Diferenciación algorítmica por números duales

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Resumen

El método de interpolación cúbica por splines, el método de Runge–Kutta y el método de Newton-Raphson se extienden a su versión dual (desarrollados en el contexto de los números duales). Esta extensión permite el cálculo de derivadas para composiciones de funciones que no necesariamente están en una forma cerrada. El código de los algorithmos se han escrito en Matlab y se presentan algunos ejemplos. Entre ellos, se usa la versión dual del método de Newton–Raphson para obtener la derivada del ángulo de salida en el mecanismo espacial RRRCR; la versión dual del método normal de interpolación cúbica por splines se usa para obtener la difusividad térmica por técnicas fototérmicas y usamos la versión dual del método de Runge–Kutta para obtener derivadas de funciones que dependen de las soluciones de la ecuación de Duffing.

Palabras Clave: Números duales, diferenciación, Runge–Kutta, Newton–Raphson, splines cúbicos.

Dual Numbers for Algorithmic Differentiation

Abstract

The cubic spline interpolation method, the Runge–Kutta method, and the Newton–Raphson method are extended to dual versions (developed in the context of dual numbers). This extension allows the calculation of the derivatives of complicated compositions of functions which are not necessarily defined by a closed form expression. The code for the algorithms has been written in Matlab and some examples are presented. Among them, we use the dual Newton–Raphson method to obtain the derivatives of the output angle in the RRRCR spatial mechanism; we use the dual normal cubic spline interpolation algorithm to obtain the thermal diffusivity using photothermal techniques; and we use the dual Runge–Kutta method to obtain the derivatives of functions depending on the solution of the Duffing equation.

Keywords: Dual numbers, Differentiation, Runge–Kutta algorithm, Newton–Raphson algorithm Cubic spline interpolation.

1 Introduction

Analogous to a complex number $z = a + ib$ where a and b are real numbers and $i^2 = -1$, a dual number is defined as $\hat{r} = a + \epsilon b$ with a and b real numbers and $\epsilon^2 = 0$. Such numbers were introduced by Clifford who also developed their algebra in the late nineteenth century [1].

The fact that $\epsilon^2 = 0$ suggests that the dual numbers can be used to differentiate functions, since in analogy to an infinitesimal dx, quantities of order dx^n with n an integer greater than or equal to two are usually neglected. It turns out that this reasoning is correct. This can be easily proved for polynomials and then via the Taylor Series, generalized for any analytic function. So, by extending a real function to a dual function one can numerically obtain its derivatives. Nonetheless, most of the applications of dual numbers are in the area of mechanics (see for example [2] where some contributions to mechanics based on dual numbers are presented) and only relatively recently have they been used to obtain

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the derivatives of functions [3–6]. Moreover, there are no papers addressing the *dualization*[1] of algorithms such as the Newton–Raphson algorithm, the Runge–Kutta algorithm, or the cubic spline interpolation method. The present paper shows that a dualization of these algorithms allows the numerical calculation of the derivatives of complicated compositions of functions which frequently arise in science and engineering applications.

The problem of numerical differentiation has been addressed by many researchers. A complete review of the literature on this topic is beyond the scope of this paper. Nevertheless we want to cite some works which represent most of the techniques used to obtain derivatives numerically [5–22].

In the case when the derivatives of a set of data are required, two excellent approaches are presented in [13,22]. However, in some applications, one deals with derivatives of the composition of functions defined by an expression rather than an explicit function or set of data. For example, one could be interested in calculating the derivatives of the composition of a function with another that is the solution of some differential equation, or in calculating the derivatives of a function which depends on another function which is the spline interpolation of some data. In such cases, the automatic differentiation methods (AD) [6,9,19,23] and in particular AD by using dual numbers are especially suited for calculating such derivatives.

As illustrative examples, the thermal diffusivity for solids is obtained by making a dual cubic spline interpolation of the amplitude of the photothermal radiometry signal [24]. The derivatives of functions depending on the solution of the Duffing equation [25–27] are calculated using the dual Runge–Kutta method. And the dual Newton–Raphson algorithm is used to obtain the derivatives of the output angle in the RRRCR spatial mechanism [28]. The Matlab code of the elemental dual functions as well as the dual version for the mentioned algorithms are provided as additional material to this article, which is available at [29].

2 Methodology

2.1 Derivatives using dual numbers

How dual numbers can be used for calculating numerical derivatives can be seen in [30, 31]. Here we briefly review the essential ideas, bearing in mind a numerical implementation.

