M.Sc. in Mathematical Modelling and Scientific Computing
Dissertation Projects

February 2023

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1 Industrial Projects

Descriptions of industrial projects have been omitted from the web version of the projects booklet. Please contact Kathryn Gillow, gillowk@maths.ox.ac.uk, if you believe you should have access to these.

2 Numerical Analysis Projects

2.1 General kernel spectral methods for equilibrium measures

Supervisors: Dr Timon Gutleb and Prof. José Carrillo
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Background and problem statement

Attractive-repulsive equilibrium measure problems appear in the modeling of the continuous limit of pair-interacting particle systems, e.g. models of animal swarms or classical physical particulates [1, 3]. From a computing point of view they are a combination of integral equation and minimization problem – the aim is to find a density $u(x)$ for a given kernel K such that the following energy E is minimized:

$$\int_{\mathrm{supp}(u)} K(|x-y|)u(y)\mathrm{d}y = E. \tag{1}$$

Power law equilibrium measures feature $K(|x-y|) = \frac{|x-y|^\alpha}{\alpha} - \frac{|x-y|^\beta}{\beta}$. In [4, 5] it was derived that the power law integral on the d-dimensional unit ball B_1 of a certain family of weighted Jacobi polynomials can be evaluated explicitly as:

$$\int_{B_1} |x-y|^\beta (1-|y|^2)^{m-\frac{\alpha+d}{2}} P_n^{(m-\frac{\alpha+d}{2},\frac{d-2}{2})}(2|y|^2-1)\mathrm{d}y = C^{\alpha,\beta}_{d,m,n} {}_2F_1\left(\begin{matrix} n-\frac{\beta}{2}, & -m-n+\frac{\alpha-\beta}{2} \\ & \frac{d}{2} \end{matrix}; |x|^2\right),$$

with available explicit forms for $C^{\alpha,\beta}_{d,m,n}$. Since these weighted Jacobi polynomials form a basis on the d-dimensional unit ball, we can use this result in a spectral method where the solution of the equilibrium measure problem in (1) is given in terms of its coefficients in this basis. Solving the problem is then as simple as using backslash along with a simple optimization routine (e.g. Newton's method).

Methods for the project

More general kernels, e.g. ℓ-Morse potentials $K(|x-y|) = C_1 e^{-\frac{|x-y|}{\ell_1}} u(y) - C_2 e^{-\frac{|x-y|}{\ell_2}}$, come up in various applications [2]. Instead of attempting to re-derive explicit results for a given kernel, one can alternatively try to use kernel expansions to derive a generic approach. Note for this purpose that the weighted basis used above satisfies:

$$P_n^{(a,b)}\left(2|x|^2-1\right) = \sum_{m=0}^{n} (-1)^{n+m} \tfrac{(n+a+b+1)_m (b+m+1)_{n-m}}{m!\,(n-m)!} |x|^{2m}.$$

Expanding a general kernel K in this basis thus leads to a series of power law terms which may be truncated at sufficient precision.

Project goals

The project would leverage kernel expansions to construct a general equilibrium measure method on the unit interval $[-1, 1]$. The d-dimensional unit ball generalization is then expected to be straightforward and can be considered as a stretch goal. Comparisons should be made with the corresponding attractive-repulsive finite particle swarm problems.

References

[1] J. A. Carrillo, M. Fornasier, G. Toscani, and F. Vecil. Particle, Kinetic, and Hydrodynamic Models of Swarming. In *Modeling and Simulation in Sci., Eng. and Tech.*, Birkhauser, Boston, 297–336, 2010.

[2] J. A. Carrillo, Y. Huang, and S. Martin. Explicit flock solutions for Quasi-Morse potentials. *European Journal of Applied Mathematics*, 25:553–578, 2014.

[3] J. A. Carrillo, A. Klar, S. Martin, and S. Tiwari. Self-propelled interacting particle systems with roosting force. *Math. Mod. Meth. Appl. Sci*, 20:1533–1552, 2010.

[4] T. S. Gutleb, J. A. Carrillo, and S. Olver. Computing equilibrium measures with power law kernels. *Mathematics of Computation*, 91(337):2247–2281, 2022.

[5] T. S. Gutleb, J. A. Carrillo, and S. Olver. Computation of power law equilibrium measures on balls of arbitrary dimension. *Constructive Approximation*: 1–46, 2022.

2.2 Modern randomised methods for optimisation and numerical linear algebra with application to weather forecasting

Supervisors: Prof. Coralia Cartis and Dr Jemima Tabeart
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Data assimilation (DA) techniques allows users to combine information from a numerical model with measurements of a physical system. Such methods are important in order to initialise weather forecasts by updating prior predictions with new observations of the atmosphere and ocean. Variational approaches, which are commonly used at many meteorological centres, are mathematically equivalent to solving a non-linear least squares optimisation problem. The dominant cost in atmospheric DA is the evaluation of the penalty function and its gradient. Due to the size of the problem (state vector having order 109 elements and assimilating order 107 observations) this is typically done in a massively parallel computing context via a series of inner (linear) and outer (non-linear) loops.

In this project the student will consider the application of modern randomised methods for optimisation and numerical linear algebra to the variational DA problem. Two possible directions are being considered depending on student interest.

The first direction focuses on applying randomised subspace iterative methods to the outer loop. In these approaches standard non-linear solvers, such as Gauss-Newton, which require full gradient information will be replaced by randomised algorithms that compute gradient information only for a random subselection of state variables. The student will:

- implement randomised optimisation algorithms, following the approach of [1], within an existing data assimilation testbed (written in Matlab).
- compare computational performance of the randomised approaches against standard optimisation algorithms.

The second direction considers the use of randomised numerical linear algebra techniques within the inner loop, where a linear system is solved using iterative methods such as conjugate gradient. Recent work has considered the use of randomised eigenvalue decomposition methods to develop preconditioners for the inner loop of the DA problem [2]. Depending on the interest of the student there are a number of avenues for this part of the project:

- Application of alternative approaches from the randomised numerical linear algebra literature to the inner DA problem (e.g. sketching techniques).
- Exploitation of the inherent structure within the linear system of interest within existing randomised NLA approaches for DA.

No special prerequisites are required. B6.2 Optimisation for data science would be useful, but is not necessary.

