Commun Nonlinear Sci Numer Simulat 19 (2014) 2614–2623

Contents lists available at ScienceDirect

Commun Nonlinear Sci Numer Simulat

journal homepage: www.elsevier.com/locate/cnsns

Dirac's formalism combined with complex Fourier operational matrices to solve initial and boundary value problems

William Labecca, Osvaldo Guimarães, José Roberto C. Piqueira *

Escola Politécnica da Universidade de São Paulo, Avenida Prof. Luciano Gualberto, travessa 3, n. 158, 05508-900 São Paulo, SP, Brazil

ARTICLE INFO

Article history:
Received 2 May 2013
Received in revised form 1 January 2014
Accepted 2 January 2014
Available online 10 January 2014

Keywords:
Bracket formalism
Fourier series
Hilbert space
Operational matrices

ABSTRACT

Approximations of functions in terms of orthogonal polynomials have been used to develop and implement numerical approaches to solve spectrally initial and boundary value problems. The main idea behind these approaches is to express differential and integral operators by using matrices, and this, in turn, makes the numerical implementation easier to be expressed in computational algebraic languages. In this paper, the application of the methodology is enlarged by using Dirac's formalism, combined with complex Fourier series.

1. Introduction

The solutions of differential equations, as is well known, often require considerable endeavor, and some of them do not have either analytic solutions by elementary functions or by infinite series with recurrence relations [10]. Consequently, alternative methods have been proposed, in order to implement numerical procedures.

Runge–Kutta [16] or Adams–Bashforth and Adams–Moulton methods are often used for initial value problems (IVP) [27], being constituent parts of specific software packets, though not applicable to boundary value problems (BVP). For BVP, variational [25] and Galerkin's methods [2,18] are used.

However there are other procedures, such as approximations by orthonormal functions [1,11,17], which, combined with optimization algorithms, presents very acceptable results with low error margins obtained spending low computational power and processing time [19,20,26,34].

Approximations by orthogonal functions have played an important role in physics and engineering, contributing to technological development and mathematical analysis evolution. In spite of this approach not being recent, its importance has significantly increased, mainly in the three last decades [12,13,17,23,32], assuming a fundamental role in the elaboration of new techniques related to the solution of problems of analysis and optimal control, for instance.

The motivation behind this kind of method is the advantages it provides in transforming differential equations into algebraic ones, simplifying solution processes. In order to formalize the ideas, the language of linear algebra is used, with linear operators representing derivative and integration operations.

The solution of differential equations by using operational matrices has been carried out by some authors, considering linear combinations of orthogonal polynomial bases. Integration matrices for Bessel functions [30], series of Fourier [31,33] and Laguerre's [4,21,24], as well as for polynomials of Chebyshev [22,29], Legendre [6,28], Bernstein [14,15,35] and Walsh [7,8] have already been determined.

* Corresponding author. Tel.: +(55) 11 3091 5221; fax: +(55) 11 3091 5718.
E-mail addresses: w.labecca@gmail.com (W. Labecca), osvaldo.guimaraes@gmail.com (O. Guimarães), piqueira@lac.usp.br (J.R.C. Piqueira).

1007-5704/$ - see front matter © 2014 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.cnsns.2014.01.001

Guimarães et al. [19] added evolutionary computation to this procedure, developing a spectral genetic algorithm which allowed the solution of non-linear differential equations by high order series. Besides, Guimarães et al. [20] deduced a form to obtain all operational matrices of polynomial bases through the *Sandwich Matrix Theorem*. Here, considering the large variety of applications for these techniques, an extension of this linear operational formalism is proposed to the complex Fourier series, by using Dirac's bracket notation [9].

The motivation for this approach is based on two ideas: over the complex field, using approximations by periodic functions is highly desirable, since many physical phenomena present periodic features and a mathematical description in these terms, along with a complex treatment, would enhance the scope and applicability of the method. Besides, the powerful simplification obtained by the use of bracket notation, provides an expansion of applicability along with more conciseness.

In the next section, the analytic foundations of the operational matrix method is presented, combined with Dirac's notation. Then, an algorithm description for complex Fourier series approximation is presented, with some examples. Closing the idea, a section describing the numerical procedures appears, followed by brief conclusions.

2. Analytic foundations

Replacing a differential equation with a linear system is based on the assumption of univocal determination of a linear operator D representing the derivative or integration operation, acting on a function, such that, if function $f(x)$ is approximated by a series $f_n(x) = \sum_{i=1}^{n} c_i b_i(x)$, where c_i are its coefficients and $b_i(x)$ the basis of the elected series, then the following can be written:

$$\frac{d}{dx} f(x) \to D f_n(x).$$

Here $f_n(x)$ is the n-terms finite series that represents the approximation of the function. In this case, the derivative linear operator D must be represented by a square $n \times n$ matrix, as in [28] for example.

The approximated series must be described by the inner product of a vector, defined by the series coefficients, by another one, composed of the basis elements, which may be polynomial, exponential or of any type. Then:

$$f_n(x) = \langle C, B(x) \rangle,$$

where C is the coefficient vector and B, the basis vector.

The same result can be obtained by the multiplication of a n-column row matrix by a n-row column matrix. This result, despite being a vector in the Hilbert space, is scalar in the discrete n-dimension space of the approximative series.

The same idea applies to its derivative, which may be obtained by the application of a linear operator to the approximate function, generating a new function, described in the original basis by other coefficients, according to the equation

$$f_n'(x) = \langle C_D, B(x) \rangle.$$

2.1. Dirac's formalism

In order to work with complex variables, it is more convenient to use Dirac's bracket formalism [9]. In this way, the inner product between two vectors $|u\rangle$ and $|v\rangle$ will be defined by:

$$\langle u | v \rangle := \sum_{i=1}^{n} \widetilde{u}_i^* v_i,$$

where u_i are the coordinates of $|u\rangle$ in the original Hilbert space, expressed as a column matrix, whereas its conjugate transpose $|u\rangle^{T*} \equiv |u\rangle^{*T}$, denoted by dagger †, i.e., $|u\rangle^{\dagger}$, with coordinates $\widetilde{u}_i^*$, is a covector.

Consequently, a dual vector $|u\rangle^{\dagger} = \langle u|$, expressed by a row matrix, obeying the condition $\langle u|u\rangle = \|u\|^2$, is associated. Then, a covector $\langle v|$ is a vector in the dual space associated to the original Hilbert space, given by $\langle v| = |v\rangle^{\dagger}$.

Considering the above hypothesis, a function approximation by a n-terms series can be expressed as:

$$f_n(x) = \langle C | B(x) \rangle,$$

where $\langle C| := (c_1, \ldots, c_n)$ are the covector components.

Besides,

$$|B(x)\rangle = \begin{bmatrix} b_1(x) \\ \vdots \\ b_n(x) \end{bmatrix}$$

is the vector associated to the chosen finite basis. For a canonical n-dimensional polynomial basis, for example, $b_k(x) = x^{k-1}$, $(k = 1, \ldots, n)$.