Meshless methods

Session at the *5th Dolomites Workshop on Constructive Approximation and Applications*

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List of contributions

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Greedy selection for learning by exponential splines

Rosanna Campagna
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Abstract: Smoothing splines are a state-of-the-art technique for learning data; indeed, recently splines have been investigated also as activation functions for deep neural networks. The main drawbacks of smoothing splines consist in possible overfitting and consequent boundary oscillations. We propose a strategy to better select the fitting data with the aim to combine complexity reduction and accuracy in capturing the data trend. Greedy methods [1], starting by a reduced data set, optimize the fitting points by an incremental selection based on the minimization either of the residual (f -greedy) or of an upper bound for the approximation error [2]. The former strategy depends on the functional values. Thus for the greedy selection, we present a theoretical upper bound designed for a class of exponential smoothing splines [3], depending only on the nodes. This grants an adaptive selection of the quasi-optimal nodes, providing an efficient fitting, particularly for data sets sampled at the same points.

This is a joint work with S. De Marchi, E. Perracchione, G. Santin.

References

[1] V. Temlyakov, Greedy approximation, Acta Numerica, 17 (2008), 235–409.

[2] R. Schaback, H. Wendland, Adaptive greedy techniques for approximate solution of large RBF systems, Numer. Algorithms 24 (2000), 239–254.

[3] R. Campagna, C. Conti, S. Cuomo, Smoothing exponential-polynomial splines for multiexponential decay data, Dolomites Research Notes on Approximation (2019), 12, 86–100.

Selection of sets of influence in meshless finite difference methods

Oleg Davydov
Universtity of Giessen

Abstract: I will present recent research on algorithms for stencil selection for RBF-FD and polynomial type meshless finite difference methods. The goal of these algorithms is to generate as small as possible stencils of desired accuracy, in order to maximize sparsity of the system matrix. The results are obtained in part jointly with Dang Thi Oanh, Ngo Manh Tuong, Mansour Safarpoor.

Kernel-based methods for reduced order modeling in environmental hydrodynamics

Sourav Dutta
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Abstract: Computational models are becoming increasingly important for achieving the U.S. Army Corps of Engineer's mission of delivering vital public and military engineering services. For instance, the depth-averaged 2D shallow water equations (SWE) are a well-studied hyperbolic or near-hyperbolic system of partial differential equations (PDEs) that has wide applications ranging from large-scale ocean modeling to granular flows, from river morphodynamics to dam break. However, fully-resolved numerical simulations of parameterized SWE can pose a significant computational challenge for multi-query, real-time and fast-replay applications. Reduced order modeling (ROM) encompasses a wide array of approaches that aim to drastically reduce computational burden versus reference, high-fidelity simulations. In particular, non-intrusive reduced order methods (NIROMs) that employ different regression-based approaches to design response functions for relevant system dynamics in the latent space, are gaining in popularity due to their high-fidelity-model agnostic nature and ease of deployment. In this work, we study the utility of several techniques that include classical kernel-based methods like radial basis function (RBF) interpolation, Bayesian non-parametric approaches like Gaussian process regression (GPR), and dynamic mode decomposition (DMD) to make a posteriori predictions for state evolution using a suitable latent space representation. These are compared to a modern deep learning-based algorithm called neural ordinary differential equations (NODE). RBF NIROMs [1] offer the promise of applicability to very high-dimensional parametric problems, the stochastic GPR model predictions are automatically endowed with an uncertainty estimate, and the DMD approach is extremely efficient in extracting latent coherent transient structures in the flow. The NODE framework leverages the connection between residual networks and ordinary differential equations to approximate the evolution of modal coefficients in the latent space [2]. We compare long-term predictive accuracy, efficiency, and computational stability properties using a variety of real-world examples characterized by estuarine flows, largescale geophysical flows, and riverine hydrodynamics that play crucial roles in navigability and flood risk assessment.

References

[1] Dutta, S., Farthing, M.W., Perracchione, E., Savant, G., and Putti, M. A greedy non-intrusive reduced order model for shallow water equations, arXiv:2002.11329, (2020).

