MANCHESTER 1824

The University of Manchester

# Bringing New Algorithms in Numerical Linear Algebra to Industry


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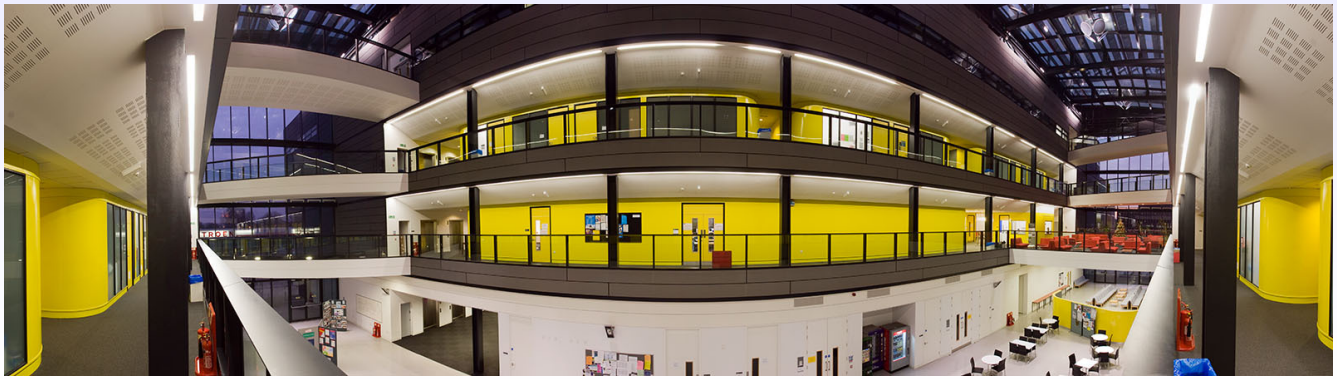
**Hartree Centre Workshop:**
**HPC as a Service for Industry**



# Questions

- Why do we need new algorithms?
- Who develops new algorithms and how?
- How are the algorithms made available to industry?

# Why Do We Need New Algorithms?

Existing algorithms

- may not exist for given problem,
- not be sufficiently **fast** or **accurate**,
- may not run well at **higher precision** (e.g., IEEE 754-2008 quadruple precision),
- may perform poorly on **multicore/manycore** systems.

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There will always be a need for new algorithms!

# Who Develops New Algorithms and How?

- An intrinsic part of research in mathematical fields.
- Research in new or improved algorithms is funded by RCUK, Royal Society, charities.
- Done by MSc and PhD students, postdocs, academics.

# How Are Algorithms Made Available to Industry?

- Open source software,
  e.g. (Scal)LAPACK, on own sites or netlib,
  Google Code, Github, MATLAB Central File Exchange.
- Through commercial program libraries,
  e.g., NAG Library.
- Consultancy for development or implementation.
- Knowledge Transfer Partnerships (TSB) for implementation.

# Nearest Correlation Matrix

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**Question from London Fund Management Company (2000)**

"Given a real symmetric matrix $A$ which is almost a correlation matrix ... what is the best approximating (in Frobenius norm?) correlation matrix? Is it unique? Can we compute it?

Typically we are working with $1400 \times 1400$ at the moment, but this will probably grow to $6500 \times 6500$."

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- Problem was unknown in numerical linear algebra community.

- There is a unique solution.

# Development

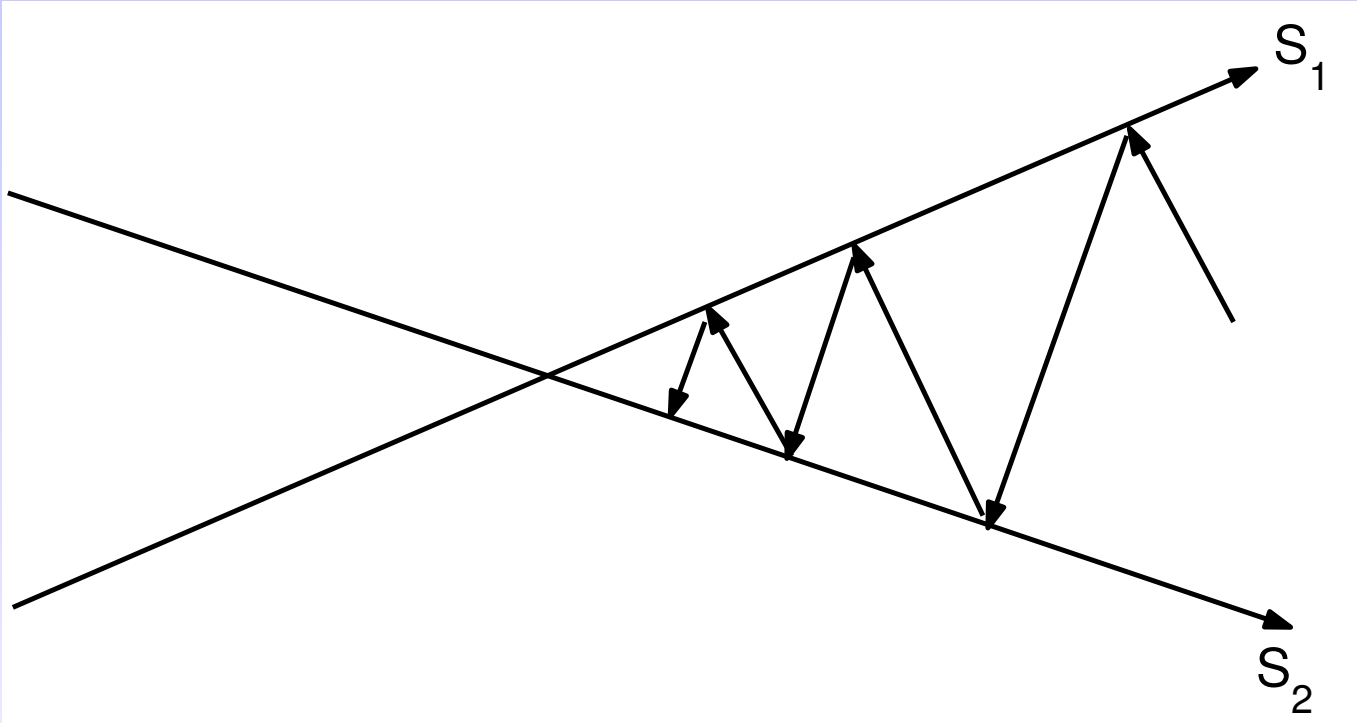
Derived theory and algorithm:

