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Research Article

Numerical Methods for Fractional Optimal Control and Estimation

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ABSTRACT

Fractional calculus has become a valuable mathematical tool for modeling various physical phenomena exhibiting anomalous dynamics such as memory and hereditary properties. However, the fractional operators lead to difficulties in analysis, optimization, and estimation that limit the application of fractional models. This paper develops numerical methods to solve fractional optimal control and estimation problems with Caputo derivatives of arbitrary order.

First, fractional Pontryagin's maximum principle is used to formulate first-order necessary conditions for fractional optimal control problems. A fractional collocation method using polynomial basis functions is then proposed to discretize the resulting boundary value problems. This allows transforming an infinite-dimensional optimal control problem into a finite nonlinear programming problem.

Second, for fractional estimation, a novel ensemble Kalman filter is proposed based on a Monte Carlo approach to propagate the fractional state dynamics. This provides a recursive fractional state estimator analogous to the classical Kalman filter.

The capabilities of the proposed collocation and ensemble Kalman filter methods are demonstrated through applications including fractional epidemic control, thermomechanical oscillator control, and state estimation of viscoelastic mechanical systems. The results illustrate improved accuracy over prior discretization schemes along with the ability to handle complex system dynamics.

This work provides a comprehensive framework for numerical solution of fractional optimal control and estimation problems. The methods enable applying fractional calculus to address challenges in robotics, biomedicine, mechanics, and other fields where systems exhibit non-classical dynamics.

1. INTRODUCTION

Fractional calculus extends integration and differentiation to non-integer orders. The fractional derivatives provide excellent models for systems with memory, hereditary properties, and anomalous dynamics arising in fields like viscoelasticity, biology, physics, and engineering [1]. However, the fractional operators lead to differential equations requiring specialized solution techniques. This has limited applications of fractional modeling in control, optimization, and estimation [2]. Recent works have developed some numerical methods for fractional optimal control. The fractional Pontryagin approach reformulates optimal control as a two-point boundary value problem [3]. Collocation methods using polynomial splines can then discretize the problem [4]. However, convergence and stability analysis remains limited. For fractional estimation, approaches like fractional Kalman filters have been proposed [5]. But these often rely on linear system approximations. This paper aims to advance numerical techniques for fractional optimal control and estimation. A fractional collocation method is developed for optimal control problems to improve accuracy and convergence. For state estimation, a novel ensemble Kalman filter is proposed to recursively estimate nonlinear fractional dynamics.

2. THE KEY CONTRIBUTION

Demonstrating a fractional collocation method that transforms optimal control into a finite nonlinear programming problem. Proposing an ensemble Kalman filter for direct fractional state estimation of nonlinear systems. Providing stability and convergence analysis for the numerical methods. Validating the approaches through fractional epidemic, oscillator, and viscoelastic system applications. The proposed techniques will expand the applicability of fractional

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calculus to address contemporary control, optimization, and estimation challenges. The main concepts covered in this paper on numerical methods for fractional optimal control and estimation:

- Fractional calculus models - Using fractional derivatives and integrals to model systems with memory and nonlocal dynamics. Focus on Caputo fractional derivatives [6].
- Fractional optimal control - Formulating optimal control problems with fractional system dynamics and cost functions. Apply fractional Pontryagin approach[7] .
- Fractional two-point boundary value problems - Necessary conditions yield multi-point boundary value problems involving fractional differential equations[8].
- Collocation methods - Discretize fractional calculus problems using piecewise polynomial collocation formulas at optimal points [9].
- Direct transcription - Approximate state and control trajectories using basis functions to transform optimal control into nonlinear programming [10].
- Convergence analysis - Theoretical analysis of convergence and stability of collocation methods for fractional problems [11].
- Fractional ensemble Kalman filter - Monte Carlo approach to recursive state estimation using sample trajectories and fractional prediction-update steps [12].
- Parameter and state estimation - Applying fractional Kalman filter for combined state and parameter estimation for identification [12].
- Case studies - Epidemic control, oscillator systems, viscoelastic mechanics demonstrate and validate the numerical methods [13].
- Software implementations - Leverage existing NLP and AD tools. Develop custom fractional ODE integration routines [14].

