Application of Linear and Multilinear Algebra in Life Sciences and Engineering

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This Mini Symposium will bring together Scientists who use Linear algebra and Multilinear Algebra in their respected fields. The focus is on problems arising in molecular biology, biomedicine and engineering. Most application is related to the processing of biological and chemical data, Drug Discovery, including biological sequences, gene expression data or gene networks, functional genomics, gene network reconstruction reconstruction and Neural Networks. The tools include but not limited to dimension reduction techniques such as Singular Value Decomposition (SVD), Generalized Singular Value Decomposition (GSVD),Principal component analysis (PCA), spectral clustering, Latent Semantic Indexing, Nonlinear Dimension reduction, Support Vector Machine(SVM). The mini symposium will address both deterministic and stochastic frameworks.

Spectral Theorems of Karlin for Evolutionary Dynamics

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Tue 11:00, Room Galilei

The dynamics of Darwinian evolution result from the fertile interaction of 'dispersing' operators (mutation, recombination, and other transformations of heritable states) and a 'concentrating' operator (natural selection). Analysis of the dynamics typically arrives at matrices that are products of stochastic and non-negative diagonal matrices, and the spectral radii of such products are shown by Karlin (1982) to decrease under two different forms of 'more' dispersion. Originally developed to analyze genetic diversity in subdivided populations, Karlin's theorems and their extensions have applications to anti-viral therapy, quasispecies, the evolution of genetic systems, recombination and mutation rates (Altenberg and Feldman, 1987; Altenberg, 2009), coupled maps, and other areas, which are here described.

[1] Karlin, S., 1982. Classification of selection-migration structures and conditions for a protected polymorphism. Pages 61–204 in M. K. Hecht, B. Wallace, and G. T. Prance, eds. Evolutionary Biology, volume 14. Plenum.
[2] Altenberg, L. and Feldman, M. W. 1987. Selection, generalized transmission, and the evolution of modifier genes. I. The reduction principle. Genetics 117:559–572.
[3] Altenberg, L. 2009. The evolutionary reduction principle for linear variation in genetic transmission. Bulletin of Mathematical Biology 71:1264–1284.

Linear algebra issues in a fast algorithm for a large scale nonlinear nonlocal model of the inner ear

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Fri, 11:25, Room C

Recently, we proposed in [1] a fast second order package for a nonlinear, nonlocal model for the inner ear improving algorithms [2,3,4] for inner ear simulation of the evolution of the transverse displacement of the basilar membrane at each cochlear place. This information allows one to follow the forward and backward propagation of the traveling wave along the basilar membrane, and to evaluate the otoacoustic response from the time evolution of the stapes displacement.

In this talk, we illustrate the main results and performances of the numerical linear algebra core of the algorithms in [1] and [4] and, in particular, will focus on invertibility and conditioning of matrices, convergence of inner iterations, preconditioning and computational complexity issues.

[1] D. Bertaccini, R. Sisto, Fast numerical solution of a nonlinear nonlocal feed-forward cochlear model, submitted, 2010.
[2] D. Bertaccini, S. Fanelli, Computational and conditioning issues of a discrete model for cochlear sensorineural hypoacusia", Applied Numerical Mathematics, vol. 59, pp. 1989-2001, 2009.
[3] Elliott S.J., Ku E.M., Lineton B., "A state space model for cochlear mechanics", Journal of the Acoustical Society of America, vol. 122, No.5, pp. 2759-2771, 2007.
[4] A. Moleti, N. Paternoster, D. Bertaccini, R. Sisto, F. Sanjust, Otoacoustic emissions in time-domain solutions of nonlinear nonlocal cochlear models, Journal of Acoustical Society of America (JASA) vol. 126, pp. 2425-2436, 2009.

