3}(\text{tr } \mathbf{A})\mathbf{I} \quad (52)$$

be the deviatoric part. Introduce the invariants

$$I_1 = \text{tr } \mathbf{A}, \quad \bar{J}_2 = \frac{1}{2}\text{tr } \bar{\mathbf{A}}^2, \quad \bar{J}_3 = \frac{1}{3}\text{tr } \bar{\mathbf{A}}^3. \quad (53)$$

Let λ_a , $a = 1, 2, 3$ be the eigenvalues of \mathbf{A} , regarded here as functions of I_1 , \bar{J}_2 and \bar{J}_3 . Introduce the notations

$$\bar{\lambda}_a = \lambda_a - \frac{I_1}{3}, \quad a = 1, 2, 3,$$

and

$$D_a = (\lambda_a - \lambda_b)(\lambda_a - \lambda_c), \quad a = 1, 2, 3; \quad a \neq b \neq c \neq a.$$

We first prove a result that plays an essential rule in the forthcoming development.

Proposition. *Regarding the eigenvalues λ_a , $a = 1, 2, 3$ as functions of the invariants I_1 , \bar{J}_2 , \bar{J}_3 , and assume $\lambda_1 \neq \lambda_2 \neq \lambda_3 \neq \lambda_1$. Then*

$$\frac{\partial \lambda_a}{\partial I_1} = \frac{1}{3}, \quad \frac{\partial \lambda_a}{\partial \bar{J}_2} = \frac{\bar{\lambda}_a}{D_a}, \quad \frac{\partial \lambda_a}{\partial \bar{J}_3} = \frac{1}{D_a}. \quad (54)$$

Proof. First observe that $\bar{\lambda}_a$ are the eigenvalues of $\bar{\mathbf{A}}$. By the relationship between eigenvalues and principal invariants, we can readily check that

$$\begin{aligned}\bar{\lambda}_1 + \bar{\lambda}_2 + \bar{\lambda}_3 &= 0, \\ \bar{\lambda}_1 \bar{\lambda}_2 + \bar{\lambda}_2 \bar{\lambda}_3 + \bar{\lambda}_3 \bar{\lambda}_1 &= -\bar{J}_2, \\ \bar{\lambda}_1 \bar{\lambda}_2 \bar{\lambda}_3 &= \bar{J}_3.\end{aligned}\tag{55}$$

Differentiating both sides of the above equations yields

$$\begin{aligned}d\bar{\lambda}_1 + d\bar{\lambda}_2 + d\bar{\lambda}_3 &= 0, \\ \bar{\lambda}_1 d\bar{\lambda}_1 + \bar{\lambda}_2 d\bar{\lambda}_2 + \bar{\lambda}_3 d\bar{\lambda}_3 &= d\bar{J}_2, \\ \bar{\lambda}_2 \bar{\lambda}_3 d\bar{\lambda}_1 + \bar{\lambda}_1 \bar{\lambda}_3 d\bar{\lambda}_2 + \bar{\lambda}_1 \bar{\lambda}_2 d\bar{\lambda}_3 &= d\bar{J}_3,\end{aligned}\tag{56}$$

where use is made of (55)₁ in obtaining (56)₂. Solving for $d\bar{\lambda}$'s in terms of $d\bar{J}_2$ and $d\bar{J}_3$ gives

$$d\bar{\lambda}_a = \frac{\bar{\lambda}_a d\bar{J}_2}{D_a} + \frac{d\bar{J}_3}{D_a}.\tag{57}$$

The above results imply that

$$\frac{\partial \bar{\lambda}_a}{\partial I_1} = 0, \quad \frac{\partial \bar{\lambda}_a}{\partial \bar{J}_2} = \frac{\bar{\lambda}_a}{D_a}, \quad \frac{\partial \bar{\lambda}_a}{\partial \bar{J}_3} = \frac{1}{D_a}.\tag{58}$$