References

[1] Coralia Cartis, Jaroslav Fowkes, and Zhen Shao. A randomised subspace Gauss-Newton method for nonlinear least-squares. arXiv preprint, arXiv:2211.05727, 2022.

[2] Ieva Daužickaitė, Amos S Lawless, Jennifer A Scott, and Peter Jan Van Leeuwen. Randomised preconditioning for the forcing formulation of weak-constraint 4d-var. *Quarterly Journal of the Royal Meteorological Society*, 147(740):371–3734, 2021.

2.3 Preconditioners for changing weather observation networks

Supervisor: Dr Jemima Tabeart
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In numerical weather prediction systems, measurements of the atmosphere and ocean are combined with a numerical model of the Earth in order to produce accurate forecasts. Observation information is weighted by an inverse error covariance matrix, which can be ill-conditioned and have complex structures. In recent years, the use of correlated (full) covariance matrices has become more feasible. However, inverting and preconditioning observation terms can be computationally expensive and difficult due to time constraints. One reason for this is that the observation network changes in time (e.g. due to weather conditions, or quality control), meaning that a different matrix needs to be used at each time-step.

In practice, a changing observation network means that different rows/columns of a larger observation error covariance matrix will be selected each time. Typically the user has access to the whole covariance matrix, which can be ill-conditioned (specifically they often suffer from small minimum eigenvalues). It is possible to compute an exact inverse or a good preconditioner for the full matrix offline, but it is too expensive in terms of storage to do this for all possible choices of sub-matrix, and expensive in terms of computation time to compute good preconditioners within a numerical routine. In this project we want to use a “good” preconditioner for the full problem to obtain preconditioners for the sub-problem. The student will study existing and alternative methods to deal with covariance matrices arising from changing observation networks. Initial areas of research would include

- Implementing existing techniques for spatial correlations (e.g. wavelet or Fourier approaches) [1, 2, 5]. This relates to a spatial setting where we might start with an evenly spaced grid of observations, and remove specific observations.
- Using linear algebra theory (such as Cauchy interlacing theorem) to consider whether information from a full preconditioner can be used to obtain a good preconditioner for the reduced network.

Depending on student interest extensions to the project include:

- Extend techniques for regular spacing to apply to broader type of problems
- Develop new preconditioners for the non-spatial setting, based on existing classes of preconditioner for the full problem [4, 3].

In addition to theoretical work, the student will conduct numerical experiments using toy problems and real numerical weather prediction data.

Areas: numerical linear algebra, preconditioners, correlation matrices.

References

[1] Vincent Chabot, Maëlle Nodet, and Arthur Vidard. Multiscale representation of observation error statistics in data assimilation. *Sensors*, 20(5), 2020.

[2] O. Guillet, A. T. Weaver, X. Vasseur, Y. Michel, S. Gratton, and S. Gürol. Modelling spatially correlated observation errors in variational data assimilation using a diffusion operator on an unstructured mesh. *Quarterly Journal of the Royal Meteorological Society*, 145(722):1947–1967, 2019.

[3] J. M. Tabeart, S. L. Dance, A. S. Lawless, N. K. Nichols, and J. A. Waller. Improving the condition number of estimated covariance matrices. *Tellus A: Dynamic Meteorology and Oceanography*, 72(1):1–19, 2020.

[4] J. M. Tabeart and J. W. Pearson. Saddle point preconditioners for weak-constraint 4d-var, 2022. https://arxiv.org/abs/2105.06975.

[5] M. Yaremchuk, J. M. D'Addezio, G. Panteleev, and G. Jacobs. On the approximation of the inverse error covariances of high-resolution satellite altimetry data. *Quarterly Journal of the Royal Meteorological Society*, 144(715):1995–2000, 2018.

2.4 Partitions of unity and blending functions

Supervisor: Prof. Nick Trefethen
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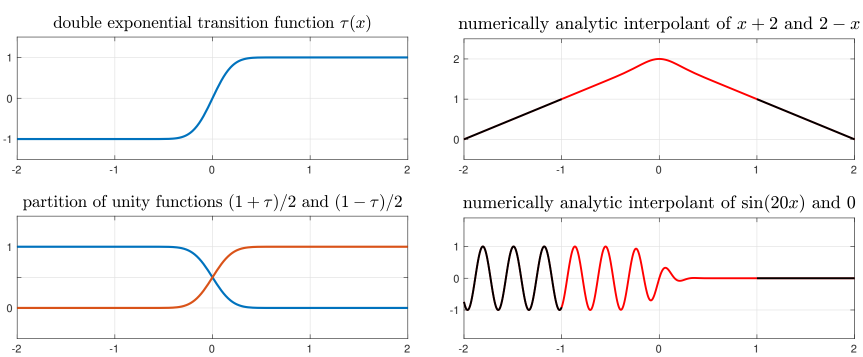
Background and problem statement

It is well known that a C^∞ function may be zero on one interval and nonzero on another: a classic example is $\exp(-1/x)$ for $x \geq 0$. From here one can devise tools such as C^∞ "bump functions" with compact support, partitions of unity, and "blending functions" to introduce a smooth transition from one function to another.

What's the best way to do such things in practice? There seems to be no consensus. The aim of this project is to seek an answer, and to explore in particular methods derived from the "double-exponential transition function" $\tau(x) = \tanh((\pi/2)\sinh(3.2x))$. Mathematically, $-1 < \tau(x) < 1$ for all x, but in standard 16-digit arithmetic, $\tau(x) = -1$ for $x \leq -1$ and $\tau(x = 1$ for $x \geq 1$.

The bump function $b(x) = (\tau(x+1) - \tau(x-1))/2$, for example, is a nonzero "analytic function with compact support." We put this in quotes since such a thing is mathematically impossible — but it's possible in 16-digit accuracy.



Description of the approach planned and the techniques needed

One important part of this project will be a presentation of the mathematical background, including the crucial distinction between C^∞ and analytic. Another will be a survey of some methods that have been proposed and applications for which they have been used. The third will be an exploration with both theorems and computations of methods related to $\tau(x)$ and $b(x)$.

What you'd hope to achieve

The ideal outcome would be a proposal of a family of transition/bump/blending/partition of unity functions that are convincingly good for all kinds of purposes.

References

Start from Section 5 of Trefethen, "Numerical analytic continuation," online at https://people.maths.ox.ac.uk/trefethen/papers.html. Beyond this a good deal of exploration of literature will be involved.

