RICAM Special Semester on Optimization

Workshop 2
Optimal control and optimization for nonlocal models

Book of Abstracts


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LECTURE I: Introduction to fractional calculus

Abner J. Salgado
Univeristy of Tennessee, TN, USA
asalgad1@utk.edu

Abstract

We will discuss several approaches to extend the notion of a derivative to a fractional order, their meaning, limitations, and possible applications. For some of these, we will study the existence, uniqueness, and regularity of solutions to initial boundary value problems with these operators, and their implications for optimization and numerical approximations.

LECTURE II: Introduction to nonlocal operators and equations

Tadele Mengesha
The University of Tennessee, Knoxville
mengesha@utk.edu

Abstract

Nonlocal models are becoming commonplace across applications. Typically these models are formulated using integral operators and integral equations, in lieu of the commonly used differential operators and differential equations. In this introductory lecture, I will present main properties of these nonlocal operators and equations. Tools of analyzing them such as nonlocal calculus, methods of showing well posedness of models, as well as corresponding solution/function spaces will be discussed. Behavior of solutions of nonlocal equations as a function of a measure of nonlocality will be analyzed. For example, with proper scaling, we will confirm consistency of models by showing that in the event of vanishing nonlocality, a limit of such solutions solve a differential equation. We will demonstrate all these in two model examples: a nonlocal model of heat conduction and a system of coupled equations from nonlocal mechanics.

On the properties of the nonlocal Cahn–Hilliard model with the double obstacle potential

Olena Burkovska
Florida State University, FL, USA,
oburkovska@fsu.edu

Abstract

We consider a nonlocal Cahn–Hilliard model with the double-well obstacle potential on a bounded domain, which is motivated by the problem of phase separation in copolymer melts. While different types of nonlocality can appear in the model, we study the case that includes both local and nonlocal operators. The latter one corresponds to a nonlocal Ginzburg-Landau energy functional and describes long-range interactions between particles in the model. We also discuss several ways how to prescribe nonlocal boundary fluxes that are analogous to the local Neumann boundary conditions.

We analyze structural properties of the solution and derive suitable discretization techniques. In contrast to the local Cahn–Hilliard problem, which always leads to a diffuse interface, the proposed nonlocal model can lead to a strict separation into pure phases of the substance for nontrivial interactions. Concretely, we show that a sharp interface can already occur for certain critical (non-zero) value of the interface parameter. Here, the choice of the obstacle potential plays an important role in our analysis, since it guarantees the strict separation into pure phases. However, the corresponding additional inequality constraints are challenging for the numerical discretization. Mathematically, they lead to a coupled-system involving nonstandard parabolic variational inequalities. We employ implicit Euler time stepping scheme combined with a finite element discretization in space. The computation of the solution at each time instance can be restated as a constrained optimization problem, which we solve by using the primal-dual active set strategy.

Finally, we provide various one and two dimensional numerical experiments to verify our theoretical results and to conduct a comparative study of the nonlocal problem and its local limit, corresponding to a vanishing radius of nonlocal interactions.

This work is in collaborative work with Max Gunzburger (Florida State University, FL, USA).

nPINNs: nonlocal Physics-Informed Neural Networks

Marta D'Elia
Sandia National Laboratories, NM, USA
mdelia@sandia.gov

Abstract

Nonlocal models provide an improved predictive capability thanks to their ability to capture effects that classical partial differential equations fail to capture. Among these effects we have multiscale behavior (e.g. in fracture mechanics) and anomalous behavior such as super- and sub-diffusion. These models have become incredibly popular for a broad range of applications, including mechanics, subsurface flow, turbulence, plasma dynamics, heat conduction and image processing. However, their improved accuracy comes at a price of many modeling and numerical challenges.

In this work we focus on the estimation of model parameters, often unknown, or subject to noise. In particular, we address the problem of model identification in presence of sparse and possibly noisy measurements. Our approach to this inverse problem is based on the combination of **1.** Machine Learning and Physical Principles and **2.** a Unified Nonlocal Vector Calculus and Versatile Surrogates such as neural networks (NN). The outcome is a flexible tool that allows us to learn existing and new nonlocal operators.

We refer to our technique as nPINNs (nonlocal Physics-Informed Neural Networks); here, we model the nonlocal solution with a NN and we solve an optimization problem where we minimize the residual of the nonlocal equation and the misfit with measured data. The result of the optimization are the weights and biases of the NN and the set of unknown model parameters.

In this talk we briefly present the unified vector calculus, introduce nPINNs, describe its properties, and provide several numerical results that illustrate our findings.