[2] Dutta, S., Rivera-Casillas, P., and Farthing, M.W. Neural ordinary differential equations for data-drivenreduced order modeling of environmental hydrodynamics, Proceedings of the AAAI MLPS Spring Symposium, Stanford,CA, USA, (2021).

Kernel-based approximation for feedback control of dynamical systems

Bernard Haasdonk
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Abstract: Greedy kernel approximation schemes are efficient techniques for sparse function approximation and surrogate modelling. Here efficiency both refers to provable rapid error decay by convergence rates in terms of the expansion size, as well as computational efficiency reflected in the computation time being linear in the training set size. We show, how these techniques can be involved in feedback control of dynamical systems with and without state constraints.

This is a joint work with Tobias Ehring.

Machine learning and dynamical systems meet in Reproducing Kernel Hilbert Spaces

Boumediene Hamzi
Imperial College London

Abstract: Since its inception in the 19th century through the efforts of Poincaré and Lyapunov, the theory of dynamical systems addresses the qualitative behaviour of dynamical systems as understood from models. From this perspective, the modeling of dynamical processes in applications requires a detailed understanding of the processes to be analyzed. This deep understanding leads to a model, which is an approximation of the observed reality and is often expressed by a system of Ordinary/Partial, Underdetermined (Control), Deterministic/Stochastic differential or difference equations. While models are very precise for many processes, for some of the most challenging applications of dynamical systems (such as climate dynamics, brain dynamics, biological systems or the financial markets), the development of such models is notably difficult. On the other hand, the field of machine learning is concerned with algorithms designed to accomplish a certain task, whose performance improves with the input of more data. Applications for machine learning methods include computer vision, stock market analysis, speech recognition, recommender systems and sentiment analysis in social media. The machine learning approach is invaluable in settings where no explicit model is formulated, but measurement data is available. This is frequently the case in many systems of interest, and the development of data-driven technologies is becoming increasingly important in many applications. The intersection of the fields of dynamical systems and machine learning is largely unexplored and the objective of this talk is to show that working in reproducing kernel Hilbert spaces offers tools for a data-based theory of nonlinear dynamical systems. In this talk, we introduce a data-based approach to estimating key quantities which arise in the study of nonlinear autonomous, control and random dynamical systems. Our approach hinges on the observation that much of the existing linear theory may be readily extended to nonlinear systems - with a reasonable expectation of success- once the nonlinear system has been mapped into a high or infinite dimensional Reproducing Kernel Hilbert Space. In particular, we develop computable, non-parametric estimators approximating controllability and observability energies for nonlinear systems. We apply this approach to the problem of model reduction of nonlinear control systems. It is also shown that the controllability energy estimator provides a key means for approximating the invariant measure of an ergodic, stochastically forced nonlinear system. We also show how kernel methods can be used to detect critical transitions for some multi scale dynamical systems. We also use the method of kernel flows to predict some chaotic dynamical systems. Finally, we show how kernel methods can be used to approximate center manifolds, propose a data-based version of the centre manifold theorem and construct Lyapunov functions for nonlinear ODEs. This is joint work with Jake Bouvrie (MIT, USA), Peter Giesl (University of Sussex, UK), Christian Kuehn (TUM, Munich/Germany), Romit Malik (ANNL), Sameh Mohamed (SUTD, Singapore), Houman Owhadi (Caltech), Martin Rasmussen (Imperial College London), Kevin Webster (Imperial College London), Bernard Hasasdonk, Dominik Wittwar (University of Stuttgart), and Gabriele Santin (Bruno Kessler Foundation).

Strict positive definiteness of non-radial kernels on two-point compact homogeneous spaces

Janin Jaeger
University of Giessen

Abstract: Isotropic positive definite functions are used in approximation theory and are for example applied in geostatistics and physiology. They are also of importance in statistics where they occur as correlation functions of homogeneous random fields for example on spheres. We study a class of function applicable for interpolation of arbitrary scattered data on $\mathbb{M}^d$, where $\mathbb{M}^d$ is a d-dimensional two-point compact homogenouse space, by linear combinations of a kernel

$$K : \mathbb{M}^d \times \mathbb{M}^d \to \mathbb{C}$$

evaluated at the interpolation points in the second argument. The isotropic kernels are a special case of this approach and where studied and characterised in recent years, [2]. We study kernels with more general form, for example convolutional kernels, or axially symmetric kernels in special cases.