2.5 Sequences of splines and finite elements

Supervisor: Dr Kaibo Hu
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The broad background of this project is to extend splines and other numerical approximations to vector- and tensor-valued problems in the framework of finite element exterior calculus. Splines are piecewise polynomials with certain (e.g., C^r) continuity. For problems involving vector and tensor fields (e.g., fluid and solid mechanics and general relativity), it is important to construct more spaces such that differential operators (e.g., grad, curl and div) map one space to another. Such sequences are referred to as the de Rham complex or differential complex in the literature. A general introduction of the background can be found in [2, pages 5–13].

In this project, one may start with a scalar spline space [1] and differentiate it in order to complete the sequence. There are both theoretical and practical questions. For theories, one may show that the obtained sequence is "exact". For practice, such sequences can be used to solve continuum models with microstructures, for example. Standard background in calculus and linear algebra is enough for carrying out the project (although some questions in this area find surprising connections in algebraic geometry and remain open). To solve problems numerically with the resulting spaces, some familiarity with (numerical) PDEs will be helpful.

The goal of this project is to 1) construct a sequence starting with a scalar spline space, 2) (optional) solve a PDE problem from continuum mechanics using the resulting space.

References

[1] Ming-Jun Lai and Larry L. Schumaker Spline functions on triangulations. Cambridge University Press, 2010.

[2] MFO, Oberwolfach Reports, no. MFO Workshop 2225, MFO, 2022. Workshop on "Hilbert Complexes: Analysis, Applications, and Discretizations", held 19 Jun–25 Jun 2022. https://doi.org/10.14760/OWR-2022-29

2.6 Finite element exterior calculus

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Please also feel free to contact me if you are interested in another problem in finite element exterior calculus. It should also be possible to figure out a project related to topological data analysis in the direction of [1] or orthogonal polynomials (e.g., symmetric OPs for vector fields) and applications.

References

[1] Lek-Heng Lim. Hodge Laplacians on graphs. *SIAM Review*, 62(3):685–715, 2020.

2.7 Numerical linear algebra

Supervisor: Prof. Yuji Nakatsukasa
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I would be happy to supervise MMSC dissertations on topics in numerical linear algebra (NLA). Many involve randomisation, which is an exciting and highly successful idea that has brought significant advances in the field. Depending on your preference, the focus can be theoretical, computational/algorithmic, or application oriented. Potential projects include

- Randomised matrix estimation [1, 18] and applications. Estimating matrices via XX^TA, where X is a random (e.g. scaled Gaussian) matrix, is a powerful idea that can be useful in a variety of contexts, including approximating bilinear forms [2], sparse approximation [17, 19], and trace estimation [6, 12]. The project will explore these problems, and ideally develop and analyse efficient algorithms and implement them.
- Use of (randomised) NLA in related fields. For example (i) Model order reduction, in particular DEIM [5], a widely popular algorithm for nonlinear dimension reduction, (ii) Optimisation, for example quasi-Newton methods, and (iii) Statistics [8, 13, 10].
- Algorithms in randomised NLA (the survey [11] is a great general reference). The goal is to explore and investigate:
  - Properties and extensions of the randomised SVD algorithms [9, 14], the primary example where randomisation has been successful.
  - The randomised linear/eigen solver in [16], which can sometimes bring enormous speedup but currently has limited applicability.
  - Algorithms for the generalised SVD; a decomposition that is sure to grow in importance [7], but an effective randomised algorithm is currently lacking.
- Topics in classical NLA. These include perturbation theory [4, 15], efficient computation of null space, and stability analysis, e.g. of iterative refinement [3].

Prerequisite: love of numerical linear algebra!

References

[1] R. A. Baston and Y. Nakatsukasa. Stochastic diagonal estimation: probabilistic bounds and an improved algorithm. *CoRR*, abs/2201.10684, 2022.

[2] M. Benzi and P. Boito. Matrix functions in network analysis. *GAMM-Mitteilungen*, 43(3):e202000012, 2020.

[3] E. Carson and N. J. Higham. A new analysis of iterative refinement and its application to accurate solution of ill-conditioned sparse linear systems. *SIAM J. Sci. Comp.*, 39(6):A2834–A2856, 2017.

[4] V. Charisopoulos, A. R. Benson, and A. Damle. Communication-efficient distributed eigenspace estimation. *SIAM Journal on Mathematics of Data Science*, 3(4):1067–1092, 2021.

[5] S. Chaturantabut and D. C. Sorensen. Nonlinear model reduction via discrete empirical interpolation. *SIAM J. Sci. Comp.*, 32(5):2737–2764, 2010.

[6] A. Cortinovis and D. Kressner. On randomized trace estimates for indefinite matrices with an application to determinants. *Found. Comput. Math.*, 22(3):875–903, 2022.

[7] A. Edelman and Y. Wang. The GSVD: Where are the ellipses?, matrix trigonometry, and more. *SIAM J. Matrix Anal. Appl.*, 41(4):1826–1856, 2020.

[8] M. Gavish and D. L. Donoho. The optimal hard threshold for singular values is $4/\backslash\sqrt{3}$. *IEEE Trans. Inf. Theory*, 60(8):5040–5053, 2014.

[9] N. Halko, P.-G. Martinsson, and J. A. Tropp. Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions. *SIAM Rev.*, 53(2):217–288, 2011.

[10] T. Hastie, A. Montanari, S. Rosset, and R. J. Tibshirani. Surprises in high-dimensional ridgeless least squares interpolation. *Ann. Math.*, 50(2):949–986, 2022.

[11] P.-G. Martinsson and J. A. Tropp. Randomized numerical linear algebra: Foundations and algorithms. *Acta Numer.*, pages 403–572, 2020.

[12] R. A. Meyer, C. Musco, C. Musco, and D. P. Woodruff. Hutch++: Optimal stochastic trace estimation. In *Symposium on Simplicity in Algorithms (SOSA)*, pages 142–155. SIAM, 2021.

[13] B. Nadler. Finite sample approximation results for principal component analysis: A matrix perturbation approach. *The Annals of Statistics*, 36(6):2791–2817, 2008.

[14] Y. Nakatsukasa. Fast and stable randomized low-rank matrix approximation. arXiv:2009.11392.