This is joint work with George E. Karniadakis and Guofei Pang (Brown University) and Michael Parks (Sandia National Laboratories, NM).

Optimal parameter selection in nonlocal image denoising

Juan Carlos De los Reyes
MODEMAT, Escuela Politécnica Nacional, Quito, Ecuador,
juan.delosreyes@epn.edu.ec

Abstract

We propose a bilevel learning approach for the determination of optimal weights in nonlocal image denoising. We consider both spatial weights in front of the nonlocal regularizer, as well as weights within the kernel of the nonlocal operator. In both cases we investigate the differentiability of the solution operator in function spaces and derive a first order optimality system that characterizes local minima. For the numerical solution of the problems, we propose a second- order optimization algorithm in combination with a finite element discretization of the nonlocal denoising models.

This is joint work with Andrés R Miniguano Trujillo (Escuela Politécnica Nacional, Quito, Ecuador) and Marta D'Elia (Sandia National Laboratories, NM, USA).

Machine Learning of Space-Fractional Differential Equations

Mamikon Gulian
Sandia National Laboratories, NM, USA,
mgulian@sandia.gov

Abstract

Data-driven discovery of differential equations has recently been approached by embedding the discovery problem into a Gaussian Process regression of spatial data, treating unknown equation parameters as hyperparameters of a modified physics-informed Gaussian Process kernel. This kernel includes the parametrized differential operators applied to a prior covariance kernel. We extend this framework to linear space-fractional differential equations. Our methodology is compatible with a variety of fractional operators and stationary covariance kernels, including the Matern class. The fractional physics-informed GP kernel is given by d-dimensional Fourier integral formulas amenable to generalized Gauss-Laguerre quadrature.

The method allows for discovering fractional-order PDEs for systems characterized by heavy tails or anomalous diffusion, which are of increasing prevalence in physical and financial domains. A single fractional-order archetype allows for a derivative of arbitrary order to be learned, with the order itself being a parameter in the regression. Thus, the user is not required to assume a "dictionary" of derivatives of various orders, and directly controls the parsimony of the models being discovered. We illustrate on several examples, including fractional-order interpolation of advection-diffusion and modeling relative stock performance in the S&P 500 with alpha-stable motion via a fractional diffusion equation.

Joint work with Maziar Raissi (Nvidia), Paris Perdikaris (University of Pennsylvania), and George Karniadakis (Brown University).

Control and parameter identification for nonlocal models of diffusion and mechanics

Max Gunzburger
Florida State University, FL, USA
mgunzburger@fsu.edu

Abstract

Optimal control and parameter identification problems constrained by nonlocal steady diffusion equations that arise in several applications are studied. The control is the right-hand side forcing function, the parameter to be identified is a coefficient function, and the objective to be minimized is a standard matching functional. A calculus for nonlocal operators is used to demonstrate the existence and uniqueness of solutions of the problems and to derive optimality systems. We also demonstrate the convergence, as the extent of nonlocal interactions vanishes, to corresponding PDE problems. Error estimates for continuous and discontinuous finite element discretizations are derived. Numerical examples are provided that show that nonlocal models provide, compared to local PDE models, superior matching to target functions with a lower cost of control and also better estimates for non-smooth and discontinuous coefficients.

This joint work with M. D'Elia (Sandia National Laboratories, NM, USA).

Learning nonlocal regularization operators

Gernot Holler
University of Graz, Graz, Austria,
gernot.holler@uni-graz.at

Abstract

We aim at learning an operator from a class of nonlocal operators that is optimal for the regularization of an ill-posed inverse problem. The considered class of nonlocal operators is motivated by the use of fractional order Sobolev semi-norms as regularization operators. First fundamental results from the theory of regularization with local operators are extended to the nonlocal case. Then a framework based on a bilevel optimization strategy is developed which allows to choose nonlocal regularization operators from a given class which i) are optimal with respect to a suitable performance measure on a training set, and ii) enjoy particularly favorable properties. Finally, numerical experiments are presented.

The talk is based on joint work with Karl Kunisch, University of Graz, Austria.