A class of kernels for which the resulting interpolation problem is uniquely solvable for any distinct point set $\Xi \subset \mathbb{M}^d$ are strictly positive definite kernels. We use the series expansion of the kernel in eigenfunctions of the Laplace-Beltrami Operator on $\mathbb{M}^d$ to derive some necessary and some sufficient conditions for strict positive definiteness.

In the case of the sphere the results extend a necessary and sufficient characterisation of strict positive definite isotropic basis functions on $(d-1)$-dimensional spheres by Chen et al. proven in [1] to a non-radial kernel class.

References

[1] Chen, D. and Menegatto, V. A. and Sun, X.: A necessary and sufficient condition for strictly positive definite functions on spheres, Proceedings of the American Mathematical Society, 131, 2733-2740, 2003.

[2] Barbosa, V. V. and Menegatto, V. A., Strict positive definite kernels on two-point compact homogeneous space, Mathematical Inequalities and Applications, 19, 743–756, 2016.

Estimation of the kernel scaling parameter

Toni Karvonen
The Alan Turing Institute

Abstract: In Gaussian process (GP) interpolation the power function from kernel-based approximation is interpreted as a conditional standard deviation and used as a statistical measure of interpolation uncertainty. However, as the power function does not depend on data no information about the data-generating function is encoded in these uncertainty estimates. The simplest approach to remedy this problem is to introduce a scaling parameter for the positive-definite covariance kernel of the GP prior and fit this parameter using some data-dependent method. In this talk we discuss connections of the maximum likelihood estimate (MLE) and a certain cross-validated estimate of the kernel scaling parameter to quantities from kernel-based approximation. We also review some bounds on these parameter estimates and their implications on reliability of GP interpolation. Of particular interest to us is the MLE and its rate of decay which is seemingly too fast by a square-root rate for functions in the reproducing kernel Hilbert space of the covariance kernel.

Kernel-based particle methods for the Vlasov–Poisson equation

Matthias Kirchhart
RWTH Aachen

Abstract: Particle methods have a long history in the numerical simulation of plasmas. Particle-in-Cell (PIC) methods are still widely considered state of the art and in common use. These methods interpret particles as quadrature rules and only yield fairly noisy results. In this work we show that drastic improvements can be achieved by using kernel based interpolation instead.

This is a joint work with Paul Wilhelm.

Solving PDEs in thin structures extracted from noisy point clouds using RBF-PUM

Elisabeth Larsson
University of Uppsala

Abstract: Manual segmentation of a medical image results in a noisy point cloud. We construct an infinitely smooth geometry based on such point clouds using a radial basis function partition of unity method (RBF-PUM). We especially focus on thin structures such as the diaphragm, which is the main muscle in the respiratory function. We also show that we can use this representation to solve a PDE in the reconstructed geometry. We present results for real patient data and consider both the quality of the reconstruction and the performance of the PDE solver. This work is part of a larger effort to numerically simulate the respiratory system..

Interpolation with variably scaled kernels

Leevan Ling
Hong Kong Baptist University

Abstract: "Within kernel–based interpolation and its many applications, it is a well–documented but unsolved problem to handle the scaling or the shape parameter" by R. Schaback, et. al. [IMA Numer. Anal. 35 (1): 199-219, 2015]. In this talk, we numerically demonstrate some potential benefits from leaving the optimal constant shape behind and, instead, working with non-constant (i.e., variable and random) shape parameters. Theoretically, we show that, subject to some restrictions on the data under analysis, Gaussian asymmetric interpolation matrix is almost surely invertible even when using non-constant shape parameters.

