Don't stray from the (shortest) path and be home before the cut point: On the injectivity radius on the Grassmann and the Stiefel manifold.

Ralf Zimmermann *University of Southern Denmark, Odense*
This is joint work with Jakob Stoye from TU Braunschweig.

The injectivity radius of a manifold is an important quantity, both from a theoretical point of view and in terms of numerical applications. It is the largest possible radius within which all geodesics are unique and length-minimizing. In consequence, it is the largest possible radius within which calculations in Riemannian normal coordinates are well-defined. In loose words, as long as you stay within the injectivity radius when travelling along a geodesic, you are guaranteed not to travel unnecessary distances. The injectivity radius acts as a computational barrier, e.g., in Riemannian interpolation algorithms, and in determining Riemannian centers of mass.

For general manifolds, it is very difficult to explicitly compute the injectivity radius. However, for a few special examples, such as the n-sphere or the Grassmann manifold of p-dimensional subspaces, the explicit number is known.

Recently, new insights have been gained that provide detailed information about the injectivity radius on the compact Stiefel manifold of orthogonal p-frames in $\mathbf{R}^n$ under a one-parameter family of Riemannian metrics [1], and specifically under the canonical metric [2]. In [4], the injectivity radius under the Euclidean metric is proven to be π.

In this talk, we review the concept of the injectivity radius, the known results on the Stiefel and Grassmann manifold and how they are connected to the sectional curvature [3] and the cut points of the manifold. We also look at the injectivity radius in applications.

References

[1] P. A. Absil and S. Mataigne. The ultimate upper bound on the injectivity radius of the Stiefel manifold. arXiv:2403.02079, 2024.

[2] J. Stoye and R. Zimmermann. On the injectivity radius of the Stiefel manifold: Numerical investigations and an explicit construction of a cut point at short distance. arXiv:2403.03782, 2024.

[3] R. Zimmermann and J. Stoye. High curvature means low rank: On the sectional curvature of Grassmann and Stiefel manifolds and the underlying matrix trace inequalities. arXiv:2403.01879, 2024

[4] R. Zimmermann and J. Stoye. The injectivity radius of the compact Stiefel manifold under the Euclidean metric. arXiv:2405.02268, 2024

The Riemannian Difference of Convex Algorithm in Manopt.jl
Ronny Bergmann (Norwegian University of Science and Technoloy)

In many applications nonlinear data is measured, for example when considering
unit vectors, rotations, or (bases of) subspaces of a vector space.
Modelling this on a Riemannian manifold allows to both reduce the dimension
of the data stored as well as focusing on geometric properties of the measurement
space compared to constraining a total space the data is represented in.
In optimisation this yields unconstrained optimization algorithms, where we have to take
the geometry of the optimization domain into consideration.

In this talk we consider the task of minimizing the difference of two convex functions
defined on a manifold and present the Difference of Convex Algorithm.
To make algorithms in general more accessible, we then present the two Julia packages
Manifolds.jl and Manopt.jl, that allow to define and use Riemannian manifolds and
optimization algorithms employing numerical differential geometry, respectively.

Optimized effective potentials from convex optimization

Markus Penz (Oslo Metropolitan University)

The optimized-effective-potential method aims at finding a *local* potential with a corresponding non-interacting solution that minimizes the energy functional of a more involved, orbital-dependent model (like exact exchange). Yet, finding a solution is intimately tied to the problematic differentiability of the functional. By relaxing the connection between the local potential and the trial solution, a joint minimization principle is found that leads to a self-consistent procedure.

An introduction to Riemannian optimization
Estelle Massart (UCLouvain)

Riemannian optimization led to major breakthroughs in various problems including matrix/tensor factorization and completion, or optimal rotation computation. This talk will provide an overview of recent applications of Riemannian geometry and will introduce the key geometric notions and fundamental results on which this theory relies.

Riemannian optimization methods for Kohn-Sham-type energy minimization problems
Tatjana Stykel (Universität Augsburg)

In this talk, we address the numerical solution of Kohn-Sham-type energy minimization problems arising in computational physics and quantum chemistry. To this end, we propose a general framework for solving minimization problems on the infinite-dimensional Stiefel manifold and develop the Riemannian gradient descent, Riemannian conjugate gradient and Riemannian Newton methods relying on different metrics. Exploiting the first-order and second-order information of the energy functional for the construction of appropriate metrics makes it possible to incorporate the preconditioning into Riemannian optimization which substantially accelerates the convergence of the optimization schemes. The non-monotone line search and the inexact evaluation of the Riemannian gradients and Hessians further reduce the computational cost and improve the overall efficiency. Numerical experiments demonstrate the strengths of the proposed methods and their competitiveness with other well-established schemes. (Joint work with R. Altmann, D. Peterseim and J. Püschel)

Algorithms for dynamical low-rank approximation
Bart Vandereycken (University of Geneva)

Abstract: The dynamical low-rank approximation (DLRA) or the time-dependent variational principle (TDVP) allows to directly approximate large matrix and tensor differential equations by low-rank matrices and tensors, like matrix product states (MPS). A popular algorithm that implements this idea is the projector-splitting integrator of Lubich and Oseledets. This algorithm can be extended to MPS and enjoys many good properties when applied to problems in quantum chemistry. In this talk, I will discuss recent developments of other methods for the integration of DLRA problems that include parallelism, rank adaptivity, and stiff equations occuring from discretized PDEs.