Some inverse problems for subdiffusion equations

Barbara Kaltenbacher
Alpen-Adria-Universität Klagenfurt, Austria,
Barbara.Kaltenbacher@aau.at

Abstract

Reaction-diffusion equations are among the most common partial differential equation models. They arise as the combination of two physical processes: a driving force $f(u)$ that depends on the state variable u and a diffusive mechanism that spreads this effect over a spatial domain. Application areas include chemical processes, heat flow models and population dynamics. The direct or forward problem for such equations is now very well-developed and understood, especially when the diffusive mechanism is governed by Brownian motion resulting in an equation of parabolic type. Recently, various anomalous processes have been used to generalize the case of classical Brownian motion diffusion. Amongst the most popular is one that replaces the usual time derivative by a subdiffusion process based on a fractional derivative of order $\alpha \leq 1$. This leads to a PDE with a nonlocal in time differential operator, with several crucial implications for the related inverse problems of backwards diffusion or coefficient identification. In this talk, we will present some of these, along with numerical reconstruction methods based on fixed point and Newton type methods.

This is joint work with William Rundell (Texas A&M University, College Station, USA).

Unique determination of several coefficients in a fractional diffusion(-wave) equation by a single measurement

Yikan Liu
Hokkaido University, Hokkaido, Japan,
ykliu@ms.u-tokyo.ac.jp

Abstract

In this talk, we investigate some inverse problems on determining several coefficients simultaneously in a nonlocal diffusion process described by a time-fractional diffusion equation by a single measurement on the boundary. With a suitably chosen Dirichlet boundary condition, we prove the uniqueness for these coefficient inverse problems by employing Laplace transform. Further, we generalize some of the above results to the case of Riemannian manifolds.

This is a joint work with Kian Yavar (Aix-Marseille University), Zhiyuan Li (Shandong University of Technology) and Masahiro Yamamoto (The University of Tokyo).

Time Optimal Control of Linear Fractional Systems

Ivan Matychyn
University of Warmia and Mazury in Olsztyn, Poland,
matychyn@matman.uwm.edu.pl

Abstract

The presentation provides an overview of the recent results on control of linear fractional systems, i.e. systems described by linear fractional differential equations with both constant and variable coefficients. Fractional differential equations involving Riemann–Liouville as well as Caputo derivatives are under consideration.

The presented results are based on explicit, closed-form solutions of the linear fractional systems. Those solutions are expressed in terms of matrix Mittag-Leffler functions in case of constant coefficients and generalized Peano–Baker series for variable ones.

Due to importance of the matrix Mittag-Leffler function in the theory of linear fractional systems, the problem of its computation is discussed.

Sufficient and necessary conditions for controllability and observability are derived using fractional Gramian matrices.

Problem of time-optimal control of linear fractional systems is examined using technique of reachable sets and their support functions.

A method to construct a control function that transfers trajectory of the system to a strictly convex terminal set in the shortest time is elaborated. The proposed method uses technique of set-valued maps and represents a fractional version of Pontryagin's maximum principle.

Theoretical results are supported by examples, in which optimal control of "bang-bang" type is obtained.

Optimal design problems governed by the nonlocal p-Laplacian equation

Julio Muñoz
Universidad de Castilla-La Mancha, Toledo, Spain,
julio.munoz@uclm.es

Abstract

It is well-known that nonlocal integral models are suitable to approximate integral functionals or partial differential equations. In this talk, a nonlocal optimal design model is going to be considered as approximation of the corresponding classical or local optimal design problem. The new model is driven by the nonlocal p-Laplacian equation, the design is the diffusion coefficient and the cost functional belongs to a broad class of nonlocal functional integrals. The purpose is to prove existence of optimal design for the new model. This work is complemented by showing that the limit of the nonlocal p-Laplacian state equation converges towards the corresponding local problem. Also, as in the linear case, the G-convergence of the nonlocal optimal design problem toward the local version is studied. This task is successfully performed in two different cases: when the cost to minimize is the compliance functional, and when an additional nonlocal constraint on the design is assumed.

A nonlocal variational model related to the spatially variable fractional Laplacian

Carlos N. Rautenberg
George Mason University, VA, US,
crautenb@gmu.edu

Abstract

A variational model in weighted Sobolev spaces with non-standard weights is proposed together with applications to image processing. The associated weights are, in general, not of Muckenhoupt type and hence non-standard analysis tools are required. For special cases, the resulting variational problem is known to be equivalent to the fractional Poisson problem. The discretized problem is solved via a finite element scheme and for image denoising we propose an algorithm to identify the unknown weights. The approach is illustrated on several test problems and it yields better results when compared to the existing total variation techniques.