[15] Y. Nakatsukasa. Sharp error bounds for Ritz vectors and approximate singular vectors. *Math. Comp.*, 89(324):1843–1866, 2020.

[16] Y. Nakatsukasa and J. A. Tropp. Fast & accurate randomized algorithms for linear systems and eigenvalue problems. arXiv 2111.00113.

[17] H. Rauhut and R. Ward. Sparse Legendre expansions via ℓ_1-minimization. *J. Approx. Theory*, 164(5):517–533, 2012.

[18] M. Udell and A. Townsend. Why are big data matrices approximately low rank? *SIAM Journal on Mathematics of Data Science*, 1(1):144–160, 2019.

[19] Z. Yao, A. Gholami, S. Shen, M. Mustafa, K. Keutzer, and M. Mahoney. Adahessian: An adaptive second order optimizer for machine learning. In *proceedings of the AAAI conference on artificial intelligence*, volume 35, pages 10665–10673, 2021.

Topics in Numerical Linear Algebra and Numerical Methods for Partial Differential Equations

Supervisor: Prof. Andy Wathen
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I'm happy to supervise generally projects in the area of Numerical Linear Algebra and Numerical Methods for Partial Differential Equations, so please come and talk with me about any ideas if you wish. Specific suggestions this year are below.

2.8 Iterative solution methods in non-standard inner products

Supervisor: Prof. Andy Wathen
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Krylov subspace iterative methods like Conjugate Gradients and GMRES construct orthogonal set of vectors via iteration. Usually the standard Euclidean inner product is employed, but these methods are defined for any inner product on vectors. Some work along these lines appears in the 2008 paper of Martin Stoll and myself [1], though this was not its main contribution.

This project would be to derive and program in Matlab these iterative methods for arbitrary inner products and to investigate both theoretically and via computation their properties. Thus both the theory of Krylov subspace methods (Numerical Linear Algebra) and computer implementation would be required.

It seems like there might be situations where such generality could be used to give more effective solution algorithms for certain problems; I have some ideas, but this is certainly a somewhat open-ended project!

References

[1] M. Stoll and A. J. Wathen. Combination preconditioning and the Bramble-Pasciak+ preconditioner. *SIAM J Matrix Anal. Appl.*, 30(2):582–608, 2008.

2.9 The iterative solution of linear least squares problems

Supervisor: Prof. Andy Wathen
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The QR factorization is the standard way to solve linear least squares problems, but it complexity means that it is only applicable for small dimensions. There are several ideas for solving large dimensional sparse linear least squares problems all largely related to the solution of the normal equations. An inherent difficulty with such an approach is that the condition number is squared when going to the normal equations and this almost always implies much slower iterative convergence.

This project is to explore some ideas for replacing the normal equations with other nonsymmetric linear systems for the least squares solution that do not square the condition number, thus may allow more rapid iterative convergence (though the squandering of the symmetry of the normal equations could lead to other difficulties as yet unknown!)

References

[1] G. H. Golub and C. F. van Loan. *Matrix Computations* (3rd Edition), The Johns Hopkins University Press, 1996. Chapter 5.

2.10 Adaptive Newton methods for finite element discretisations of aeroelasticity

Supervisors: Dr Francis Aznaran and Dr Charles Parker
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Background and problem statement

In the field of aeroplane design, the optimisation of the shape of wings and the prediction of their behaviour under heavy loads plays a key role for their safety, economic efficiency of manufacturing, and fuel efficiency. A commonly simulated problem is the deformation of the wing, modelled by nonlinear elasticity. This project seeks to study and improve Newton's method for the approximate solution of the underlying PDEs. We will also compare the solutions of the nonlinear model to linear models of elasticity which engineers commonly assume instead (as a simplification), in order to evaluate the validity of such assumptions. We will apply the finite element method to approximately solve the linearised systems in the Newton iteration.

Newton's method is the standard technique for the numerical solution of nonlinear PDEs. Adaptive variants of Newton's method are more sophisticated in providing a more accurate solution and/or making more efficient use of computational resources.

Approach planned and the techniques needed

First, we will study the derivation and nondimensionalisation of the hyperelastic model, posed in an appropriate Sobolev space, before defining the Newton–Kantorovich iteration for a nonlinear equation posed in an abstract Banach space. Then we will collect together different adaptations to Newton's method: their definitions, properties, and (for example) convergence theorems.

This includes many different possibilities, and from the start we will experiment with them computationally on the hyperelastic model; relevant topics include alternatives to Newton linearisation (such as the Picard iteration), quasi-Newton and inexact Newton methods, conditions of local or global convergence of these iteration schemes, convergence with respect to weaker norms and topologies, affine covariance of Newton, linearisation vs. discretisation and whether these commute, use and estimation of different metrics of convergence (such as error vs. residual), continuation with respect to physical parameters or the magnitude of the body forces, problematic parameter regimes in the physics such as incompressibility of the solid material, basins of attraction and choice of initial guess, globalisation via linesearch (i.e. choice and scaling of Newton step), adapting the tolerance of the linear algebraic solver, and refining with respect to mesh size or polynomial degree as part of the Newton algorithm. Many of these aspects might be symbiotic, or in tradeoff.

We both will study the abstract theory of Newton's method in Banach spaces, and code numerical experiments in the Firedrake finite element library to give results with which to compare the theory; the latter will require familiarity with the python language (and the student will learn about git version control). Beyond this, the project can either be more theoretical or more computational according to the student's taste.

C6.4 Finite Element Methods for PDEs is a requirement. Other relevant courses are C6.1 Numerical Linear Algebra, C4.3 Functional Analytic Methods for PDEs, C5.2 Elasticity and Plasticity, C6.2 Continuous Optimisation, B6.1 Numerical Solution of Partial Differential Equations.

Planned outcome

An algorithm for the adaptive solution of the hyperelastic model, which possibly includes heuristics but also automated aspects; a collection of computational results trying different techniques; possibly (ambitiously), theoretical proofs which explain the numerical phenomena observed. Computational experiments will be carried out on examples of realistic mesh geometries taken from the engineering literature, and then visualised and interpreted physically. We will also postprocess some physically relevant quantities as outputs of the simulation which are of interest to aeronautical engineers.

