Journal of Computational Physics 305 (2016) 1–28

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Well-conditioned fractional collocation methods using fractional Birkhoff interpolation basis

Yujian Jiao [a,b,1], Li-Lian Wang [c,*,2], Can Huang [d,3]

[a] *Department of Mathematics, Shanghai Normal University, Shanghai, 200234, China*
[b] *Scientific Computing Key Laboratory of Shanghai Universities, China*
[c] *Division of Mathematical Sciences, School of Physical and Mathematical Sciences, Nanyang Technological University, 637371, Singapore*
[d] *School of Mathematical Sciences and Fujian Provincial Key Laboratory on Mathematical Modeling & High Performance Scientific Computing, Xiamen University, Fujian, 361005, China*

ARTICLE INFO

Article history:
Received 27 March 2015
Received in revised form 17 October 2015
Accepted 19 October 2015
Available online 23 October 2015

Keywords:
Fractional differential equations
Caputo fractional derivative
(Modified) Riemann–Liouville fractional derivative
Fractional Birkhoff interpolation
Interpolation basis polynomials
Well-conditioned collocation methods

ABSTRACT

The purpose of this paper is twofold. Firstly, we provide explicit and compact formulas for computing both Caputo and (modified) Riemann–Liouville (RL) fractional pseudospectral differentiation matrices (F-PSDMs) of any order at general Jacobi–Gauss–Lobatto (JGL) points. We show that in the Caputo case, it suffices to compute F-PSDM of order $\mu \in (0,1)$ to compute that of any order $k+\mu$ with integer $k \ge 0$, while in the modified RL case, it is only necessary to evaluate a fractional integral matrix of order $\mu \in (0,1)$. Secondly, we introduce suitable fractional JGL Birkhoff interpolation problems leading to new interpolation polynomial basis functions with remarkable properties: (i) the matrix generated from the new basis yields the exact inverse of F-PSDM at "interior" JGL points; (ii) the matrix of the highest fractional derivative in a collocation scheme under the new basis is diagonal; and (iii) the resulted linear system is well-conditioned in the Caputo case, while in the modified RL case, the eigenvalues of the coefficient matrix are highly concentrated. In both cases, the linear systems of the collocation schemes using the new basis can be solved by an iterative solver within a few iterations. Notably, the inverse can be computed in a very stable manner, so this offers optimal preconditioners for usual fractional collocation methods for fractional differential equations (FDEs). It is also noteworthy that the choice of certain special JGL points with parameters related to the order of the equations can ease the implementation. We highlight that the use of the Bateman's fractional integral formulas and fast transforms between Jacobi polynomials with different parameters, is essential for our algorithm development.

* Corresponding author.
E-mail address: lilian@ntu.edu.sg (L.-L. Wang).

[1] This author is supported in part by NSFC grants (Nos. 11171227, 11371123 and 11571151), Natural Science Foundation of Shanghai (No. 13ZR1429800), and the State Scholarship Fund of China (No. 201308310188).

[2] The research of this author is partially supported by Singapore MOE AcRF Tier 1 Grants (RG15/12 and RG27/15), Singapore MOE AcRF Tier 2 Grant (MOE 2013-T2-1-095, ARC 44/13) and Singapore A*STAR-SERC-PSF Grant (122-PSF-007).

[3] The research of the this author is supported by the NSFC (No. 11401500) and the Fundamental Research Funds for the Central Universities (No. 20720150007).

http://dx.doi.org/10.1016/j.jcp.2015.10.029
0021-9991/

1. Introduction

Fractional differential equations have been found more realistic in modelling a variety of physical phenomena, engineering processes, biological systems and financial products, such as anomalous diffusion and non-exponential relaxation patterns, viscoelastic materials, among others. Typically, such scenarios involve long-range temporal cumulative memory effects and/or long-range spatial interactions that can be more accurately described by fractional-order models (see, e.g., [38,36,24,12,13] and the references therein).

One challenge in numerical solutions of FDEs resides in that the underlying fractional integral and derivative operators are global in nature. Indeed, it is not surprising to see the finite difference/finite element methods based on "local operations" lead to full and dense matrices (cf. [35,32,40,34,15,16,42,22] and the references therein), which are expensive to compute and invert. It is therefore of importance to construct fast solvers by carefully analysing the structures of the matrices (see, e.g., [44,31]). This should be in marked contrast with the situations when they are applied to differential equations of integer order derivatives. In this aspect, the spectral method using global basis functions appears to be well-suited for non-local problems. However, only limited efforts have been devoted to this very promising approach (see, e.g., [29,30,28,49,48,9]), when compared with a large volume of literature on finite difference and finite element methods.