Let $f : \mathbb{R} \to \mathbb{R}$ be an analytic function. Expanding this function in a Taylor Series and evaluating at $\hat{x} = x + \epsilon$ (note that we have taken the dual part to be

1) we get

$$f(x + \epsilon) = f(x) + f'(x)\epsilon + O(\epsilon^2). \tag{1}$$

As we can see, $f(x) + f'(x)\epsilon$ is a dual number, so we associate the dual function

$$\hat{f}(\hat{x}) = f(x) + f'(x)\epsilon \tag{2}$$

to it. As in the case of the complex numbers, there is an isomorphism between the dual numbers and $\mathbb{R}^2$, thus a dual number can be written as

$$\hat{r} = \{a, b\}. \tag{3}$$

From now on we will use the notation given by Eq. (3), thus Eq. (2) will be written as

$$\hat{f}(\hat{x}) = \{f_0, f_1\}, \tag{4}$$

where $f_0 = f(x)$ and $f_1 = f'(x)$.

The next step is to dualize the composition of $f(x)$ with another function $g(x)$. From the chain rule, we get

$$\hat{f}(\hat{g}) = \{f_0(g_0), f_1(g_0)g_1\}. \tag{5}$$

For instance, if $h(x) = f(g(u(x)))$, the dual component of $\hat{h}(\hat{x}) = \hat{f}(\hat{g}(\hat{u}(\hat{x})))$ will be $h'(x)$. That is the power of the dual method of obtaining derivatives. We only need to implement the chain rule once. This makes the dual number method of obtaining derivatives an AD method (forward mode of AD).

The generalization to second derivatives is straightforward. To this end we define a *new dual* number

$$\begin{aligned} \tilde{r} &= a + b\,\epsilon_1 + c\,\epsilon_2, \\ \tilde{r} &= \{a, b, c\}, \end{aligned} \tag{6}$$

with a, b and c being real numbers and ϵ_1 and ϵ_2 having the following multiplication table

	1	ϵ_1	ϵ_2
1	1	ϵ_1	ϵ_2
ϵ_1	ϵ_1	ϵ_2	0
ϵ_2	ϵ_2	0	0

$$\tag{7}$$

Now, evaluating the Taylor expansion for $f(x)$ in $\tilde{x} = x + \epsilon_1$ we have,

$$f(\tilde{x}) = f(x) + f'(x)\epsilon_1 + \frac{1}{2!}f''(x)\epsilon_1^2, \tag{8}$$

$$f(\tilde{x}) = f(x) + f'(x)\epsilon_1 + \frac{1}{2!}f''(x)\epsilon_2. \tag{9}$$

These expressions are of the form of Eq. (6) so we can write

$$\tilde{f}(\tilde{x}) = \{f(x),\ f'(x),\ \frac{1}{2!}f''(x)\}. \tag{10}$$

The fact that the third component is a half of the second derivative does not matter. We can choose

$$\tilde{f}(\tilde{x}) = \{f(x),\ f'(x),\ f''(x)\} \tag{11}$$

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[1]From now on the term *dualization* will refer to extending a function or algorithm to the context of dual numbers.

as our definition for this *new dual* function (in fact, by choosing $\epsilon_1^2 = 2\epsilon_2$ the factor $1/2$ disappears). Also the inappropriate name, *new dual* function, can be changed to dual function; leaving to the context of the problem (number of components of f) if we are talking about a simple dual function or of an extended dual function of 3 components. Clearly Eq. (10) can be generalized to obtain higher order derivatives. For instance, to obtain derivatives until order n, define $\epsilon_0 = 1$, ϵ_1, ϵ_2, ..., ϵ_n having the multiplication table

$$\epsilon_i \cdot \epsilon_j = \begin{cases} 0 & \text{if } i+j > n, \\ \\ \epsilon_{i+j} & \text{otherwise,} \end{cases} \quad (12)$$

with i, $j = 0, 1, \ldots, n$.

It is also interesting to prove Eqs. (8, 9, 10) from a matrix algebra point of view. To this end we define the following matrices having the multiplication table (7),

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{\epsilon_1} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\boldsymbol{\epsilon_2} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (13)$$

Now, since

$$\mathbf{X} = x\,\mathbf{I} + \boldsymbol{\epsilon_1} \quad (14)$$

is in its Jordan canonical form, we will have [32]

$$f(\mathbf{X}) = \begin{pmatrix} f(x) & f'(x) & f''(x)/2! \\ 0 & f(x) & f'(x) \\ 0 & 0 & f(x) \end{pmatrix}, \quad (15)$$

$$f(\mathbf{X}) = f(x)\,\mathbf{I} + f'(x)\,\boldsymbol{\epsilon_1} + \frac{1}{2!}f''(x)\,\boldsymbol{\epsilon_2}. \quad (16)$$

Thus, the derivatives of f are determined by calculating the matrix function $f(\mathbf{X})$. This matrix function can be calculated by using the Cauchy integral formula for operator-value functions (see for example Sec. 16.8 of [33]).