A multivariate rational interpolation with conditionally positive definite kernels

Davoud Mirzaei
University of Isfahan

Abstract: Rational approximations are known to be much more efficient than standard (linear) ones for functions with poles or other singularities on or near the domain of approximation, or on unbounded domains. Univariate polynomial rational approximations have a long history, but some new robust algorithms are recently being developed. However, not much research has been devoted to multivariate rational approximations. In recent decades, the radial basis function (RBF) approximation/interpolation has provided an outstanding tool for scattered data approximation on multidimensional cases. It is natural to ask for a multivariate rational RBF approximation for functions with steep gradients and/or singularities. Poles and singularities may be well captured if polynomial terms are appended to RBF expansions in numerator and denominator. Thus, conditionally positive definite kernels with respect to polynomial spaces, such as polyharmonic splines, should play an important role to enrich the available rational RBF approximations. However, the recent rational RBF method [1, 2] has some limitations in using conditionally positive definite kernels. In this talk, a reformulation of the method is given that avoids those limitations and allows to implement the rational polyharmonic-based algorithm on a scaled data to prevent the instability of the involved RBF systems. Sufficient number of numerical examples in one, two and three dimensions are given to show the efficiency and the accuracy of the method.

This is a joint work with Elham Farazandeh.

References

[1] S. De Marchi, A. Mart inez, and E. Perracchione. Fast and stable rational RBF-based partition of unity interpolation. Journal of Computational and Applied Mathematics, 349:331–343, 2019.

[2] S. Jakobsson, B. Andersson, and F. Edelvik. Rational radial basis function interpolation with applications to antenna design. Applied Numerical Mathematics, 233:889–904, 2009.

Feature augmentation in high energy solar imaging

Michele Piana
University of Genova

Abstract: Modern high energy solar imaging provides experimental observations that correspond to sparse samples of the fourier transform of the incoming photon flux. this talk illustrates how feature augmentation can be exploited to realize an interpolation/extrapolation approach to image reconstruction for this kind of imaging modalities. examples involving both synthetic data and real measurements will be discussed.

Kernel methods for parametric equations

Christian Rieger
Unviersity of Marburg

Abstract: Parametric equations give rise to a variey of coupled approximation problems.

Kernel methods have been proven useful in many of those problems.

Especially the coupling of different approximation processes makes kernel methods an interesting choice.

We will present recent progress on those approximation problems and discuss also future challenges.

A high-order meshless semi-Lagrangian method for PDEs on surfaces

Varun Shankar
University of Utah

Abstract: We present a high-order meshless method based on radial basis function finite differences (RBF-FD) for the solution of partial differential equations on surfaces. Our method consists of recently-developed Tangent Plane RBF-FD method for approximating spatial operators, and a meshless semi-Lagrangian method for approximating advection terms. Our results show that the resulting method is high-order accurate, efficient, and easily parallelizable. We also present applications of our method to PDEs arising from physiology.

HJB-RBF based approach for the control of PDEs

Hugo Souza Oliveira
PUC-Rio

Abstract: Semi-Lagranian schemes for discretization of the dynamic programming principle are based on a time discretization projected on a state-space grid. The use of a structured grid makes this approach not feasible for high-dimensional problems due to the curse of dimensionality. Here, we present a new approach for infinite horizon optimal control problems where the value function is computed using Radial Basis Functions (RBF) and Shepard's moving least squares approximation method on scattered grids. We propose a new method to generate a scattered mesh driven by the dynamics and the selection of the shape parameter in the RBF using an optimization routine. Numerical tests for high dimensional problems will show the effectiveness of the proposed method. Joint work with A. Alla (PUC-Rio, Brazil) and G. Santin (FBK, Italy).

Registration-based model reduction of parameterized advection-dominated PDEs

Tommaso Taddei
Inria Bordeaux

Abstract: We propose a model reduction procedure for rapid and reliable solution of parameterized advection-dominated problems. Accurate approximation of travelling parameter-dependent waves is extremely challenging for traditional model reduction approaches based on linear approximation spaces: to address this issue, we propose an adaptive registration-based data compression procedure to align local features in a fixed reference domain, to ultimately improve the linear compressibility of the solution manifold. We further develop an hyper-reduced projection-based (Petrov-Galerkin) framework for the computation of the mapped solution. Numerical results for the Euler equations and for the shallow water equations show the potential of the method.