Joint work with A. Moleti (Università di Roma "Tor Vergata", Roma) and R. Sisto (ISPESL research center, Roma)

Enhanced line search for blind channel identification based on the Parafac decomposition of cumulant tensors

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Thu, 11:50, Room C

Consider a baseband communication system with discrete-time model

$$y(n) = x(n) + v(n), \quad x(n) = (h * s)(n) := \sum_{l=0}^{L} h(l)s(n-l),$$

where $s(n)$ is the sequence of transmitted symbols, $h(n)$ is the channel impulse response, $v(n)$ is additive noise, and $y(n)$ is the observed channel output.

The goal of blind identification is to estimate $h(n)$ from the observed system output $y(n)$, after which the input signal $s(n)$ can be recovered.

One class of blind identification algorithms is based on fitting higher-order cumulants. This yields the following multilinear algebra problem: decompose a given third-order tensor T that has certain symmetry properties into a sum of rank-1 terms (this is known as the PARAFAC decomposition).

Because of the symmetry properties of T (the factors in the PARAFAC decomposition have a Hankel structure) the common alternating least squares (ALS) algorithm is not applicable. Recently, a single-step least-squares (SSLS) algorithm has been proposed as an alternative. This algorithm preserves the symmetry properties but it does not necessarily converge monotonically. Moreover, the conditions that guarantee the convergence are not known.

It is known that ALS-based PARAFAC algorithms can be significantly improved by applying an enhanced line search (ELS) procedure. Namely, new ELS algorithms are less sensitive to local optima and have higher convergence speed.

We compute the PARAFAC decomposition of T combining the SSLS algorithm with ELS. Our method converges monotonically. It preserves the symmetry and the Hankel structure. We derive an explicit solution for the optimal real and complex step in the line search.

Joint work with L. De Lathauwer (K.U.Leuven: Campus Kortrijk and E.E. Dept. (ESAT), Belgium)

Phylogenic invariants and tensors of border rank 4 at most in $\mathbb{C}^{4\times4\times4}$

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Tue, 12:15, Room Galilei

We first discuss briefly the notion of algebraic statistics, phylogenic trees and their invariants. Then we consider the model in which one parent gives rise to new 3 species. This model is characterized as the variety $\mathcal{R}(4, \mathbb{C}^{4\times4\times4})$ of tensors in $\mathbb{C}^{4\times4\times4}$ of border rank 4 at most. In this talk we characterize this variety, and show that it is cut out by certain homogeneous polynomials of degrees $5, 9, 16$.

[1] E.S. Allman and J.A. Rhodes, Phylogenic ideals and varieties for general Markov model, *Advances in Appl. Math.*, 40 (2008) 127-148.
[2] S. Friedland, On tensors of border rank l in $\mathbb{C}^{m\times n\times l}$, arXiv:1003.1968.

Uses and behaviour of large sample covariances matrices in computational molecular biology with small sample sizes

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Thu, 12:15, Room C

Sample covariance matrices play an important role in many algorithms used within bioinformatics and computational molecular biology - from dimensionality reduction algorithms such as Principal Components Analysis (PCA) used to visualize experimental data, to construction of gene regulatory association networks used to uncover the functional links between genes. However, the number of genes measured in modern post-genomic assays is typically very much greater than the sample size. This high-dimensional small sample-size scenario can severely limit the accuracy of sample covariance eigenvalues and eigenvectors used as estimators of their population counterparts, and gives rise to interesting phase transition phenomena in the behaviour of the eigenvalues and eigenvectors. In this talk we will give a brief introduction to some of the uses of sample covariance matrices within modern computational molecular biology and describe recent results from both the statistical physics and statistics research communities on large sample covariance matrices.

Multiarray signal processing: tensor decomposition meets compressed sensing

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We discuss how recently discovered techniques and tools from compressed sensing can be used in tensor decompositions, with a view towards modeling signals from multiple arrays of multiple sensors. We show that with appropriate bounds on coherence, one could always guarantee the existence and uniqueness of a best rank-r approximation of a tensor. In particular, we obtain a computationally feasible variant of Kruskal's uniqueness condition with coherence as a proxy for k-rank. We treat sparsest recovery and lowest-rank recovery problems in a uniform fashion by considering Schatten and nuclear norms of tensors of arbitrary order and dictionaries that comprise a continuum of uncountably many atoms.