A generalization of Eqs. (15, 16) to obtain higher order derivatives, can be done by calculating $f(\mathbf{X})$ with

$$\mathbf{X} = x\,\mathbf{I}_{(n+1)\times(n+1)} + \boldsymbol{\epsilon}_{1;(n+1)\times(n+1)}, \quad (17)$$

$\left[\boldsymbol{\epsilon}_{\alpha;(n+1)\times(n+1)}\right]_{i,j} = \delta_{i,j-\alpha}$; being $\delta_{i,j}$ the Kronecker's delta function, and $\alpha = 1, 2, \ldots, n$.

From Eq. (10), the analog of $\hat{x} = \{x, 1\}$ will be $\tilde{x} = \{x, 1, 0\}$ and the analog of Eq. (4) will be

$$\tilde{f}(\tilde{x}) = \{f_0, f_1, f_2\}, \quad (18)$$

where $f_0 = f(x)$, $f_1 = f'(x)$ and $f_2 = f''(x)$. Similarly, we will have

$$\tilde{f}(\tilde{g}) = \{f_0(g_0), f_1(g_0)g_1, f_2(g_0)g_1^2 + f_1(g_0)g_2\}, \quad (19)$$

for the composition of two dual functions.

Eq. (19), is of central importance in dualizing a function or algorithm. Notice that, unlike the finite difference methods, the use of Eq. (19) to obtain derivatives does not have the problems of truncation or cancellation errors.

2.2 Matlab implementation

In order to facilitate the use of the dual number given by Eq. (6), it is convenient to introduce a class for this kind of number. In the Matlab programming language, this can be done as:

```
classdef dual
%Class for dual numbers
    properties
        f0;%function
        f1;%first derivative
        f2;%second derivative
    end

 methods
  function obj = dual(g0,g1,g2)
    if (nargin ~= 0)
        if (nargin == 1&&isnumeric(g0))
            g1 = zeros(size(g0));
            g2 = g1;
        elseif(nargin == 1&&isa(g0,'dual'))
            obj = g0;
            return
        end
        obj.f0 = g0;
        obj.f1 = g1;
        obj.f2 = g2;
    end
  end
 end
end
```

Now, the dual number of Eq. (6) can be written as $\tilde{r} = $ `dual(a,b,c)`. This class as well as many other overloaded functions are included in the additional material to this article.

2.3 Dualization of algorithms

2.3.1 Dual Newton–Raphson algorithm

Let us suppose that we are given equation

$$F(u(x), x) = 0 \quad (20)$$

and that $u'(x_0)$ is required. In the case when a closed form expression for $u(x)$ can be obtained, the derivatives can be calculated by writing $u(x)$ in its dual form $\tilde{u}(\tilde{x})$.

If there is no closed form expression for $u(x)$, applying the chain rule yields

$$u'(x_0) = -\frac{1}{\partial F/\partial u(u(x_0), x_0)} \frac{\partial F}{\partial x}(u(x_0), x_0). \quad (21)$$

Assuming that there are closed form expressions for $\partial F/\partial x$ and $\partial F/\partial u$, the derivative $u'(x_0)$ can be calculated by solving numerically Eq. (20) and substituting $u(x_0)$ into Eq. (21). If $\partial F/\partial x$ and $\partial F/\partial u$ cannot be obtained in closed form, its numerical values can be obtained using AD. Nevertheless, by coding the dual version of some numerical solution method to solve Eq. (20), we will obtain $u(x_0)$ and automatically its derivatives. In the present paper, we dualize the Newton–Raphson method [34, 35].