References

[1] C. Beentjes. *Computing bifurcation diagrams with deflation.* M.Sc. dissertation, University of Oxford, 2015. https://cbeentjes.github.io/files/Ramblings/MScBeentjes.pdf

[2] D. Braess. *Finite elements: Theory, fast solvers, and applications in solid mechanics*, Cambridge University Press, Cambridge, 3rd ed., 2007. https://doi.org/10.1088/0957-0233/13/9/704

[3] P. G. Ciarlet and C. Mardare. On the Newton–Kantorovich theorem. *Analysis and Applications*, 10(3):249–269, 2012. https://doi.org/10.1142/S0219530512500121

[4] P. Deuflhard. *Newton methods for nonlinear problems: affine invariance and adaptive algorithms*, vol. 35, Springer Science & Business Media, 2005. https://doi.org/10.1007/978-3-642-23899-4

[5] S. C. Eisenstat and H. F. Walker. Choosing the forcing terms in an inexact Newton method. *SIAM Journal on Scientific Computing*, 17:16–32, 1996. https://doi.org/10.1137/0917003

[6] P. Heid and T. Wihler. Adaptive iterative linearization Galerkin methods for nonlinear problems. *Mathematics of Computation*, 89:2707–2734, 2020. https://doi.org/10.1090/mcom/3545

[7] P. Howell, G. Kozyreff, and J. Ockendon. *Applied solid mechanics.* Cambridge University Press, Cambridge, 2009. https://doi.org/10.1017/CBO9780511611605

[8] B. Shamsaei and J. Newman. *Comparison of linear and non-linear elasticity large displacement mesh deformation in computational fluid dynamics*, in 46th AIAA Fluid Dynamics Conference, 06 2016. https://doi.org/10.2514/6.2016-3183

[9] J. Xia, P. E. Farrell, and S. G. P. Castro. Nonlinear bifurcation analysis of stiffener profiles via deflation techniques. *Thin-Walled Structures*, 149:106662, 2020. https://doi.org/10.1016/j.tws.2020.106662

3 Biological and Medical Application Projects

3.1 From microscopic to macroscopic description of liquid-liquid phase separation

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Liquid-liquid phase separation (LLPS) is a process by which liquids separate into different phases. In this project, we will consider applications of LLPS to modelling of intracellular processes, where LLPS has been recently shown to have a potential for being an important physical mechanism behind the formation of certain types of cell organelles.

From the mathematical point of view, the candidate will use a combination of molecular dynamics (MD) and Brownian dynamics (BD) techniques, which are discussed in the Special Topic course "Stochastic Modelling of Biological Processes". The candidate will learn and implement coarse-grained models that incorporate sequence-specific information into modelling of LLPS [1, 2]. One of the aims of the project is to connect these microscopic models with LLPS modelling based on more classical mean-field (Flory-Huggins or Voorn-Overbeek) type descriptions of charged macromolecules which have been developed during the last 70 years [3] with the aim to inform parameters of macroscopic models by sequence-specific information available in the microscopic models of charged macromolecules, such as intrinsically disordered proteins or nucleic acids (DNA, RNA).

References

[1] R. M. Regy, W. Zheng, and J. Mittal. Using a sequence-specific coarse-grained model for studying protein liquid–liquid phase separation. *Methods Enzymol.*, 646:1–17, 2021.

[2] S. Kmiecik, D. Gront, M. Kolinski, L. Wieteska, A. E. Dawid, and A. Kolinski. Coarse-grained protein models and their applications. *Chem. Rev.*, 116(14):7898–7936, 2016.

[3] J. T. G. Overbeek, and M. J. Voorn. Phase separation in polyelectrolyte solutions. Theory of complex coacervation. *Journal of Cellular and Comparative Physiology*, 49(S1):7–26, 1957.

3.2 Characterising the solution space of tumour blood flow

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Background and problem statement

It has long been hypothesised that the abnormal and heterogeneous architecture of tumour vascular networks promotes spatio-temporal variations in blood flow rates, red blood cell (RBC) distribution, and consequent oxygen delivery. These irregularities drive heterogeneity in the oxygenation landscape in tumours, where some regions experience either chronic or transient hypoxia. Exposure to such variability in oxygen levels is assumed to select for, and promote, metastatic spread and resistance of the tumour to radio- and chemo-therapy. Consequently, understanding the structural and fluid-dynamic mechanisms that promote heterogeneities in tumour blood flow is of great importance.

In this project we will simulate steady-state blood flow in vessel networks. The bi-phasic nature of blood (which is essentially composed of plasma and RBCs) leads to the emergence of nonlinearities that promote heterogeneities in the flow between different vessels and multiple equilibria for some network geometries [1]. We aim to characterise the steady-state solution space for different network architectures and, by comparing to the topological analysis of these networks, to reveal the structural features that promote blood flow heterogeneities.

Approach and techniques

We will generate a set of artificial vessel networks that differ in their topological features (e.g., random, tree-type, honeycomb networks). We will solve for the steady-state blood flow and RBC distribution in these networks using existing models [1]. By continuously varying key biophysical parameters (e.g., boundary conditions, vessel diameters and lengths), we will obtain a set of equilibrium solutions for a given network topology. We will use existing techniques to quantify topological features of the networks [2], and then use clustering methods (e.g., K-means, UMAP, PCA) to characterise the heterogeneity of the solution space and to link it with specific features of the network.

Objectives

By the end of this project, we aim to develop a pipeline for systematically analysing the solution space of steady-state blood flow and relating this solution space to a network feature summary of the vascular network structure. This will increase our understanding of how network architecture affects the spatial distribution of blood flow and oxygen.

Ultimately, this project may be extended to biological networks acquired via photoacoustic imaging [3], to facilitate comparisons between tumour and healthy tissues, and between different tumours. This will contribute to a better understanding of the mechanisms that promote blood flow and oxygen heterogeneities in tumours.