Sparse optimal control for fractional diffusion

Abner J. Salgado
Univeristy of Tennessee, TN, USA
asalgad1@utk.edu

Abstract

We consider an optimal control problem that entails the minimization of a nondifferentiable cost functional, fractional diffusion as state equation and constraints on the control variable. We provide existence, uniqueness and regularity results together with first-order optimality conditions. In order to propose a solution technique, we realize fractional diffusion as the Dirichlet-to-Neumann map for a nonuniformly elliptic operator and consider an equivalent optimal control problem with a nonuniformly elliptic equation as state equation. The rapid decay of the solution to this problem suggests a truncation that is suitable for numerical approximation. We propose a fully discrete scheme: piecewise constant functions for the control variable and first-degree tensor product finite elements for the state variable. We derive a priori error estimates for the control and state variables.

This is joint work with Enrique Otárola (UTFSM, Chile).

External optimal control of fractional parabolic PDEs

Deepanshu Verma
George Mason University, VA, USA,
dverma2@gmu.edu

Abstract

In this talk, we introduce a new notion of optimal control, or source identification in inverse, problems with fractional parabolic PDEs as constraints. This new notion allows a source/control placement outside the domain where the PDE is fulfilled. We tackle the Dirichlet, the Neumann and the Robin cases. The need for these novel optimal control concepts stems from the fact that the classical PDE models only allow placing the source/control either on the boundary or in the interior where the PDE is satisfied. However, the nonlocal behavior of the fractional operator now allows placing the control in the exterior. We introduce the notions of weak and very-weak solutions to the parabolic Dirichlet problem. We present an approach on how to approximate the parabolic Dirichlet solutions by the parabolic Robin solutions (with convergence rates). A complete analysis for the Dirichlet and Robin optimal control problems has been discussed. The numerical examples confirm our theoretical findings and further illustrate the potential benefits of nonlocal models over the local ones.

Shape optimization for identifying interfaces in nonlocal models

Christian Vollmann
Trier University, Trier, Germany,
vollmann@uni-trier.de

Abstract

Shape optimization methods have been proven useful for identifying interfaces in models governed by partial differential equations. For instance, shape calculus can be exploited for parameter identification in models, where the diffusivity is structured by piecewise constant patches.

On the other hand, nonlocal models, which are governed by integral operators instead of differential operators, have attracted increased attention in recent years. This is due to the large variety of applications including, e.g., peridynamics, image processing, nonlocal heat conduction or anomalous diffusion.

In this talk we bring together these two fields by considering a shape optimization problem which is constrained by a nonlocal convection-diffusion model. We discuss the constraint equation, derive a novel shape derivative of the associated nonlocal bilinear form and present numerical results of the implemented optimization algorithm.

This has been joint work with Prof. Dr. Volker Schulz (Trier University, Trier, Germany).

A variable-order fractional differential equation and its optimal control

Hong Wang
University of South Carolina, Columbia, SC, USA,
hwang@math.sc.edu

Abstract

Fractional differential equations were shown to provide competitive modeling capabilities of challenging phenomena such as anomalously diffusive transport. Moreover, laboratory experiments and field tests showed that the order of fractional differential equations may vary, e.g., as the structure of the media changes.

We report some preliminary results on the analysis and numerical approximations of variable-order fractional differential equations and their optimal control problems.

Error analysis of fully-discrete finite element approximations for stochastic time-fractional PDEs driven by space-time white noise

Jilu Wang
Beijing Computational Science Research Center, Beijing, China,
wangjilu03@gmail.com

Abstract

In this work, we consider the convergence rates of numerical methods for solving a stochastic time-fractional PDE in a convex polygon/polyhedron. For this model, both the time-fractional derivative and the stochastic process result in low regularity of the solution. Hence, the numerical approximation of such problems and the corresponding numerical analysis are very challenging. In our work, the stochastic time-fractional equation is discretized by a backward Euler convolution quadrature in time with piecewise continuous linear finite element method in space for which a sharp-order convergence is established in multidimensional spatial domains with nonsmooth initial data. Numerical results are presented to illustrate the theoretical analysis. Results on optimal control will also be presented.

A nonlocal feature-driven exemplar-based approach for image inpainting

Clayton Webster
Oak Ridge National Laboratory and The University of Tennessee, Knoxville,
webstercg@ornl.gov

Abstract

We will present a nonlocal variational image completion technique which admits simultaneous inpainting of multiple structures and textures in a unified framework. The recovery of geometric structures is achieved by using general convolution operators as a measure of behavior within an image. These are combined with a nonlocal exemplar-based approach to exploit the self- similarity of an image in the selected feature domains and to ensure the inpainting of textures. We also introduce an anisotropic patch distance metric to allow for better control of the feature selection within an image and present a nonlocal energy functional based on this metric. Finally, we derive an optimization algorithm for the proposed variational model and examine its validity experimentally with various test images.