Let $f(q)$ be a real function of a real variable. The Newton–Raphson method allows finding a solution of the equation $f(q) = 0$. Starting to look for a solution in q_0, the algorithm determines an approximate solution as[2]

$$q_1 = q_0 - \frac{f(q_0)}{f'(q_0)}$$

$$\vdots$$

$$q_{n+1} = q_n - \frac{f(q_n)}{f'(q_n)}. \quad (22)$$

In order to obtain $u'(x_0)$ from Eq. (20) we proceed as follows: Write $\tilde{F}$ for the dual version of the function F. Define the dual starting point $\tilde{u}_0 = \{u_0, 0, 0\}$. Since we need $F'(u)$, we define $\tilde{x}_0 = \{x_0, 0, 0\}$ and $\tilde{u} = \{u_0, 1, 0\}$, then from $\tilde{f}_1 = \tilde{F}(\tilde{u}, \tilde{x}_0)$ we obtain the first and second derivatives of F with respect to u. This is an extra bonus of the method: we do not need to worry about the derivative of F. In practice, this is an issue, and the derivative must be provided by hand. Finally, write Eq. (22) in its dual form, keeping in mind that since we want $u'(x)$ we need to evaluate $\tilde{F}$ in $\tilde{u}_0$ and $\tilde{x} = \{x_0, 1, 0\}$.

Putting $\tilde{u}_0 = $ u0d, $\tilde{x}_0 = $ x0d, and $\tilde{F} = $ fd; the essential part of the method is

```
x0d = dual(x0);
u0d = dual(u0);
for k = 1:n
    fx  = fd(u0d, dual(x0,1,0));
    fu  = fd(dual(u0d.f0,1,0), x0d);
    u0d = u0d - fx/(fu.f1);
end
```

This algorithm will produce $\tilde{u}(x)$. Using Eq. (19), we can construct the general dual function for u: $\tilde{u}(\tilde{g})$. The complete algorithm is coded in the function NR_-dual of the additional material. We also coded Halley's

method [37], so the user can choose between the simple Newton–Raphson method or Halley's method. Some examples are presented in Section 3.

2.3.2   Dual cubic spline interpolation

Let $P : A \subset \mathbb{R} \rightarrow B \subset \mathbb{R}$ be the function representing a cubic spline interpolation and let f be a real function such that $f(P(x), x)$ is defined. The problem is to find $f'(P(x), x)$ with $x \in A$. We solve this problem by writing the dual version of the natural cubic spline interpolation.

Natural cubic splines

Suppose that we have n data points $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, $n > 1$. A cubic spline is a spline constructed of piecewise third-order polynomials

$$Y_i(t) = a_i + b_i\,t + c_i\,t^2 + d_i\,t^3; \ \ t \in [0, 1], \ \ i = 1, \ldots, n-1, \quad (23)$$

which pass through this set of points.

In determining the coefficient of the ith piece of the spline, a linear system of $4(n-1) - 2$ equations and $4(n-1)$ unknowns will appear [38]. Two more equation can be obtained by demanding that $Y''(0) = 0$ and $Y''(1) = 0$. This yields the so called natural cubic spline interpolation. With this, the coefficients of Y_i are given by

$$a_i = y_i$$
$$b_i = D_i$$
$$c_i = 3(y_{i+1} - y_i) - 2D_i - D_{i+1}$$
$$d_i = 2(y_i - y_{i+1}) + D_i + D_{i+1} \quad (24)$$

where the D_s numbers are determined by solving the symmetric tridiagonal system:

$$\mathbf{T}\,\mathbf{D} = \mathbf{R} \quad (25)$$

with

$$\mathbf{T} = \begin{pmatrix} 2 & 1 & & & & & \\ 1 & 4 & 1 & & & & \\ & 1 & 4 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1 & 4 & 1 & \\ & & & & 1 & 4 & 1 \\ & & & & & 1 & 2 \end{pmatrix} \quad (26)$$

$$\mathbf{D} = \begin{pmatrix} D_1 \\ D_2 \\ D_3 \\ \vdots \\ D_{n-2} \\ D_{n-1} \\ D_n \end{pmatrix} \quad (27)$$

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[2] The convergence of the Newton–Raphson method is not a trivial subject. In some cases, a small variation of q_0 causes a convergence/divergence of the method. For a study of the convergence of the method, we refer the reader to [36].

$$\mathbf{R} = 3 \begin{pmatrix} y_2 - y_1 \\ y_3 - y_1 \\ y_4 - y_2 \\ \vdots \\ y_{n-1} - y_{n-3} \\ y_n - y_{n-2} \\ y_n - y_{n-1} \end{pmatrix}. \qquad (28)$$

The inversion of an $n \times n$ tridiagonal matrix can be done by an $O(n)$ algorithm [34], and in general it is this kind of algorithm which is used in order to find the inverse of the matrix $\mathbf{T}$ in Eq. (26). However, as we will show, an analytical formula for the inverse of $\mathbf{T}$ can be obtained.