References

[1] Y. Ben-Ami, G. W. Atkinson, J. M. Pitt-Francis, P. K. Maini, and H. M. Byrne Structural features of microvascular networks trigger blood flow oscillation. *Bulletin of Mathematical Biology*, 84, 85, 2022. doi:10.1007/s11538-022-01046-y

[2] B. J. Stolz, J. Kaeppler, B. Markelc, F. Braun, F. Lipsmeier, R. J. Muschel, H. M. Byrne, and H. A. Harrington. Multiscale topology characterizes dynamic tumor vascular networks. *Science Advances*, 8, eabm2456, 2022. doi:10.1126/sciadv.abm2456

[3] E. L. Brown, T. L. Lefebvre, P. W. Sweeney, B. J. Stolz, J. Gröhl, L. Hacker, Z. Huang, D.-L. Couturier, H. A. Harrington, H. M. Byrne, and S. E. Bohndiek. Quantification of vascular networks in photoacoustic mesoscopy. *Photoacoustics*, 26:100357, 2022. doi:10.1016/j.pacs.2022.100357

3.3 Modelling cell transport and growth in a nanofiber scaffold

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Collaborators: Dr Rudolf Hellmuth, Dr Yuan-Tsan Tseng, and Dr Najma Latif (Magdi Yacoub Institute)

Background and objectives

Tissue engineering has the potential to provide replacements for damaged tissues or organs. The generation of artificial tissues typically involves seeding cells in a scaffold, which is then placed in a bioreactor to provide necessary nutrients and mechanical forces for cell growth and tissue formation. However, the biophysical mechanisms that govern this process remain poorly understood. The aims of this project are thus to

- Develop a continuum model of cell transport and growth in a scaffold
- Apply the model to examine the impact of scaffold microstructure characteristics, such as density and porosity, on cell distribution
- Validate the model against experimental data

This project will improve our understanding of the impact of scaffold geometry on tissue generation, and inform future scaffold designs for tissue engineering applications.

Approaches and techniques

The student will work closely with experimental collaborators at the Magdi Yacoub Institute to develop and validate the model [1]. The scaffold has been scanned using nano-scale computer tomography. Topological data representing the scaffold geometry will be provided at the start of this project. The scaffold will be treated as a porous medium incorporating its topological properties, and fluid flow through the scaffold will be modelled by Darcy's law [2]. Cell growth and expansion will be simulated using a reaction-diffusion equation for the cell density [3], and the impact of cell growth on scaffold porosity will be incorporated [4]. The final cell distribution will be validated against in vitro experiments using scaffolds with different geometries.

Prerequisites

Knowledge of fluid mechanics, mathematical biology and numerical methods for solving differential equations would be helpful, but not necessary.

References

[1] J. Sohier, I. Carubelli, P. Sarathchandra, N. Latif, A. H. Chester, and M. H. Yacoub. The potential of anisotropic matrices as substrate for heart valve engineering. *Biomaterials*, 35:1833–1844, 2014. doi:10.1016/j.biomaterials.2013.10.061

[2] R. J. Shipley and S. L. Waters. Fluid and mass transport modelling to drive the design of cell-packed hollow fibre bioreactors for tissue engineering applications. *Mathematical Medicine and Biology*, 29:329–359, 2012. doi:10.1093/imammb/dqr025

[3] M. Shakeel, P. C. Matthews, R. S. Graham, and S. L. Waters. A continuum model of cell proliferation and nutrient transport in a perfusion bioreactor. *Mathematical Medicine and Biology*, 30:21–44, 2013. doi:10.1093/imammb/dqr022

[4] R. D. O'Dea, M. R. Nelson, A. J. el Haj, S. L. Waters, and H. M. Byrne. A multiscale analysis of nutrient transport and biological tissue growth in vitro. *Mathematical Medicine and Biology*, 32:345–366, 2015. doi:10.1093/imammb/dqu015

3.4 The role of fluid mechanics in stem cell delivery for liver disease

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Background

Cell therapy for liver disease aims to inject donor cells into the vasculature to engraft and regenerate regions of diseased liver. Fluid mechanical stresses are sensed by cells as they transit to the injury site and can lead to upregulation of integrin expression. Integrins are receptors that bind to extracellular matrix, which in turn promotes engraftment of the donor cells into the injured tissue. This MMSC project will contribute to a wider interdisciplinary effort involving teams at the Universities of Oxford, Birmingham and Edinburgh, in which we combine in-silico, in-vitro and in-vivo approaches to understand the relationship between fluid flow conditions and integrin expression, and the impact of these factors on cell engraftment in diseased livers.

Problem statement

To mimic the liver circulation, our collaborators at the University of Birmingham have developed an in-vitro system that drives flow through a closed tube using a peristaltic pump. This project will use lubrication theory to model fluid flow through the system, exploiting the small aspect ratio of the tube. We will model the transport of donor cells via an advection-diffusion equation. The governing equations will be solved using a combination of analytical and numerical techniques. We will then perform a parameter sensitivity analysis to determine how the fluid mechanical stresses experienced by the donor cells depend on system parameters, including peristaltic pump settings and system geometry. Finally, we aim to relate the predicted cell experienced stress to the experimentally determined changes in integrin expression.

Outcomes

This project will result in theoretical predictions for the transport of donor cells in the in-vitro system. We will then exploit the theoretical model to determine the mechanical stress and corresponding levels of integrin expression experienced by donor cells in in-vivo scenarios.

Expertise required

A background in fluid dynamics, and analytical and numerical methods is desirable. No prior knowledge of biology is required. There is scope within the project to visit the collaborative team at the University of Birmingham to get first-hand experience of the in-vitro system.

3.5 Modelling Human papilloma virus (HPV) with agent-based models: HPVSim development and application to England

Supervisor: Dr Jasmina Panovska-Griffiths (The Big Data Institute and The Queen's College)
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Collaborators: Dr Jamie Cohen and Dr Robyn Stuart (Institute for Disease Modelling, Bill and Melinda Gates Foundation, USA) and Dr Thomas Bailey (UK Health Security Agency, UK)

During the COVID-19 pandemic, mathematical and statistical modelling has been very useful in informing and advising policy decision making. Utilising existing methods across different disciplines and furnishing them with novel adaptations has been an important part of the pandemic response over the last three years. One stream of modelling that has been popularised during the pandemic is agent-based or individual-based models (ABMs/IBMs). Notably, Covasim [1] is an ABM that was developed in early 2020 to model the transmission of different SARS-CoV-2 strains and incorporate interventions such as contract tracing which are difficult to model with population-based compartmental models. Covasim has been widely used to track the COVID-19 epidemic across a number of countries. Notably in the UK it has been used to provide ongoing informed scientific advice to the UK Health Security Agency and the Department of Health and Social Care.