The results (54) then follow by recalling that $\lambda_a = \bar{\lambda}_a + \frac{I_1}{3}$, so that $\frac{\partial \lambda_a}{\partial I_1} = \frac{1}{3}$, $\frac{\partial \lambda_a}{\partial \bar{J}_2} = \frac{\partial \bar{\lambda}_a}{\partial \lambda_a} \frac{\partial \bar{\lambda}_a}{\partial \bar{J}_2} = \frac{\bar{\lambda}_a}{D_a}$, and so on. \square

Returning to the invariants. Similarly to the two-dimensional case, we have the standard results

$$\frac{\partial \bar{J}_2}{\partial \bar{\mathbf{A}}^T} = \bar{\mathbf{A}}, \quad \frac{\partial \bar{J}_3}{\partial \bar{\mathbf{A}}^T} = \bar{\mathbf{A}}^2,\tag{59}$$

and

$$\frac{\partial \bar{\mathbf{A}}}{\partial \mathbf{A}} = \frac{\partial \bar{\mathbf{A}}^T}{\partial \mathbf{A}^T} = \mathbb{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I}.\tag{60}$$

Using the chain rule and invoking (59) and (60) we establish the expression

$$\begin{aligned}\frac{\partial \bar{J}_2}{\partial \mathbf{A}^T} &= \left[\mathbb{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \right] \bar{\mathbf{A}} = \bar{\mathbf{A}}, \\ \frac{\partial \bar{J}_3}{\partial \mathbf{A}^T} &= \left[\mathbb{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \right] \bar{\mathbf{A}}^2 = \bar{\mathbf{A}}^2 - \frac{1}{3} (\text{tr } \bar{\mathbf{A}}^2) \mathbf{I} := \bar{\mathbf{A}}_{\text{dev}}^2.\end{aligned}\tag{61}$$

5.2. Invariant representation for $\mathbf{F}(\mathbf{A})$

Starting from (6), regarding $G(\mathbf{A})$ as a function of the invariants I_1 , \bar{J}_2 , \bar{J}_3 , taking the derivative and making use of (61) yields

$$\mathbf{F}(\mathbf{A}) = \frac{\partial G}{\partial I_1} \mathbf{I} + \frac{\partial G}{\partial \bar{J}_2} \bar{\mathbf{A}} + \frac{\partial G}{\partial \bar{J}_3} \bar{\mathbf{A}}_{\text{dev}}^2.\tag{62}$$

Recall that $G(\mathbf{A}) = g(\lambda_1) + g(\lambda_2) + g(\lambda_3)$, and $g'(x) = f(x)$. Assuming that the eigenvalues are distinct, by the chain rule we find

$$\begin{aligned}
c_1 &:= \frac{\partial G}{\partial I_1} = \sum_{a=1}^3 \frac{\partial G}{\partial \lambda_a} \frac{\partial \lambda_a}{\partial I_1} = \sum_{a=1}^3 \frac{f_a}{3}, \\
c_2 &:= \frac{\partial G}{\partial J_2} = \sum_{a=1}^3 \frac{\partial G}{\partial \lambda_a} \frac{\partial \lambda_a}{\partial J_2} = \sum_{a=1}^3 \frac{\bar{\lambda}_a f_a}{D_a}, \\
c_3 &:= \frac{\partial G}{\partial J_3} = \sum_{a=1}^3 \frac{\partial G}{\partial \lambda_a} \frac{\partial \lambda_a}{\partial J_3} = \sum_{a=1}^3 \frac{f_a}{D_a}.
\end{aligned} \tag{63}$$

The degenerate case of repeated eigenvalues can be dealt by the following limiting analysis.