Let us consider the $n \times n$ nonsingular tridiagonal matrix

$$\mathbf{M} = \begin{pmatrix} a_1 & b_1 & & & \\ c_1 & a_2 & b_2 & & \\ & c_2 & \ddots & \ddots & \\ & & \ddots & \ddots & b_{n-1} \\ & & & c_{n-1} & a_n \end{pmatrix}.$$

The inverse of such a matrix can be written as [39]:

$$\mathbf{M}_{ij}^{-1} = \begin{cases} (-1)^{i+j} \, b_i \ldots b_{j-1} \, \theta_{i-1} \, \phi_{j+1}/\theta_n & \text{if } i \leqslant j, \\ (-1)^{i+j} \, c_j \ldots c_{i-1} \, \theta_{j-1} \, \phi_{i+1}/\theta_n & \text{if } i > j, \end{cases} \qquad (29)$$

where θ_i is obtained by solving the recurrence equation

$$\theta_i = a_i \, \theta_{i-1} - b_{i-1}c_{i-1}\theta_{i-2}, \text{ for } i = 2, \ldots, n, \qquad (30)$$

with $\theta_0 = 1$ and $\theta_1 = a_1$. Then ϕ_i is obtained by solving the recurrence equation

$$\phi_i = a_i \, \phi_{i+1} - b_i c_i \phi_{i+2}, \text{ for } i = n-1, \ldots, 1, \qquad (31)$$

with $\phi_{n+1} = 1$ and $\phi_n = a_n$.

The use of Eq. (29) is not an efficient way to find the inverse of a tridiagonal matrix. However it can be used to deduce an analytical formula for the inverse of the matrix $\mathbf{T}$.

Applying Eqs. (29, 30 and 31) to Eq. (26), we get

$$\theta_s = \begin{cases} \dfrac{\left(2-\sqrt{3}\right)^s + \left(2+\sqrt{3}\right)^s}{2} & \text{if } s \neq n, \\[2ex] \dfrac{\left(2+\sqrt{3}\right)^n\left(-3+2\sqrt{3}\right) - \left(2-\sqrt{3}\right)^n\left(3+2\sqrt{3}\right)}{2} & \text{if } s = n, \end{cases} \qquad (32)$$

$$\phi_s = \begin{cases} \dfrac{\left(2-\sqrt{3}\right)^{1+n}\left(2+\sqrt{3}\right)^s + \left(2-\sqrt{3}\right)^s\left(2+\sqrt{3}\right)^{1+n}}{2} & \text{if } s \neq 1, \\[2ex] \dfrac{\left(2+\sqrt{3}\right)^n\left(-3+2\sqrt{3}\right) - \left(2-\sqrt{3}\right)^n\left(3+2\sqrt{3}\right)}{2} & \text{if } s = 1. \end{cases} \qquad (33)$$

Defining inv as

$$inv(s,k) = (-1)^{s+k}\theta_{s-1}\,\phi_{k+1}/\theta_n, \qquad (34)$$

writing explicitly ϕ_{k+1}/θ_n and carrying out some elementary algebra, we obtain

$$inv(s,k) = \frac{(-1)^{s+k}}{2} \frac{1 + (\alpha^\dagger/\alpha)^{s-1}}{\beta^\dagger - (\alpha^\dagger/\alpha)^n \, \beta} \left[\alpha \, e^{(k+1)\ln \alpha^\dagger + (s-1)\ln \alpha} + \alpha^\dagger \, e^{(s+k)\ln \alpha + n \, \ln(\alpha^\dagger/\alpha)} \right], \qquad (35)$$

with

$$\alpha = 2 + \sqrt{3}$$
$$\alpha^\dagger = 2 - \sqrt{3}$$
$$\beta = 2\sqrt{3} + 3$$
$$\beta^\dagger = 2\sqrt{3} - 3. \qquad (36)$$

From this, the inverse of the matrix $\mathbf{T}$ is

$$\mathbf{T}_{sk}^{-1} = \begin{cases} inv(s,k) & \text{if } s \leqslant k, \\ inv(k,s) & \text{if } s > k. \end{cases} \qquad (37)$$

Thus the coefficients D_s are given by

$$D_s = \sum_{k=1}^{n} \mathbf{T}_{sk}^{-1}\mathbf{R}_k, \ s = 1, \ldots, n. \qquad (38)$$

Now that all the coefficients have been determined, the parametric equation for the interpolated points will be

$$\mathbf{r}_i(t) = \{x_i + (x_{i+1} - x_i)\, t, \ Y_i(t)\}. \qquad (39)$$

Eliminating the parameter t, the equation for the ith polynomial of the normal cubic spline will be

$$P_i(x) = Y_i\left(\frac{x - x_i}{x_{i+1} - x_i}\right), \ x \in [x_i, x_{i+1}]. \qquad (40)$$

The interpolated points in the whole interval $[x_1, x_n]$ are

$$P(x) = \bigcup_{i=1}^{n-1} P_i(x). \qquad (41)$$

Once $P(x)$ has been promoted to a dual function (see the function `NCSplinedual` of the aditional material), the derivatives of an arbitrary function $f = f(P(x), x)$ for any $x \in [x_1, x_n]$, as well as $P'(f(x), x)$, are calculated by writing f in its dual form. Some examples are presented in Section 3.