This M.Sc. project will utilise the knowledge from the technical framework and the development of Covasim, to develop an England specific ABMs to model the transmission and vaccination against Human Papilloma Virus (HPV). A prototype model called HPVSim has been built recently, and within the project this prototype will be tested and further developed. Importantly, the aim of the work is to adapt the design to develop an HPVSim for England — taking care of the correct HPV transmission networks for this setting and modelling the current vaccination strategies against HPV [2] as well as future possible extensions.

The work of the project will comprise:

1. Undertaking of a systematic review of HPV modelling and convince yourself of the advantage of using an ABM over compartmental model for HPV transmission.

2. Learning to use the Covasim technical framework and building a simple Oxford University model taking care of the networks you want to include. Can be an adaptation of the application of Covasim to Boston University in [3].

3. Learning to use the HPVSim modeling and noting the differences between Covasim and HPVSim.

4. Undertaking a scoping/systematic review of existing vaccines and possible future candidates.

5. Developing HPVSim for England based on the transmission network modelled in [2] and what we learned about current and possible vaccine candidates.

There is a scope to change/adapt/extent the above points if there is a direction that the student is particularly interested in exploring. Please get in touch if this is the case.

Outputs from the project could be used to offer informed advice to the Joint Committee for Vaccination and Immunisation (JCVI) who evaluate all the immunisation programmes in England, and its HPV sub-committee who evaluate the ongoing HPV immunisation programme.

References

[1] C. C. Kerr, R. M. Stuart, D. Mistry, R. G. Abeysuriya, K. Rosenfeld et al. Covasim: An agent-based model of COVID-19 dynamics and interventions. *PLOS Computational Biology*, 17(7):e1009149, 2021. https://doi.org/10.1371/journal.pcbi.1009149

[2] H. C. Johnson, E. I. Lafferty, R. M. Eggo, K. Louie, K. Soldan, J. Waller, and W. J. Edmunds. Effect of HPV vaccination and cervical cancer screening in England by ethnicity: a modelling study. *Lancet Public Health*, 3(1):e44–e51, 2018.

[3] D. H. Hamer, L. F. White, H. E. Jenkins et al. Assessment of a COVID-19 Control Plan on an Urban University Campus During a Second Wave of the Pandemic. *JAMA Netw Open.*, 4(6):e2116425, 2021.

4 Physical Application Projects

4.1 Repeatable snap-through mechanism for a jumping robot

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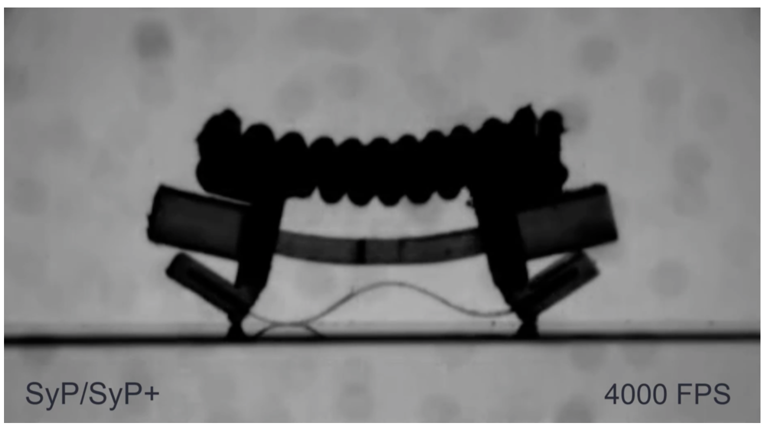
Elastic instabilities are fascinating phenomena that occur when an elastic material under stress suddenly relaxes to a new configuration. In biological systems, elastic instabilities are believed to sculpt a variety of complex shapes, from the wrinkles on the edges of leaves to the villi in the human gut. Moreover, because some elastic instabilities are accompanied by a sudden release of elastic energy, they can be harnessed to achieve fast dynamics. For example, insects such as click beetles, use a snap-through instability to perform impressive jumps, easily leaping many times their body length. Unlike jumps in humans, these leaps are not performed on demand, limited by the power supplied by muscle; instead, the energy is stored slowly over time, and then suddenly released to achieve impressive relative heights.



Recently, engineers have turned to mimicking this jumping mechanism at a range of scales and with different mechanisms [1, 2, 3], each of which is able to achieve multiple jumps. However, the design of each mechanism is often driven by trial-and-error, leaving jumping optimisation to chance rather than a rational approach.

This dissertation will focus on developing a mathematical model for the loading phase of one such robot, reported in [3]. The modelling will involve understanding the deformation of an elastic beam in response to an increasing compression and how this ultimately leads to a rapid snap-through event. Some knowledge of beam theory (for example by having sat in on lectures in the Part C course ‘Elasticity and Plasticity’) would be useful. However, the background relevant material can easily be taught as necessary.

The aim of the project is to understand the geometrical properties of the robot presented in [3] for which repeatable jumping is observed.

References

[1] Y. Kim, J. van den Berg, and A. J. Crosby. Autonomous snapping and jumping polymer gels. *Nat. Mater.*, 20:1695–1701, 2021.

[2] T. S. Hebner, K. Korner, C. N. Bowman, K. Bhattacharya, and T. J. White. Leaping liquid crystal elastomers. *Sci Adv.*, 9(3):eade1320, 2023.

[3] Y. Wang, Q. Wang, M. Liu, and S. Tawfick. Insect-scale jumping robots enabled by a dynamic buckling cascade. *Proc. Natl Acad. Sci. USA*, 120(5):e2210651120, 2023.

4.2 Modelling the evolution of marine ice sheets with bed sedimentation

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Marine ice sheets terminate in the ocean, where they form floating ice shelves that break off to form ice bergs. Both the Antarctic and Greenland ice sheets are examples. The ice becomes afloat across the so-called grounding line, and the dynamics of the ice sheet are thought to be particularly sensitive to changes in the location of this interface. Retreat of the grounding line is generally associated with rapid ice loss and sea-level changes. There is therefore a lot of interest in understanding what controls the grounding line location, and being able to predict how it will change in response to changing climate.

Simplified models exist to describe how the grounding line behaves in a two-dimensional setting, under certain idealised assumptions (eg. [1]). This project would try to extend such models to account for erosion and deposition of the underlying sediments on which the ice rests. There have been suggestions that the shape of the bed directly under the groundling line exerts a big influence on the stability of the grounding line's position (e.g. [2]).