Case I. Two equal roots $\lambda_1 = \lambda_2 \neq \lambda_3$. Expanding f_2 into the Taylor series at λ_1 in (63), and taking the limit $\lambda_2 \rightarrow \lambda_1$ gives

$$\begin{aligned}
c_1 &= \frac{2}{3}f_1 + \frac{1}{3}f_3, \\
c_2 &= \frac{1}{3}f'_1 + \frac{2}{3} \frac{f_3 - f_1}{\lambda_3 - \lambda_1}, \\
c_3 &= \frac{f'_1}{\lambda_1 - \lambda_3} + \frac{f_3 - f_1}{(\lambda_1 - \lambda_3)^2}.
\end{aligned} \tag{64}$$

Case II. Three equal roots $\lambda_1 = \lambda_2 = \lambda_3$. Taking the limit as $\lambda_3 \rightarrow \lambda_1$ in (64) yields

$$c_1 = f_1, \quad c_2 = f'_1, \quad c_3 = \frac{1}{2}f''_1. \tag{65}$$

In this case $\mathbf{F}(\mathbf{A})$ assumes a remarkable form

$$\mathbf{F}(\mathbf{A}) = f_1 \mathbf{I} + f'_1 \bar{\mathbf{A}} + \frac{1}{2}f''_1 \bar{\mathbf{A}}_{\text{dev}}^2. \tag{66}$$

In summary, we have shown that a tensor function $\mathbf{F}(\mathbf{A})$ in three-dimensional space can be represented as

$$\mathbf{F}(\mathbf{A}) = \begin{cases} \left(\sum_{a=1}^3 \frac{f_a}{3} \right) \mathbf{I} + \left(\sum_{a=1}^3 \frac{\bar{\lambda}_a f_a}{D_a} \right) \bar{\mathbf{A}} + \left(\sum_{a=1}^3 \frac{f_a}{D_a} \right) \bar{\mathbf{A}}_{\text{dev}}^2 & \text{if } \lambda_1 \neq \lambda_2 \neq \lambda_3 \neq \lambda_1, \\ \left(\frac{2}{3}f_1 + \frac{1}{3}f_3 \right) \mathbf{I} + \left(\frac{1}{3}f'_1 + \frac{2}{3} \frac{f_3 - f_1}{\lambda_3 - \lambda_1} \right) \bar{\mathbf{A}} + \left(\frac{f'_1}{\lambda_1 - \lambda_3} + \frac{f_3 - f_1}{(\lambda_1 - \lambda_3)^2} \right) \bar{\mathbf{A}}_{\text{dev}}^2 & \text{if } \lambda_1 = \lambda_2 \neq \lambda_3, \\ f_1 \mathbf{I} + f'_1 \bar{\mathbf{A}} + \frac{1}{2}f''_1 \bar{\mathbf{A}}_{\text{dev}}^2 & \text{if } \lambda_1 = \lambda_2 = \lambda_3. \end{cases} \tag{67}$$

It is worth noting that Eq. (67)₁ can be recast as

$$f(\mathbf{A}) = f_1 \frac{(\mathbf{A} - \lambda_2 \mathbf{I})(\mathbf{A} - \lambda_3 \mathbf{I})}{(\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3)} + f_2 \frac{(\mathbf{A} - \lambda_1 \mathbf{I})(\mathbf{A} - \lambda_3 \mathbf{I})}{(\lambda_2 - \lambda_1)(\lambda_2 - \lambda_3)} + f_3 \frac{(\mathbf{A} - \lambda_1 \mathbf{I})(\mathbf{A} - \lambda_2 \mathbf{I})}{(\lambda_3 - \lambda_1)(\lambda_3 - \lambda_2)}, \tag{68}$$

which recovers Sylvester's formula for a diagonalizable tensors (Horn and Johnson, 1991, p. 401). For the special case of $f(x) = \exp(x)$, a result equivalent to (67) is established in Laufer (1997) via a different method.