2.3.3   Dual Runge–Kutta algorithm

Let us consider the following ordinary differential equation (ODE)

$$f''(t) = F(t, f, f'), \qquad (42)$$

with initial conditions $f(t_0) = f_0$ and $f'(t_0) = v_0$. Let $g(t)$ be a function defined in such a way that $f(g(t))$ and $g(f(t))$ are defined. The problem we want to address is to find the derivatives of the composition of the functions f and g.

Dual Runge–Kutta 4th order method

One of the most often used methods for numerically solving ODEs is the Runge–Kutta Method [34,35,40]. In order to calculate $f'(g(t))$, $f''(g(t))$, $g'(f(t))$ and $g''(f(t))$, we will dualize the 4th order Runge–Kutta method (RK4). Putting $x_2 = f'$, $x_1 = f$, $u_1(t, x_1, x_2) = x_2$, $u_2(t, x_1, x_2) = F(t, x_1, x_2)$, the RK4 method produces x_2 and x_1 and hence $f''(t)$. From this, the dual version of f as a function of the real variable t (see the rk4 function of the additional material) is

$$\tilde{f}(t) = \{f(t), f'(t), f''(t)\}. \qquad (43)$$

The dual version of f for any dual variable $\tilde{u}$, namely $\tilde{f}(\tilde{u})$, can be constructed following Eq. (19). (See the rk4dual function of the additional material). Once we have $\tilde{f}(\tilde{u})$, the derivatives are calculated from the compositions $\tilde{f}(\tilde{g}(\tilde{t}))$ and $\tilde{g}(\tilde{f}(\tilde{t}))$—actually, we can calculate the derivatives of any function $G(f(t), t)$. Some examples are presented in Section 3.

3   Results

All the examples and required folders are included in the additional material to this article.

3.1   Dual Newton–Raphson example 1

Suppose that $u(x)$ is defined by the equation $f(u, x) = 0$ where

$$f(u, x) = \cos(u\,x) - u^3 + x + \sin(u^2\,x).$$

Let us consider the functions $g_1(x) = \sin(u(x)) + x$ and $g_2(x) = u(\sin x + x^2)$. The problem is to find

$u(x_0)$, $u'(x_0)$, $u''(x_0)$, $g_1(x_0)$, $g_1'(x_0)$, $g_1''(x_0)$, $g_2(x_0)$, $g_2'(x_0)$, $g_2''(x_0)$, with $x_0 = 0.7$. This can be accomplished by writing the Newton–Raphson algorithm in its dual form. Such an algorithm is coded in the function `NR_dual(NRkind,u0,n,fd,gdual)`. In this function, `NRkind` is the kind of method used. `NRkind = NR1` is for the simple Newton–Raphson method and `NRkind = NR2` is for Halley's method, `u0` is the dual point where the method starts to look for a solution, `n` is the number of iterations, `fd` is the equation to solve; in this example it will be $\tilde{f}(\tilde{u}, \tilde{x})$, the dual version of $f(u, x)$; `gdual` is the dual point where we want to evaluate the functions. The following script computes the required values.

```
addpath('01DualNumberF;02DualAlgs')

x = 0.7;
u0 = 1.6d0;
xd = dual(x,1,0);
n = 10;

f = @(u,x) cos(u*x) - u^3 + x + sin(u^2*x);

disp(['The function u and its derivatives' ...
    ' in x = 0.7 are'])
disp(NR_dual('NR1',u0,n,f,xd))

disp(['The function g1 and its derivatives'...
    ' in x = 0.7 are'])
disp(sin(NR_dual('NR1',u0,n,f,xd)) + xd)

disp(['The function g2 and its derivatives'...
    ' in x = 0.7 are'])
disp(NR_dual('NR1',u0,n,f,sin(xd) + xd*xd))
```

Notice the advantages of this method: we can calculate very complicated derivatives involving $u(x)$ by using the dual functions. The results are shown in Table 1.