Stability and uniqueness in inverse problems for viscoelasticity equations by Carleman estimates

Masahiro Yamamoto
The University of Tokyo, Tokyo, Japan
myama@ms.u-tokyo.ac.jp

Abstract

The subject is inverse problems of determining spatially varying factors of source terms and coefficients by a finite number of boundary measurement data. Our main result is the conditional stability for such inverse problems and the main tool is Carleman estimates.

We plan to discuss several model equations for the viscoelasticity and one model is the linear viscoelasticity:

$$\rho(x)\partial_t^2\mathbf{u}(x,t) - L_{\lambda,\mu}\mathbf{u}(x,t) + \int_0^t L_{\widetilde{\lambda},\widetilde{\mu}}\mathbf{u}(x,\eta)d\eta = \mathbf{F}(x,t) \quad \text{in } \Omega\times(-T,T), \qquad (*)$$

where $\mathbf{u}(x,t) = (u_1(x,t), u_2(x,t), u_3(x,t))^T$, ^{T} denotes the transpose of vectors, and $\lambda(x)$, $\mu(x)$, and $\widetilde{\lambda}(x,t,\eta)$, $\widetilde{\mu}(x,t,\eta)$, and for $(a,b) = (\lambda(x),\mu(x))$ and $(a,b) = (\widetilde{\lambda}(x,t,\eta), \widetilde{\mu}(x,t,\eta))$, we define the partial differential operator $L_{a,b}$ is defined by

$$L_{a,b}\mathbf{u}(x,t) = b\Delta\mathbf{u} + (a+b)\nabla\mathrm{div}\,\mathbf{u} + (\mathrm{div}\,\mathbf{u})\nabla a + (\nabla\mathbf{u} + (\nabla\mathbf{u})^T)\nabla b.$$

We use boundary data limited to some suitable sub-boundary and so we need Carleman estimate for the Lamé system (*) with nonlocal term for functions not having compact supports, which requests a lot of calculus and estimates. On the basis of such Carleman estimates, one can apply the methodology by Bukhgeim and Klibanov (1981) to prove the stability results.

This talk is based on joint works with Professor O.Y. Imanuvilov (Colorado State University), and Professors P. Loreti and D. Sforza (Sapienza University of Rome).

A probabilistic numerical scheme for nonlocal diffusion equations and its applications to training residual neural networks (ResNets)

Guannan Zhang
Oak Ridge National Laboratory, TN, USA
zhangg@ornl.gov

Abstract

We will present a new probabilistic numerical scheme for a class of semi-linear nonlocal diffusion equations with integral kernels in three-dimensional irregular domains with volume constraints. The nonlocal Fokker-Planck operator is firstly converted to its adjoint and then approximated by the mathematical expectation with respect to the associated the stochastic process. The volume constraints are handled by utilizing the first exit time of the underlying stochastic process. Error analysis will be provided to show first-order in temporal discretization and p-th order convergence in spatial discretization. In addition, we will show preliminary results on applying the developed scheme to training nonlocal ResNets with random dropouts by exploiting the connection between ResNets training and optimal control of nonlocal backward Kolmogorovs equations.

Pointwise-in-Time Error Estimates for an Optimal Control Problem with Subdiffusion Constraint

Zhi Zhou
The Hong Kong Polytechnic University, Hong Kong, China,
zhi.zhou@polyu.edu.hk

Abstract

In this talk, we will study numerical analysis for a distributed optimal control problem, with box constraint on the control, governed by a subdiffusion equation which involves a fractional derivative of order $\alpha \in (0,1)$ in time. The fully discrete scheme is obtained by applying the conforming linear Galerkin finite element method in space, L1 scheme/backward Euler convolution quadrature in time, and the control variable by a variational type discretization. With a space mesh size h and time stepsize τ, we establish the following order of convergence for the numerical solutions of the optimal control problem: $O(\tau^{\min(1/2+\alpha-\epsilon,1)} + h^2)$ in the discrete $L^2(0,T;L^2(\Omega))$ norm and $O(\tau^{\alpha-\epsilon} + \ell_h^2 h^2)$ in the discrete $L^\infty(0,T;L^2(\Omega))$ norm, with any small $\epsilon > 0$ and $\ell_h = \ln(2 + 1/h)$. The analysis relies essentially on the maximal L^p-regularity and its discrete analogue for the subdiffusion problem.