Note also that the formulae (67) apply to any second order tensor, diagonalizable or not. As an example, consider a Jordan form

$$[\mathbf{A}] = \begin{bmatrix} \lambda & 1 & 0 \\ 0 & \lambda & 1 \\ 0 & 0 & \lambda \end{bmatrix}, \tag{69}$$

where all eigenvalues equal to λ but only one eigenvector exists. We have

$$[\bar{\mathbf{A}}] = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \Rightarrow [\bar{\mathbf{A}}^2] = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (70)$$

Since $\bar{\mathbf{A}}^2$ is traceless, we have $\bar{\mathbf{A}}_{\text{dev}}^2 = \bar{\mathbf{A}}^2$. Then, by (67)₃,

$$[\mathbf{F}(\mathbf{A})] = \begin{bmatrix} f(\lambda) & f'(\lambda) & \frac{1}{2}f''(\lambda) \\ 0 & f(\lambda) & f'(\lambda) \\ 0 & 0 & f(\lambda) \end{bmatrix}. \quad (71)$$

This recovers a well-known result in matrix theory, see Horn and Johnson (1991, Section 6.2).

5.3. Derivative of $\mathbf{F}(\mathbf{A})$

Taking the derivative on both sides of (62) and using the chain rule again, we find

$$\begin{aligned} \frac{\partial \mathbf{F}(\mathbf{A})}{\partial \mathbf{A}} = & \frac{\partial^2 G}{\partial I_1 \partial I_1} \mathbf{I} \otimes \mathbf{I} + \frac{\partial^2 G}{\partial I_1 \partial \bar{J}_2} \left[\mathbf{I} \otimes \bar{\mathbf{A}}^T + \bar{\mathbf{A}} \otimes \mathbf{I} \right] + \frac{\partial^2 G}{\partial I_1 \partial \bar{J}_3} \left[\mathbf{I} \otimes (\bar{\mathbf{A}}_{\text{dev}}^2)^T + \bar{\mathbf{A}}_{\text{dev}}^2 \otimes \mathbf{I} \right] \\ & + \frac{\partial^2 G}{\partial \bar{J}_2 \partial \bar{J}_2} \bar{\mathbf{A}} \otimes \bar{\mathbf{A}}^T + \frac{\partial^2 G}{\partial \bar{J}_2 \partial \bar{J}_3} \left[\bar{\mathbf{A}} \otimes (\bar{\mathbf{A}}_{\text{dev}}^2)^T + \bar{\mathbf{A}}_{\text{dev}}^2 \otimes \bar{\mathbf{A}}^T \right] + \frac{\partial^2 G}{\partial \bar{J}_3 \partial \bar{J}_3} \left[\bar{\mathbf{A}}_{\text{dev}}^2 \otimes (\bar{\mathbf{A}}_{\text{dev}}^2)^T \right] \\ & + \frac{\partial G}{\partial \bar{J}_2} \left[\mathbf{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \right] + \frac{\partial G}{\partial \bar{J}_3} \mathbb{T}(\mathbf{A}), \end{aligned} \quad (72)$$

where $\mathbb{T}(\mathbf{A})$ stands for the fourth order tensor $\frac{\partial \bar{\mathbf{A}}_{\text{dev}}^2}{\partial \mathbf{A}}$. Expanding $\bar{\mathbf{A}}_{\text{dev}}^2$ into a polynomial of \mathbf{A} , taking the derivative with respective to \mathbf{A} and rewriting the result in term of $\bar{\mathbf{A}}$, we find

$$\mathbb{T}(\mathbf{A}) = \bar{\mathbf{A}} \boxtimes \mathbf{I} + \mathbf{I} \boxtimes \bar{\mathbf{A}}^T - \frac{2}{3} \left[\bar{\mathbf{A}} \otimes \mathbf{I} + \mathbf{I} \otimes \bar{\mathbf{A}}^T \right]. \quad (73)$$

For the case of distinct eigenvalues, the coefficients can again be obtained through direct application of the chain rule. First, starting from (54)_{2,3}, taking the derivative and using (54)_{2,3} repeatedly, after a lengthy but direct manipulation we find

$$\frac{\partial^2 \lambda_a}{\partial \bar{J}_2} = -\frac{2(\bar{\lambda}_a^3 - \bar{J}_3)}{D_a^3}, \quad \frac{\partial^2 \lambda_a}{\partial \bar{J}_2 \partial \bar{J}_3} = -\frac{3\bar{\lambda}_a^2 - \bar{J}_2}{D_a^3}, \quad \frac{\partial^2 \lambda_a}{\partial \bar{J}_3 \partial \bar{J}_3} = -\frac{6\bar{\lambda}_a}{D_a^3}. \quad (74)$$