Work in collaboration with Dr.Lei Zhang (Inria Bordeaux).

An oversampled RBF-FD method for elliptic and hyperbolic PDEs

Igor Tominec
Uppsala University

Abstract: In the last two decades, the radial basis function generated finite difference (RBF-FD) methods have been playing an important role in the meshfree approximation to solutions of PDEs. So far, the RBF-FD discretizations were mostly used in the collocation sense, where the underlying matrices have a square shape. Recently, we introduced an approach to use the RBF-FD method in an oversampled context, where the rectangular matrices play a central role in the resulting numerical scheme.
Benefits include improved stability properties, especially for stationary PDEs with derivative boundary conditions, an ability to decouple the PDE geometry and the stencil-based interpolation problems (unfitted approach), and an access to a theoretical framework for studying stability properties of the RBF-FD operators and convergence under node refinement. In this talk we are going to focus on an oversampled RBF-FD discretization of (non)linear time-dependent transport equations, and provide our recent findings on stability properties and their practical implications for convergence of error under node refinement.

Spectral properties of kernel matrices in the flat limit

Konstantin Usevich
CNRS and University of Lorraine

Abstract: Kernel matrices are of central importance to many applied fields. In this manuscript, we focus on spectral properties of kernel matrices in the so-called ”flat limit”, which occurs when points are close together relative to the scale of the kernel. We establish asymptotic expressions for the determinants of the kernel matrices, which we then leverage to obtain asymptotic expressions for the main terms of the eigenvalues. A separate analysis yields expressions for limiting eigenvectors, which are strongly tied to discrete orthogonal polynomials. Both smooth and finitely smooth kernels are covered, with stronger results available in the univariate case. If time permits, I will discuss some implications for Gaussian process regression.

Joint work with Simon Barthelm’e (`https://arxiv.org/abs/1910.14067`).

Analysis of target data dependent greedy kernel algorithms: Convergence rates for f-, $f \cdot P$- and f/P-greedy

Tizian Wenzel
University of Stuttgart

Abstract: Data-dependent greedy algorithms in kernel spaces are known to provide fast converging interpolants, while being extremely easy to implement and efficient to run. Despite this experimental evidence, no detailed theory has yet been presented.

In this work we fill this gap by first defining a new scale of greedy algorithms for interpolation that comprises all the existing ones in a unique analysis, where the degree of dependency of the selection criterion on the functional data is measured by a real parameter. We then prove new convergence rates where this degree is taken into account and we show that, possibly up to a logarithmic factor, data dependent selection strategies provide faster convergence.

In particular, for the first time we obtain convergence rates for adaptive interpolation that are faster than the ones given by uniform points, without the need of any special assumption on the target function. The rates are confirmed by a number of examples.

This is a joint work with Gabriele Santin and Bernard Haasdonk.

Implicit surface reconstruction with a curl-free Radial Basis Function Partition of Unity Method

Grady Wright
Boise State University

Abstract: Surface reconstruction from a set of scattered points, or a point cloud, has many applications ranging from computer graphics to remote sensing. We present a new method for this task that produces an implicit surface (zero-level set) approximation for an oriented point cloud using only information about (approximate) normals to the surface. The technique exploits the fundamental result from vector calculus that the normals to an implicit surface are curl-free. By using a curl-free radial basis function (RBF) interpolation of the normals, we can extract a potential for the vector field whose zero-level surface approximates the point cloud. We use curl-free RBFs based on polyharmonic splines for this task, since they are free of any shape or support parameters. Furthermore, to make this technique efficient and able to better represent local sharp features, we combine it with a partition of unity (PU) method. The result is the curl-free partition of unity (CFPU) method. We will discuss how CFPU can be adapted to enforce exact interpolation of a point cloud and can be regularized to handle noise in both the normal vectors and the point positions. Numerical results will be presented that demonstrate how the method converges for a known surface as the sampling density increases, how regularization handles noisy data, and how the method performs on various problems found in the literature.