3.2   Dual Newton–Raphson example 2

The example here presented concerns the RRRCR spatial mechanism [28]. Following Eq. (2) of [28] and the definitions given in the aforementioned reference, the output angle ϕ as a function of the input angle θ is given by the equation

$$
\begin{aligned}
&a^2 c_1^2 c_2^2 - 2\,a\,c_1\,c_2^2\,s_1\,(b-e) - 2\,a\,c_1^2\,c_2^2\,L\cos\theta + 2\,a\,c_1\,c_2^2\,R\cos\phi - c_1^2\,c_2^2\,(b-e)^2 + 2\,c_1\,c_2^2\,L\,s_1\,(b-e)\cos\theta + \\
&2\,c_1\,c_2\,L\,s_2\,(b-e)\sin\theta - 2\,c_1\,R\,s_2\,(b-e)\sin\phi - 2\,R\,s_1\,(b-e)\cos\phi + (b-e)^2 - c_1^2\,c_2^2\,l^2 + c_1^2\,c_2^2\,L^2 + \\
&c_1^2 c_2^2 R^2 \cos^2\phi - 2c_1^2 c_2 LR \sin\theta\sin\phi - c_1^2 R^2 \left(1 - 2\sin^2\phi\right) - 2c_1 c_2^2 LR \cos\theta\cos\phi - 2c_1 c_2 LR s_1 s_2 \sin\theta\cos\phi + \\
&2c_1 R^2 s_1 s_2 \sin\phi\cos\phi + R^2 \cos^2\phi = 0.
\end{aligned}
\qquad (44)
$$

Table 1: Results for the Newton–Raphson example 1.

$u(x_0)$	$u'(x_0)$	$''u(x_0)$	$g_1(x_0)$	$g_1'(x_0)$	$g_1''(x_0)$	$g_2(x_0)$	$g_2'(x_0)$	$g_2''(x_0)$
1.3085	0.1163	-0.9337	1.6658	1.0301	-0.2551	1.2963	-0.2556	-1.1425

Table 2: Parameters used for the Newton–Raphson example 2.

Parameter	Value
L	0.3933578023
l	0.4174323687
a	0.9526245468
R	0.4484604992
s_1	0.6298138891
s_2	0.2506389576
b	2.0
e	1.0

Now, if one is interested in calculating the velocities and accelerations, complicated functions involving ϕ and $\phi'(\theta)$ will appear. As an example, let us consider the function $f(x) = 2\sin^2 x$ and the point $x_0 = 2.0$. The problem is to calculate $f(\phi(x_0))$, $f'(\phi(x_0))$, $f''(\phi(x_0))$, $\phi(f(x_0))$, $\phi'(f(x_0))$ and $\phi''(f(x_0))$ for the same set of parameters given in [28], and reproduced in Table 2 for clarity.

Analogously to the example in Section 3.1, we obtain the results shown in Table 3. Notice that the solution of Eq. (44) for $\theta = 2$ is not unique. The values in Table 3 are for $\phi = 2.1351$.

3.3 Dual cubic spline interpolation example 1

Let $y(x)$ be the normal cubic spline interpolation for the data shown in Table 4.

The values $y(x_0)$, $y'(x_0)$, $f(x_0)$, $f'(x_0)$, $g(x_0)$ and $g'(x_0)$ with $f(x) = x\sin^2(y(x))$, $g(x) = y(x\sin^2 x)$ and $x_0 = 1.75$ can be calculated by dualizing the normal cubic spline interpolation method. This has been done in the function `NCSplinedual(A,xd)`. In such a function, `A` is the matrix containing the points for which the spline will be constructed (in this case, they would be the points of Table 4) and `xd` is the dual point where we want to evaluate, in this case `xd=dual(1.75,1,0)`. For instance the first (second) component of `NCSplinedual(A,xd)` will be $y(x_0)$ ($y'(x_0)$).

The derivatives $f'(x_0)$ and $g'(x_0)$, respectively, are obtained by taking component `f1` of

```
xd*sin(NCSplinedual(A,xd))^2
```

and

```
NCSplinedual(A, xd*sin(xd)^2)
```

The results are given in Table 5.