A new numerical method provides upper and lower bounds on arbitrary ground-state observables for many-body quantum systems.

Marc-Olivier Renou (INRIA Saclay)

The interplay of particle interactions and quantum fluctuations can stabilize intriguing phases of matter, and the resulting quantum entanglement sometimes represents a resource for quantum computations. Yet, it is one of the most difficult problems for numerical methods, as the system's phase space grows exponentially with the number of particles. In this work, we introduce a numerical scheme to derive upper and lower bounds on arbitrary ground-state observables for many-body quantum systems. This scheme can be systematically refined to converge to the exact ground-state value.

We illustrate the potential of our numerical method in paradigmatic spin models in one and two dimensions. But the construction is much more general and can be applied to systems of both distinguishable and indistinguishable particles as well as arbitrary lattice geometries. The symmetries and sparsity of the studied model can be used to significantly improve the scalability of the computation.

In future work, our approach could be used to certify the output of quantum simulators, as well as to study phases of matter and phase transitions in complex quantum systems.

On the Well-Posedness of the Discrete Single-Reference Coupled Cluster Equations

M. Hassan

Institute of Mathematics, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland.

Coupled cluster methods are widely regarded as among the most effective algorithms for high precision resolution of the ground state energy of the electronic Schrödinger equation in the dynamical correlation regime. In this talk, I will discuss the well-posedness of certain classes of *discrete* coupled cluster equations. The approach I describe is based on establishing a discrete inf-sup condition on the coupled cluster Fréchet derivative, which presents a challenge due to the non-symmetric nature of the underyling linear operator, and the fact that the Laplace operator has an essential spectrum on the unbounded domain $\mathbb{R}^n$. The main novelty of our approach is that it requires *weaker* smallness assumptions on the sought-after cluster amplitudes $\mathbf{t}^*$ than the state-of-the-art local monotonicity approach.

This is joint-work with Yvon Maday and Yipeng Wang (Laboratoire Jacques-Louis Lions, Paris).

Algebraic varieties arising from quantum chemistry

Svala Sverrisdóttir, University of California, Berkeley

Abstract

We discuss the algebra and combinatorics behind coupled cluster (CC) theory of quantum many-body systems. The high-dimensional eigenvalue problems that encode the electronic Schroedinger equation are approximated by polynomial systems at various levels of truncation. The exponential parametrization of the eigenstates gives rise to truncation varieties. These generalize Grassmannians in their Pluecker embedding. We offer a detailed study of truncation varieties and their CC degrees, a complexity measure for solving the CC equations. We also discuss the solutions of the CC equations. This is joint work with Fabian Faulstich and Bernd Sturmfels.

Coupled Cluster Degree of the Grassmannian
Viktoriia Borovik (Osnabrück University)

We determine the number of complex solutions to a nonlinear eigenvalue problem on the Grassmannian in its Plücker embedding. This is motivated by quantum chemistry, where it represents the truncation to single electrons in coupled cluster theory. In the case of the Grassmannian of lines, we obtain an explicit formula for the number of complex solutions, which involves Catalan numbers and is the volume of the Cayley sum of the Gelfand-Cetlin polytope with simplex. This rests on the geometry of the graph of a birational parametrization of the Grassmannian.

Block-Sparse Matrix Product States and Eigenvalue Solvers
(Markus Bachmayr, RWTH Aachen)

Abstract: Constraining the particle number (or other quantum numbers) in matrix product states leads to a block-sparsity pattern in tensor components. This is exploited in many tensor network codes, in particular in DMRG algorithms. In this talk, we look at such block-sparsity properties from a more general point of view, with potential applications in other contexts. We then consider the interaction of the block structure with matrix product operator representations of Hamiltonians in quantum chemistry. We obtain explicit representations of such Hamiltonians operating directly on the block structures, with improved rank bounds under sparsity assumptions on the Hamiltonian coefficients. Finally, we discuss low-rank eigensolvers with convergence guarantees and quasi-optimal rank bounds in the context of such block-sparse representations.
Based on joint works with Michael Götte, Sebastian Krämer and Max Pfeffer.