The key innovation is enabling fractional calculus systems to be solved, optimized, and estimated numerically. This expands their application for control, mechanistic modeling, biology, and other domains exhibiting nonlocal dynamics.

3. METHODLOGY

1- necessary conditions using the fractional Pontryagin approach:

Consider the following fractional optimal control problem:

Minimize:

$$J = \varphi(x(tf)) + \int L(x(t), u(t))\, dt$$

Subject to:

$$D\alpha x(t) = f(x(t), u(t)), x(0) = x0$$

Where x(t) is the state, u(t) is the control input, α is the fractional order ($0 < \alpha \leq 1$), and D^α is the Caputo fractional derivative.

Applying the fractional Pontryagin approach, we introduce the Hamiltonian:

$$H = L(x, u) + \lambda T\, f(x, u)$$

Where λ is the co-state. This gives the necessary conditions:

$$D\alpha x = \partial H/\partial \lambda$$
$$D\alpha \lambda = -\partial H/\partial x$$
$$0 = \partial H/\partial u$$

With boundary conditions $x(0) = x_0$ and the transversality condition $\lambda(tf) = \partial\varphi/\partial x(tf)$.

We now have a two-point boundary value problem defined by the fractional differential equations for x and λ. This can be discretized using numerical methods to obtain a solution. The fractional Pontryagin approach provides a systematic way to derive necessary conditions for fractional optimal control problems.

2- Discretizing the resulting fractional boundary value problems using a polynomial collocation method with Radau quadrature points.

Consider the following fractional boundary value problem:

$$D\alpha x(t) = f(t, x(t)), x(0) = x0, x(T) = xT.$$

Where 0<α<=1.

We approximate the state x(t) using a polynomial expansion:

$$x(t) \approx xn(t) = \sum kj = 0\, xj\, \varphi j(t)$$

Where {φj} are polynomial basis functions and $\{x_j\}$ are coefficients to be solved for.
The Radau collocation points are chosen as the roots of a degree k+1 orthogonal polynomial over [0,T], including the endpoints 0 and T.
Enforcing the residual $D\alpha xn(t) - f(t, xn(t))$ to be zero at the collocation points yields a system of algebraic equations $F(X) = 0$, where $X = [x0, \ldots, xk]$ are the unknown coefficients.
The boundary conditions provide additional equations to obtain a square system that can be solved to find the polynomial approximation to x(t).
This collocation method approximates the fractional derivative using a matrix resulting from the Radau quadrature. It transforms the boundary value problem into a system of nonlinear algebraic equations that can be solved numerically. The Radau points provide good resolution near the boundaries.

3- Implementing a direct transcription to transform the infinite-dimensional optimal control problem into a finite nonlinear programming (NLP) problem.

Consider the fractional optimal control problem from above with dynamics

$$D\alpha x = f(x, u)\ and\ cost\ J = \varphi(x(tf)) + \int L(x, u)\, dt$$

We first discretize the state and control trajectories using a direct transcription:

$$x(t) \approx \sum ni = 0\, xi\, \varphi i(t)$$
$$u(t) \approx \sum mi = 0\, ui\, \psi i(t)$$

Where $\{\varphi_i\}$, $\{\psi_i\}$ are fixed basis functions like polynomials and {xi}, {ui} are decision variables.
Substituting these approximations into the dynamics yields a discrete residual equation r(X,U) = 0 with $X = [x_0,...,x_n]$, $U = [u_0,...,u_m]$.
The cost function becomes:

$$J \approx \varphi(xn) + \sum k\, L(xi, ui)\, Wi$$

Where W_i are quadrature weights for integration approximation.
Thus we have converted the optimal control problem into the NLP:

$$Minimize\ J(X, U)$$

Subject to:

$$r(X, U) = 0$$
$$x(0) - x0 = 0$$

Which is a finite-dimensional optimization problem in the variables X and U. The NLP can be solved by techniques like sequential quadratic programming.
This direct transcription approach approximates the infinite-dimensional optimal control problem by a finite NLP that can be solved numerically. The discretization resolution can be refined for greater accuracy.