3.4 Dual cubic spline interpolation example 2

This example concerns the determination of the thermal properties of a solid using photothermal radiometry [24]. In particular, we are interested in determining the thermal diffusivity from the experimental data of Fig. 4 from [24]. The experimental data can be extracted using EasyNData [41]. Assuming that such data are stored in the matrix `pts`, the dual cubic spline interpolation is done by `NCSplinedual(pts,x)`. Now, according to [24], the thermal diffusivity can be calculated from

$$\alpha_s = \frac{64\,L_s^2\,f_q}{9\,\pi}, \qquad (45)$$

where $L_s = 522\,\mu\text{m}$ is the thickness of the studied sample and f_q is the frequency for which the derivative of the amplitude of the radiometry signal is zero. The frequency f_q can be calculated using the Newton–Raphson algorithm. To this end we define the dual function `fej2(x)` containing the first and second derivatives of the spline. The essential part of the code is

```
function fr = fej2(x)
...
auxresult = NCSplinedual(pts,x);
fr  = dual(auxresult.f1,auxresult.f2,0);
...
```

Table 3: Results for the Newton–Raphson example 2.

$f(\phi(x_0))$	$f'(\phi(x_0))$	$f''(\phi(x_0))$	$\phi(f(x_0))$	$\phi'(f(x_0))$	$\phi''(f(x_0))$
1.4279	-1.7693	-1.2856	1.7817	-1.6171	-3.5137

Table 4: Points used for the dual cubic spline interpolation example 1.

x	y
1.	0
1.25	0.22314355
1.5	0.40546511
1.75	0.55961579
2.	0.69314718
2.25	0.81093022
2.5	0.91629073
2.75	1.0116009
3.	1.0986123

Taking `x0 = 10.0` as the initial point where the Newton–Raphson algorithm will start to look for a solution, f_q can be found by

```
...
fq = x0;

for k=1:50
  fauxd = fej2(dual(fq,1,0));
  fq    = fq - fauxd.f0/fauxd.f1;
end
...
```

After this, the obtained thermal diffusivity was $\alpha_s = 6.00 \times 10^{-6} \, \mathrm{m^2 s^{-1}}$ which is in good agreement with the value reported in [24, 42].

3.5 Dual Runge–Kutta example

Consider the Duffing equation studied in [27]

$$f''(t) + 0.4\,f'(t) + 1.1\,f(t) + f^3(t) = 2.1\,\cos(1.8\,t) \tag{46}$$

with initial conditions

$$f(0) = 0.3, \ f'(0) = -2.3. \tag{47}$$

The values $f(t)$, $(f \circ g)(t)$, $(g \circ f)(t)$, as well as their first and second derivatives at $t = 1.0$ (or at some other t where the functions are defined) for the function $g(t) =$ $\sin t$ (or some other function where the above compositions are defined) can be calculated by dualizing the Runge–Kutta algorithm. Such an algorithm is dualized in the function `rk4dual(u1,u2,t0,x10,x20,np,td)`. In this function, `x10` and `x20` are the initial conditions for $f(t_0)$ and $f'(t_0)$ respectively (see Section 2.3.3 for details and also for the definitions of u_1 and u_2); `td` is the dual point where we want to evaluate the solution; and `np` is the number of steps between t_0 and and the real component of `td`. The values for $f(t)$, $(f \circ g)(t)$, $(g \circ f)(t)$, as well as their first and second derivatives at $t = 1.0$ are shown in Table 6.

4 Conclusions

After a dualization of the normal cubic spline interpolation algorithm, the Runge–Kutta algorithm, and the Newton–Raphson algorithm, it is possible to calculate the derivatives of functions efficiently, precisely, and accurately. So we can calculate the derivatives of functions depending on the solution of algebraic or differential equations as well as functions resulting from the spline interpolation of experimental data. As an added value to the normal cubic spline interpolation algorithm, it is shown that a closed form expression for its coefficients can be obtained. Interesting applications in science and engineering were studied. Those examples can be used as a guide to dualize many other functions and algo-

Table 5: Results for the dual cubic spline interpolation example 1.

$y(x_0)$	$y'(x_0)$	$f(x_0)$	$f'(x_0)$	$g(x_0)$	$g'(x_0)$
0.5596	0.5727	0.4931	1.1836	0.5272	0.2097

Table 6: Results for the Runge–Kutta example. The functions are evaluated at $t = 1.0$.

f	f'	f''	$(f \circ g)$	$(f \circ g)'$	$(f \circ g)''$	$(g \circ f)$	$(g \circ f)'$	$(g \circ f)''$
-0.7474	-0.1282	0.8140	-0.6797	-0.0940	0.6081	-0.7144	-0.1638	0.6608

rithms. For example, it would be interesting to dualize the trapezium rule although this would be only for academic purposes since there is not much to gain because its components would be the integral, the first derivative (which is actually the function to integrate), and the second derivative (which is actually the first derivative of the function to integrate). Nevertheless, the dualization of an integration method could be necessary for dualizing some other algorithm.

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