> *N. J. Higham, Computing the Nearest Correlation Matrix—A Problem from Finance, IMA J. Numer. Anal. 22, 329–343, 2002.*

Extensions in:

> *Craig Lucas, Computing Nearest Covariance and Correlation Matrices, M.Sc. Thesis, University of Manchester, 2001.*

# Alternating Projections Algorithm




- Easy to implement.
- Guaranteed convergence, at a linear rate.
- Can add further constraints/projections.

# Questions From Finance Practitioners

*"Given a real symmetric matrix A which is almost a correlation matrix what is the best approximating (in Frobenius norm?) correlation matrix?"*

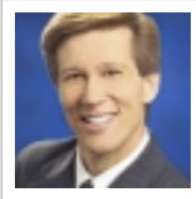
*"I am researching ways to make our company's correlation matrix positive semi-definite."*

*"Currently, I am trying to implement some real options multivariate models in a simulation framework. Therefore, I estimate correlation matrices from inconsistent data set which eventually are non psd."*

The DO Loop
Statistical programming in SAS with an emphasis on SAS/IML programs



# Computing the nearest correlation matrix



Rick Wicklin | NOVEMBER 28, 2012



Frequently someone will post a question to the SAS Support Community that says something like this:

> *I am trying to do [statistical task] and SAS issues an error and reports that my correlation matrix is not positive definite. What is going on and how can I complete [the task]?*

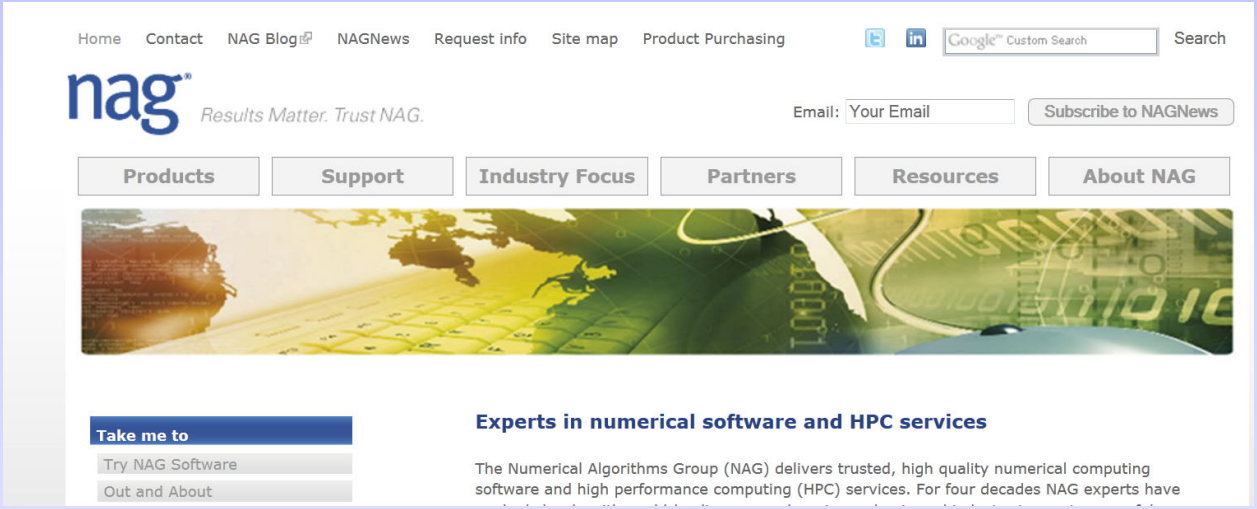
The statistical task varies, but one place where this problem occurs is in simulating multivariate normal data. I have previously written about why an estimated matrix of pairwise correlations is not always a valid correlation matrix. This article discusses what to do about it. The material in this article is taken from my forthcoming book, Simulating Data with SAS

# Newton Method

Qi & Sun (2006): **Newton method** based on theory of strongly semismooth matrix functions.