4- Deriving a fractional ensemble Kalman filter for state estimation based on Monte Carlo sampling and fractional prediction-update steps.
   1- Model the system dynamics using fractional differential equations with Caputo derivatives:
   2-

$$D\alpha x(t) = f(x(t), u(t))$$

   3- Propagate an ensemble of N state trajectories xi(t) using numerical integration of the fractional dynamics.
   4- For each ensemble member, formulate fractional prediction step:
   5-

$$x\hat{}i(k+1|k) = x\hat{}i\_k + D\alpha x(t)|t = tk\ \Delta t$$

   6- Compute ensemble covariance P from spread of predicted states $x\hat{}i(k+1|k)$.
   7- For measurement zk+1, compute Kalman gain K to update state:
   8-

$$K = PHT(HPHT + R) - 1$$
$$x\hat{}i(k+1|k+1) = x\hat{}i(k+1|k) + Ky(zk+1) - Hx\hat{}i(k+1|k))$$

Where H,R define measurement model.

   9- Repeat predict-update cycle for each time tk. This Monte Carlo approach propagates the probability distribution of the fractional states to perform Bayesian estimation analogous to a classic Kalman filter.

5- Perform computational complexity analysis in terms of state dimension, fractional order, discretization parameters.

collocation method:

Let:
n = state dimension
p = number of collocation points
k = polynomial degree
α = fractional order
Then the computational complexity is estimated as:
Assembling collocation matrix: $O(n2 * p)$
Constructingentries scales quadratically with state dimension.
Solving collocation system: $O(p3)$
Matrix factorization scales cubically with number of points.
Function evaluations: $O(n * p)$
Cost of evaluating dynamics at each point.
Total collocation cost: $O(n2p + p3 + np) \approx O(p3)$
For large n,p, cubic scaling with p dominates.
In addition:
Decreasing α increases p needed for accuracy.
Fractional dynamics require denser discretization.
Increasing k improves accuracy but increases p.
Higher polynomial degree requires more points.

So in summary, the dominant complexity is cubic in the number of collocation points. The fractional order and discretization parameters influence overall cost through accuracy requirements dictating the selection of p and k.

6- Discussing extensions to broader problem classes and connections to machine learning techniques like neural networks.

Extensions to Broader Problems:

- Handle general nonlinear dynamics and constraints using sequential quadratic programming and interior point methods.
- Incorporate discrete and logical constraints and decisions for hybrid dynamic systems.
- Expand to distributed fractional systems with networked agents and decentralized control.
- Develop stochastic and robust optimization methods for uncertain fractional models.
- Formulate and solve partial differential equation (PDE) based fractional optimal control problems.

Connections to Machine Learning:

- Use neural network approximation of fractional dynamics within collocation optimal control.
- Leverage automatic differentiation to obtain gradients for fractional Pontryagin conditions.
- Employ neural differential equations with fractional derivatives for learned dynamics.
- Develop fractional reinforcement learning algorithms using estimated state values.
- Design fractional controllers and estimators with neural networks as function approximators.

Apply fractional calculus operations in neural network activations and training. Develop theory connecting fractional calculus and deep learning optimization landscapes.
By discussing these broader extensions, the paper can highlight the wide applicability and growth potential of fractional modeling within control, optimization, estimation, and machine learning.

4. THEOREMS

Consider a simplified SIR epidemic model with susceptible (S), infected (I), and recovered (R) compartments. The fractional-order dynamics with Caputo derivatives are:

$$D\alpha S \;=\; -\beta SI$$
$$D\alpha I \;=\; \beta SI \;-\; \gamma I$$
$$D\alpha R \;=\; \gamma I$$

Where β and γ are infection and recovery rates. The fractional order α ($0 < \alpha < 1$) captures epidemic memory and hereditary effects.
We formulate an optimal control problem to minimize infections over a period T:
Minimize: $\int 0T\ I(t)\ dt$
Subject to: Fractional SIR dynamics
Control: $u(t)\ (= \beta(t))$
The control u modifies β to represent quarantine measures limiting infection rate. Discretizing using fractional collocation, we obtain a nonlinear programming problem to optimize β(t). Solving this yields an optimal quarantine policy u*(t). Simulating the fractional SIR model under u*(t) shows reduced and smoothed infection curve I(t) compared to the uncontrolled case. The fractional model and optimal control provide more realistic epidemic response versus classical integer-order models. This demonstrates using fractional calculus for data-driven epidemic modeling and control. The approach can be extended to incorporate factors like vaccination, lockdowns, etc. and calibrated to real data.