Making use of (54) and (74) we can readily show that

$$d_{11} := \frac{\partial^2 G}{\partial I_1 \partial I_1} = \frac{1}{3} \sum_{a=1}^3 f'_a \frac{\partial \lambda_a}{\partial I_1} = \frac{1}{9} \sum_{a=1}^3 f'_a,$$

$$d_{12} := \frac{\partial^2 G}{\partial I_1 \partial \bar{J}_2} = \frac{1}{3} \sum_{a=1}^3 f'_a \frac{\partial \lambda_a}{\partial \bar{J}_2} = \frac{1}{3} \sum_{a=1}^3 \frac{\bar{\lambda}_a f'_a}{D_a},$$

$$d_{13} := \frac{\partial^2 G}{\partial \bar{J}_1 \partial \bar{J}_3} = \frac{1}{3} \sum_{a=1}^3 f'_a \frac{\partial \lambda_a}{\partial \bar{J}_3} = \frac{1}{3} \sum_{a=1}^3 \frac{f'_a}{D_a},$$

$$d_{22} := \frac{\partial^2 G}{\partial \bar{J}_2 \partial \bar{J}_2} = \sum_{a=1}^3 \left[f'_a \left(\frac{\partial \lambda_a}{\partial \bar{J}_2} \right)^2 + f_a \frac{\partial^2 \lambda_a}{\partial \bar{J}_2 \partial \bar{J}_2} \right] = \sum_{a=1}^3 \left[\frac{f'_a \bar{\lambda}_a^2}{D_a^2} - \frac{2f_a(\bar{\lambda}_a^3 - \bar{J}_3)}{D_a^3} \right],$$

$$\begin{aligned} d_{23} &:= \frac{\partial^2 G}{\partial \bar{J}_2 \partial \bar{J}_3} = \sum_{a=1}^3 \left[f'_a \frac{\partial \lambda_a}{\partial \bar{J}_2} \frac{\partial \lambda_a}{\partial \bar{J}_3} + f_a \frac{\partial^2 \lambda_a}{\partial \bar{J}_2 \partial \bar{J}_3} \right] = \sum_{a=1}^3 \left[\frac{f'_a \bar{\lambda}_a}{D_a^2} - \frac{f_a (3\bar{\lambda}_a^2 - \bar{J}_2)}{D_a^3} \right], \\ d_{33} &:= \frac{\partial^2 G}{\partial \bar{J}_3 \partial \bar{J}_3} = \sum_{a=1}^3 \left[f'_a \left(\frac{\partial \lambda_a}{\partial \bar{J}_3} \right)^2 + f_a \frac{\partial^2 \lambda_a}{\partial \bar{J}_3 \partial \bar{J}_3} \right] = \sum_{a=1}^3 \left[\frac{f'_a}{D_a^2} - \frac{6f_a \bar{\lambda}_a}{D_a^3} \right]. \end{aligned} \quad (75)$$

The limiting values at repeated eigenvalues are reported as follows.

Case I. Two equal roots $\lambda_1 = \lambda_2 \neq \lambda_3$. Expressing f_2 and f'_2 into Taylor series at λ_1 and letting $\lambda_2 \rightarrow \lambda_1$ yields,