Another more distinctive challenge in solving FDEs lies in that the intrinsic singular kernels of the fractional integral and derivative operators induce singular solutions and/or data. Just to mention a simple FDE involving RL fractional derivatives of order $\mu \in (0,1)$: $\big({}_{-1}^{\;R}D_x^{\mu}\, u\big)(x) = 1$ for $x \in (-1,1)$, such that $u(-1) = 0$, whose solution behaves like $u(x) \sim (1+x)^{\mu}$. Accordingly, it only has a limited regularity in a usual Sobolev space, so the naive polynomial approximation has a poor convergence rate. Zayernouri and Karniadakis [49] proposed to approximate such singular solutions by Jacobi poly-fractonomials (JPFs), which were derived from eigenfunctions of a fractional Sturm–Liouville operator. Chen, Shen and Wang [9] modified the generalised Jacobi functions (GJFs) introduced earlier in Guo, Shen and Wang [19], and rigorously derived the approximation results in weighted Sobolev spaces involving fractional derivatives. The JPFs turned out to be special cases of GJFs, and the GJF Petrov-spectral-Galerkin methods could achieve truly spectral convergence for some prototypical FDEs. We also refer to [45] for interesting attempts to characterise the regularity of solutions to some special FDEs by Besov spaces. It is also noteworthy that the analysis of spectral-Galerkin approximation in [29,30] was under the function spaces and notion in [16], and in [22], the finite-element method was analysed for the case with smooth source term but singular solution.

It is known that by pre-computing the pseudospectral differentiation matrices (PSDMs), the collocation method enjoys a "plug-and-play" function with simply replacing derivatives by PSDMs, so it has remarkable advantages in dealing with variable coefficients and nonlinear PDEs. However, the practicers are usually plagued with the dense, ill-conditioned linear systems, when compared with properly designed spectral-Galerkin approaches (see, e.g., [8,39]). The "local" finite-element preconditioners (see, e.g., [25]) and "global" integration preconditioners (see, e.g., [11,18,20,14,46,47]) were developed to overcome the ill-conditioning of the linear systems. When it comes to FDEs, it is advantageous to use collocation methods, as the Galerkin approaches usually lead to full dense matrices as well. Recently, the development of collocation methods for FDEs has attracted much attention (see, e.g., [28,50,43,17]). It was numerically testified in [28,50] that for both Lagrange polynomial-based and JPF-based collocation methods, the condition number of the Caputo F-PSDM of order μ behaves like $O(N^{2\mu})$ which is consistent with the integer-order case. However, it seems very difficult to construct preconditioners from finite difference and finite elements as they own involve full and dense matrices and suffer from ill-conditioning.

The main purpose of this paper is to construct integration preconditioners and new basis functions for well-conditioned fractional collocation methods from some suitably defined *fractional Birkhoff polynomial interpolation problems.* In [46], optimal integration preconditioners were devised for PSDMs of integer order, which allows for stable implementation of collocation schemes even for thousands of collocation points. Following the spirit of [46], we introduce suitable fractional Birkhoff interpolation problems at general JGL points with respect to both Caputo and (modified) Riemann–Liouville fractional derivatives (note: the RL fractional derivative is modified by removing the singular factor so that it is well defined at every collocation point). As we will see, the extension is nontrivial and much more involved than the integer-order derivative case. Here, we restrict our attention to the polynomial approximation, though the ideas and techniques can be extended to JPF- and GJF-type basis functions. On the other hand, using a suitable mapping, we can transform the FDE (e.g., the aforementioned example) and approximate the smooth solution of the transformed equation, which is alternative to the direct use of JPF or GJF approximation to achieve spectral accuracy for certain special FDEs.

We highlight the main contributions of this paper in order.

- From the fractional Birkhoff interpolation, we derive new interpolation basis polynomials with remarkable properties:
  (i) It provides a stable way to compute the exact inverse of Caputo and (modified) Riemann–Liouville fractional PSDMs associated with "interior" JGL points. This offers integral preconditioners for fractional collocation schemes using Lagrange interpolation basis polynomials.
  (ii) Using the new basis, the matrix of the highest fractional derivative in a collocation scheme is identity, and the F-PSDMs are not involved. More importantly, the resulted linear systems can be solved by an iterative method converging within a few iterations even for a very large number of collocation points.
- We propose a compact and systematic way to compute Caputo and (modified) Riemann–Liouville F-PSDMs of any order at JGL points. In fact, we can show that the computation of F-PSDM of order $k+\mu$ with $k \in \mathbb{N}$ and $\mu \in (0,1)$ boils down to evaluating (i) F-PSDM of order μ in the Caputo case, and (ii) a modified fractional integral matrix of order μ