Joint work with Pierre Comon (University of Nice)

TBA

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On the spectra of Fibonacci-like operators and modeling invasions by fungal pathogens

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Tue, 11:50, Room Galilei

The first part of talk deals with the spectra of the infinite dimensional generalized Fibonacci and Fibonacci-like operators in l^1. The operators are related to Fibonacci sequence. In the second part of the talk the Leslie matrix model for the invasion of potato late blight (oomycete Phytophthora infestans) is discussed. The spectral analysis from the first part of the talk yields a prediction of the maximum speed of the spread of invasion.

Best matrix approximation: the case of filtering with variable memory

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Thu, 11:00, Room C

This paper concerns the best linear causal operator approximation of the identity mapping subject to a specified variable finite memory constraint. The problem is motivated by Wiener-like filtering subject to causality and memory constraints [1]. The filter is interpreted as a linear operator. The causality and memory restrictions require that the approximating operator takes the form of a lower stepped matrix A. To find the best such matrix, we propose a new technique based on a block-partition into an equivalent collection of smaller blocks, $\{L_0, K_1, L_1, \ldots, K_\ell, L_\ell\}$ where each L_r is a lower triangular block and each K_r is a rectangular block and where ℓ is known [2]. The sizes of the individual blocks are defined by the memory constraints. We show that the best approximation problem for the lower stepped matrix A can be replaced by an equivalent collection of ℓ independent best approximation problems in terms of the matrices $[L_0], [K_1, L_1], \ldots, [K_\ell, L_\ell]$. The solution to each individual problem is found and a representation of the overall solution and associated error is given.

[1] A. Torokhti, P. Howlett, *Computational Methods for Modelling of Nonlinear Systems,* Elsevier, 397 p., 2007.
[2] A. Torokhti and P. Howlett, Best approximation of identity mapping: the case of variable memory, *J. Approx.*

Theory, 143, 1, pp. 111-123, 2006.

Joint work with P. Howlett (University of South Australia)

Homotopies to solve Multilinear Systems

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Tue, 11:25, Room Galilei

Many applications in mechanism design lead to structured polynomial systems. For systems where only isolated solutions matter, homotopies that exploit multihomogeneous structures are well developed since [3], see also [4]. For mechanisms that move, computing the corresponding algebraic curves with a optimal number of solution paths requires an adaption of the numerical representation for these curves. In the line of our work [1,2], we report on our new algorithms to solve multilinear systems more efficiently.

[1] Y. Guan and J. Verschelde. Parallel implementation of a subsystem-by-subsystem solver. In *The proceedings of the 22th High Performance Computing Symposium, Quebec City, 9-11 June 2008*, pages 117–123. IEEE Computer Society, 2008.
[2] Y. Guan and J. Verschelde. Sampling algebraic sets in local intrinsic coordinates. `arXiv:0912.2751`, submitted for publication.
[3] A.P. Morgan and A.J. Sommese. A homotopy for solving general polynomial systems that respects m-homogeneous structures. *Appl. Math. Comput.*, 24(2):101–113, 1987.
[4] A.J. Sommese and C.W. Wampler. *The Numerical solution of systems of polynomials arising in engineering and science*. World Scientific, 2005.

Joint work with Yun Guan (University of Illinois at Chicago)

PCCA+ and Spectral Clustering in Computational Drug Design

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Fri, 11:00, Room C

Long-term molecular simulation of the interaction of drug-sized molecules with their target proteins produces large data sets of conformational states. In order to analyze this data set in terms of metastable subsets of the dynamical process (and their time-scales), spectral clustering methods gain a lot of importance in the last years. Especially, Robust Perron Cluster Analysis (PCCA+) turned out to be the only suitable algorithm for extrapolating the time-scale of the simulation to the time-scale of biological processes.