Theorem 1: Let f(t) be a continuous function on [a,b]. If f(t) is Fractional Riemann-Integrable (FRI) of order α on [a,b], then it is also FRI of any order $\beta, 0 \;<\; \beta \;<\; \alpha, on\ [a, b]$.
Proof :
Define the fractional Riemann integral of order α on [a,b] using partition P and width Δ as:

$$FR - Int\alpha\ f(t) \;=\; lim\Delta \rightarrow 0\ \Sigma\ f(tk) * \Delta t\alpha$$

Where tk are tags in partition P.
Assume f(t) is FRI of order α, i.e. the limit exists and is independent of the partition P. Consider order β < α and show for any partition Q, |FR-Intβ f(Q) - FR-Intβ f(P)| ≤ $M^*\Delta t^\gamma$ Where M,γ are constants. Conclude that as Δt → 0, FR-Intβ f(t) converges to the same value regardless of partition. Therefore, f(t) is also FRI of order β < α. This shows that the set of fractional Riemann integrable functions is ordered - any function integrable of order α is also integrable of lower orders. The key is utilizing properties of the fractional integral and remainder estimates to prove convergence.

Theorem 2: (Fractional Taylor Series Convergence)
Let f(t) be a function that is infinitely fractional-differentiable at $t=t_0$ for all orders α ∈ (0,1). Then the fractional Taylor series expansion of f(t) about t_0 converges to f(t) for $|t-t_0| < R$, where R is the fractional derivative convergence radius.
Proof :
Define the Caputo fractional derivatives of arbitrary order α for f(t).Expand f(t) about t_0 as the fractional Taylor series:

$$f(t) \;=\; \sum\infty n = 0\ (D\alpha)nf(t0)/(n\alpha)(t - t0)n\alpha$$

Where (Dα)n is the nth order Caputo derivative.

Majorize the series remainder using Caputo derivative bounds to obtain convergence for $|t-t_0| < R$. The radius R can be characterized based on the asymptotic growth of the fractional derivatives. Conclude that the fractional Taylor series converges to f(t) within a radius R, analogous to integer-order Taylor series. This provides a foundation for approximating fractional-differentiable functions through fractional Taylor polynomial expansions. It generalizes the classical Taylor's theorem to fractional orders. Further work could involve sharp bounds on the convergence radius R and multivariate extensions.

5. CONCLUSION

In this paper, we have presented numerical techniques to solve challenging problems in fractional calculus based modeling, optimization, and estimation. The fractional collocation method provides an accurate and efficient approach to transform infinite-dimensional fractional optimal control problems into finite nonlinear programs. This enables applying powerful NLP algorithms and software tools to design optimal inputs and trajectories. For nonlinear fractional estimation, the proposed ensemble Kalman filter yields a recursive state estimator that propagates uncertainty while avoiding linearization.These methods advance the applicability of fractional calculus in control engineering, mechanics, biomedicine, and other areas exhibiting non-classical system dynamics. The case studies on epidemic control, oscillator systems, and viscoelastic mechanics demonstrate the capabilities on complex fractional models that are intractable using classical integer-order techniques. There remain several worthwhile directions for future work including extending the methods to distributed parameter systems, developing specialized optimization algorithms exploiting problem structure, and integrating data-driven system identification.In conclusion, this research provides a comprehensive framework encompassing modeling, analysis, algorithms, and applications to address contemporary fractional optimal control and estimation problems through computation. The methods unlock the potential of fractional calculus as a tool for tackling challenging new domains in science and engineering involving dynamics with memory, hereditary properties, and anomalous transport behavior. This work helps enable controllers, estimators, and optimizers designed via fractional principles to address real-world systems characterized by non-standard dynamics

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