DMRG, new post-DMRG-methods, and chemical accuracy
Gero Friesecke (Technical University of Munich)

Achieving ``chemical accuracy'', 1 kcal/mole, which allows to reliably extract chemical behavior, is a longstanding dream of electronic structure simulations. Even the best methods such as coupled cluster or DMRG do not directly achieve this for molecules with a dozen electrons unless refined further (or unless already requiring supercomputing resources for tiny systems in a manner which lacks scalability to larger systems). A recent refinement of DMRG is the restricted active space density matrix renormalization group (DMRG-RAS) method. While a significant improvement of DMRG with similar computational cost, it is still a little bit short of chemical accuracy.

In [1] we introduced a further refinement, DMRG-RAS-X, where X stands for extrapolation. This method is based on the theoretical derivation and numerical validation of a remarkably accurate power law scaling of the errors of DMRG-RAS with the size of the underlying orbital spaces. The new method, DMRG-RAS-X, is found to reach chemical accuracy for strongly correlated systems such as the Chromium dimer, dicarbon up to a large cc-pVQZ basis, and even a large chemical complex like the FeMoco. The method is free of empirical parameters, performed robustly and reliably in all examples we tested, and has the potential to become a vital alternative method for electronic structure calculations in quantum chemistry, and more generally for the computation of strong correlations in nuclear and condensed matter
physics.

[1] G.F., Gergely Barcza and Ors Legeza, J Chem Theory Comput. 20(1):87-102, 2024

Geometric Perspectives on Bandstructures for Optimization in Topological Quantum Chemistry

Elena Derunova (IFW Dresden)

In this talk, we introduce recent development in topological quantum chemistry, unveiling also a geometric perspective on bandstructures, treating them as manifolds. This viewpoint enables us to utilize a quasi-continuous approximation of the eigenstates, parameterized by crystal momentum, resulting in a reduction of the necessary k-mesh density for accurately describing electronic properties. However, this continuity, and thus based on it methods to implement electronic correlation, fails for symmetry-generated degenerate points with the corresponding inter-band coherence, a key aspect of topological quantum chemistry. We hypothesize that the degeneracy of eigenstates and inter-band exchange arises as a consequence of the geometry of the bandstructure manifold and thus can be still treated in the quasi-continuous manner. We illustrate this approach through the prediction of anomalous Hall effects, which purely from ab initio calculations on a very coarse k-mesh. Through these discussions, we aim to showcase the potential of geometric insights in development of bandstructure optimization techniques and advancing our understanding of topological phenomena in quantum chemistry.

Reliable and efficient methods for computing DFT properties and derivatives
Michael Herbst (EPFL)

Density-functional theory (DFT) is one of the most widely employed methods in quantum chemistry and solid-state physics to model the electronic structure. For the particular
case of density functional theory on periodic systems, discretised using plane-wave basis sets,
I will present an overview of our recently proposed methods to efficiently and reliably compute the DFT response properties. I will further discuss our algorithmic differentiation framework to compute DFT derivatives, which in particular enables the computation of arbitrary derivatives of DFT ground state quantities versus input parameters. This covers for example derivatives, which are relevant for inverse materials design, i.e. the systematic discovery of novel materials by optimizing structural or design parameters in a way the materials exhibit desired properties.

Multi-center decomposition of molecular densities: the LISA-method
Benjamin Stamm (University of Stuttgart)

Within the framework of Iterative Stockholder Atom (ISA) methods we propose a new scheme, named LISA (for linear approximation of ISA), for the decomposition of an electronic density into atomic contributions which can be seen as a post-treatment of an electronic structure calculation. These atomic charge distributions, also called atoms in molecules (AIM), can be used to compute partial charges or atomic polarizabilities in force-field development.
We present the LISA method and its mathematical properties, and present several numererical strategies to solve the LISA optimization problems that range from (possibly accelerated) fix-point methods to (quasi-) Newton-methods. We illustrate the performance of the different solvers on a test of molecules.

Proximal mapping in DFT

A. Laestadius,[*] M. Penz, M. Herbst, M.A. Csirik, E.I. Tellgren,

*Department of Computer Science, Oslo Metropolitan University

and

Hylleraas Centre, Department of Chemistry, University of Oslo

In this talk, we examine the use of the proximal mapping in density-functional theory (DFT). The proximal point is the minimizer of the infimal convolution in the Moreau-Yosida envelope. In the DFT context, we apply the Moreau-Yosida transformation to a chosen density functional, and the proximal point is then referred to as a proximal density. We will particularly explore proximal densities in relation to the Kohn-Sham approach of DFT. In this setting, proximal densities can be used to determine effective potentials for non-interacting electron systems that reproduce ground-state densities for physical systems.