The project would involve building a model that accounts for the movement of a layer of sediment beneath the ice, using ideas from lubrication theory and some existing studies (e.g. [3]). It would then seek to find quasi-steady solutions in which the ice can be assumed to be in a steady state, but the sediment depth evolves slowly over time. We would investigate what the long term behaviour of the system is, and whether the sediment evolution can generally be expected to lead to stabilisation or destabilisation of the groundling line location.

This project would require interest in fluid dynamics, PDEs, asymptotic methods and/or numerical methods, as well as an interest in the general context of geophysical problems.

References

[1] C. Schoof. Ice sheet grounding line dynamics: Steady states, stability, and hysteresis. *J. Geophys. Res.*, 112:F03S28, 2007. doi:10.1029/2006JF000664

[2] R. B. Alley, S. Anandakrishnan, T. K. Dupont, B. R. Parizek, and D. Pollard. Effect of Sedimentation on Ice-Sheet Grounding-Line Stability. *Science*, 315(5820):1838–1841, 2007. doi:10.1126/science/1138396

[3] K. N. Kowal and M. G. Worster. The formation of grounding zone wedges: theory and experiments. *J. Fluid Mech.*, 898:A12, 2020. doi:10.1017/jfm.2020.393

4.3 Surging glaciers

Supervisor: Prof. Ian Hewitt
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Many of the world's glaciers undergo an intriguing behaviour in which they undergo quasi-periodic 'surges', during which they move much faster ($\sim$100 times faster) than their usual slow pace. The surges generally last for a few months, and occur every few years (though the timescales are quite variable). They are associated with an advance of the glacier front, which can have dramatic effects such as altering river courses and wiping out infrastructure. Despite lots of attempts to understand what causes a surge, and why some glaciers surge while some do not, there are still no clear answers to those questions.

A recent study, [1], suggested a new theory for glacier surges, based on principles of mass and energy conservation. That study described a 'lumped' ODE model for surging behaviour, which took the form of a dynamical system for the average ice thickness H and velocity u. The system can be analysed using phase-plane methods. The intention for this project would be to extend the ideas in that model to a spatially-extended model, to provide greater realism.

The project would involve constructing a PDE model for the flow of a glacier and the evolution of its energy content. It would solve the model — probably numerically using either a finite element or a finite volume discretisation — and look to examine whether the behaviour seen in the lumped ODE model carries over to the spatially-resolved model. There may be potential for comparing the model with satellite observations from surging glaciers in Svalbard.

This project would require interest in PDEs, numerical methods, and getting to grips with various interesting (but somewhat messy) physics.

References

[1] D. I. Benn, A. C. Fowler, I. Hewitt, and H. Sevestre. A general theory of glacier surges. *J. Glaciology*, 65(253):701–716, 2019. doi:10.1017/jog.2019.62

4.4 Geoscience, fluid dynamics, and solid mechanics

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I am also happy to discuss other projects in geoscience, fluid dynamics, or solid mechanics.

4.5 Reducing longterm battery degradation

Supervisor: Prof. Jon Chapman
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Collaborators: Prof. Colin Please (Oxford) and Dr Robert Timms (Ion-works)

Background and problem statement

Batteries degrade over the longterm due to a multitude of different mechanisms. It is important to try to operate batteries in a manner that makes their lifetime as long as possible. In particular the problem is complicated by the "knee" behaviour of batteries where they operate well for a long time, slowly degrading, and then suddenly degrade much more rapidly, [1]. Trying to optimise the usage to reduce this degradation requires accounting for the underlying physical processes and how they can be manipulated.

Description of the approach planned and the techniques needed

In this project existing models of the physical degradation of a battery will be considered. These models consist of partial differential equations that describe the electrochemical processes that occur i the battery. These models must be over long timescales and doing this in a computationally efficient manner, so that many different usage profiles can be considered is critical to being able to optimise the usage. To do this different numerical and analytical approaches to solving the problem, particularly those that exploit for the vast different in timescale between slow degradation processes and the rapid changes in the usage will need to be examined. The project will involve significant asymptotic analysis and numerical solution of the model, as well as some modelling and optimisation.

What you'd hope to achieve

It is hoped that a framework will be created that allows the user to explore optimal usage profiles for the battery that minimise the long term degradation.

References

[1] P. M. Attia, A. Bills, F. Brosa Planella, P. Dechent, G. Reis, M. Dubarry, P. Gasper, R. Gilchrist, S. Greenbank, D. Howey, O. Liu, E. Khoo, Y. Preger, A. Soni, S. Sripad, A. G. Stefanopoulou, and V. Sulzer. Review – "Knees" in Lithium-Ion Battery Aging Trajectories. *Journal of The Electrochemical Society*, 169(6):060517, 2022. https://dx.doi.org/10.1149/1945-7111/ac6d13.

5 Data Science

5.1 Network analysis with linear algebra techniques

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Understanding and detecting structure in large-scale networks is an important problem today in a variety of disciplines [5]. A number of concepts in network analysis involve functions of matrices [3], such as the shifted inverse $(I - \alpha A)^{-1}$ for Katz centrality, and the matrix exponential $\exp(A)$ for centrality and communicability measures.

In this project we investigate the behavior of these matrix functions, in particular when the network undergoes small changes. Theoretical and computational results in numerical linear algebra [1, 2] suggest that efficient estimates of the updates of the matrix functions should be possible. This project aims to utilise these tools together with and classical results in matrix analysis [4] to understand the behavior and develop algorithms.

Prerequisite: Familiarity with the courses Networks, and Numerical Linear Algebra.

References

[1] B. Beckermann, A. Cortinovis, D. Kressner, and M. Schweitzer. Low-rank updates of matrix functions II: Rational Krylov methods. *SIAM J. Numer. Anal.*, 59(3):1325–1347, 2021.

[2] B. Beckermann, D. Kressner, and M. Schweitzer. Low-rank updates of matrix functions. *SIAM J. Matrix Anal. Appl.*, 39(1):539–565, 2018.

[3] M. Benzi and P. Boito. Matrix functions in network analysis. *GAMM-Mitteilungen*, 43(3):e202000012, 2020.

[4] R. A. Horn and C. R. Johnson. *Matrix Analysis.* Cambridge University Press, second edition, 2012.

[5] R. Lambiotte and P. Grindrod. C5.4 Networks. *Oxford University Mathematical Institute Lecture notes.*