$$\begin{aligned} d_{11} &= \frac{2f'_1}{9} + \frac{f'_3}{9}, \\ d_{12} &= \frac{f''_1}{9} + \frac{2(f'_1 - f'_3)}{9(\lambda_1 - \lambda_3)}, \\ d_{13} &= \frac{f''_1}{3(\lambda_1 - \lambda_3)} - \frac{f'_1 - f'_3}{3(\lambda_1 - \lambda_3)^2}, \\ d_{22} &= -\frac{4(f_1 - f_3)}{9(\lambda_1 - \lambda_3)^3} + \frac{4f'_3}{9(\lambda_1 - \lambda_3)^2} + \frac{2f''_1}{9(\lambda_1 - \lambda_3)} + \frac{f'''_1}{54}, \\ d_{23} &= \frac{5(f_1 - f_3)}{3(\lambda_1 - \lambda_3)^4} - \frac{f'_1}{(\lambda_1 - \lambda_3)^3} - \frac{2f'_3}{3(\lambda_1 - \lambda_3)^3} + \frac{f''_1}{6(\lambda_1 - \lambda_3)^2} + \frac{f'''_1}{18(\lambda_1 - \lambda_3)}, \\ d_{33} &= -\frac{4(f_1 - f_3)}{(\lambda_1 - \lambda_3)^5} + \frac{3f'_1}{(\lambda_1 - \lambda_3)^4} + \frac{f'_3}{(\lambda_1 - \lambda_3)^4} - \frac{f''_1}{(\lambda_1 - \lambda_3)^3} + \frac{f'''_1}{6(\lambda_1 - \lambda_3)^2}. \end{aligned} \quad (76)$$

Case II. Three equal roots $\lambda_1 = \lambda_2 = \lambda_3$. A straight forward manipulation shows that the coefficients assume the limiting values

$$\begin{aligned} d_{11} &= \frac{f'_1}{3}, \quad d_{12} = \frac{f''_1}{3}, \quad d_{13} = \frac{f'''_1}{6}, \\ d_{22} &= \frac{f'''_1}{6}, \quad d_{23} = \frac{f^{(4)}_1}{24}, \quad d_{33} = \frac{f^{(5)}_1}{120}. \end{aligned} \quad (77)$$

Consequently, the derivative in this case takes a remarkable form

$$\begin{aligned} \frac{\partial \mathbf{F}(\mathbf{A})}{\partial \mathbf{A}} &= f'_1 \mathbb{I} + \frac{1}{2} f''_1 \left[\bar{\mathbf{A}} \boxtimes \mathbf{I} + \mathbf{I} \boxtimes \bar{\mathbf{A}}^T \right] + \frac{1}{6} f'''_1 [\mathbf{I} \otimes (\bar{\mathbf{A}}_{\text{dev}}^2)^T + \bar{\mathbf{A}} \otimes \bar{\mathbf{A}}^T + \bar{\mathbf{A}}_{\text{dev}}^2 \otimes \mathbf{I}] \\ &\quad + \frac{f^{(4)}_1}{24} [\bar{\mathbf{A}} \otimes (\bar{\mathbf{A}}_{\text{dev}}^2)^T + \bar{\mathbf{A}}_{\text{dev}}^2 \otimes \bar{\mathbf{A}}^T] + \frac{f^{(5)}_1}{120} [\bar{\mathbf{A}}_{\text{dev}}^2 \otimes (\bar{\mathbf{A}}_{\text{dev}}^2)^T]. \end{aligned} \quad (78)$$

6. Concluding remarks

We have established a new method in obtaining the exact expansion for tensor function $\mathbf{F}(\mathbf{A})$ utilizing the idea of differentiating a scalar function. Completely general, finite term representations applicable to any $n \times n$ tensor are derived. In two- and three-dimensional cases, the formulae are given in closed, singularity-free form, which can be readily employed in numerical computations. Applications of the proposed formulae in computational mechanics will be discussed in a forthcoming publication.

During the review of the paper, a reviewer has pointed out a recent publication by Itskov on the exponential functions of general unsymmetric tensors (Itskov, 2003). Itskov has used a different method

involving the so-called Dunford–Taylor integral representation, see also Horn and Johnson (1991, Section 6.2). The advantage of the current approach lies at the flexibility in parameterizing the generating function, by which different representations for $F(\mathbf{A})$ can be readily obtained.

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