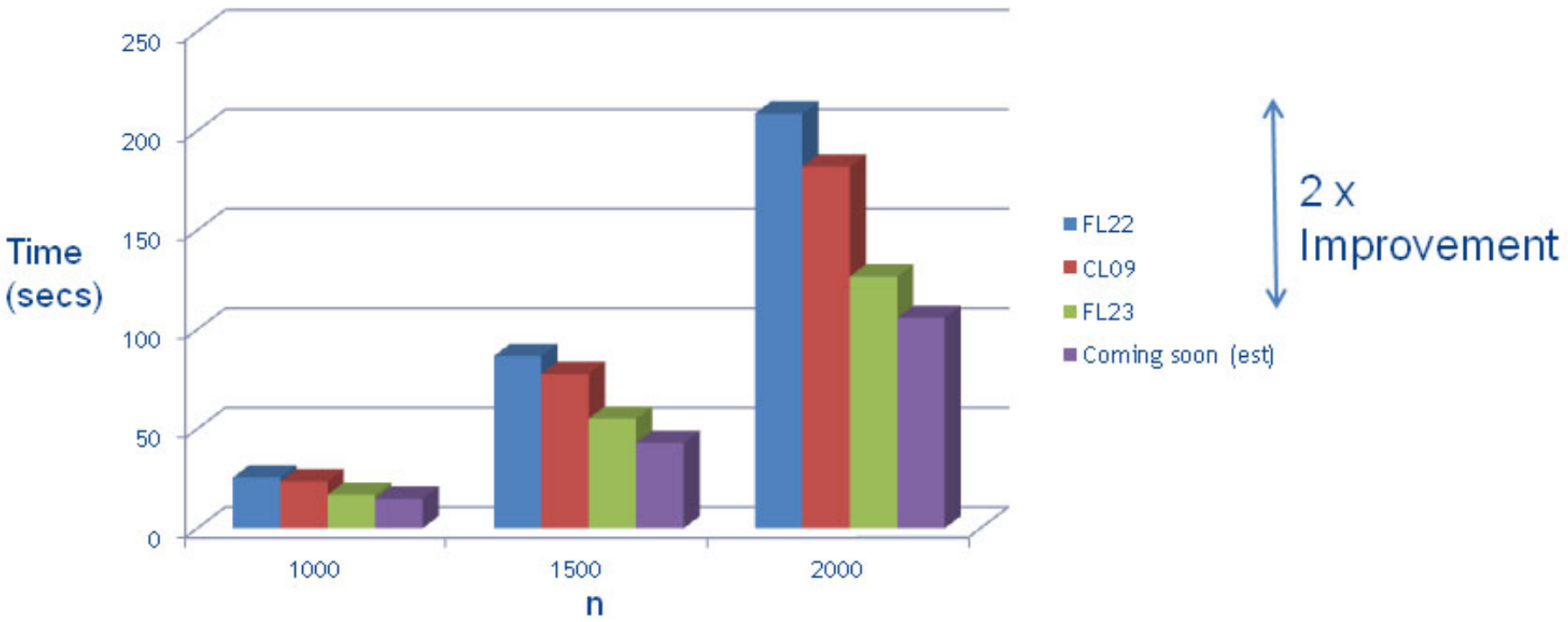
- Applies Newton to **dual** (unconstrained) of $\min \frac{1}{2}\|A - X\|_F^2$ problem.
- **Globally** and **quadratically** convergent.
- H & Borsdorf (2010) improve efficiency and reliability:
  - use minres for Newton equation,
  - Jacobi preconditioner,
  - reliability improved by line search tweaks,
  - extra scaling step to ensure unit diagonal.

# NAG Collaboration




- Collaborated on implementing Newton alg for NAG Library.
  `g02aaf` (Mark 22, 2011)
- Input from NAG customers has led to extensions of the original code.
  `g02abf`: weights, lower bounds on e'vals (Mark 23, 2012).

# Performance of NAG Codes



# Unexpected Applications

Some recent papers:

- **Applying stochastic small-scale damage functions to German winter storms** (2012)
- **Estimating variance components and predicting breeding values for eventing disciplines and grades in sport horses** (2012)
- **Characterisation of tool marks on cartridge cases by combining multiple images** (2012)
- **Experiments in reconstructing twentieth-century sea levels** (2011)

# Factor Structure

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# Factor Structure

Nearest correlation matix **with factor structure**.

- *Principal factors method* (Andersen et al., 2003) has no convergence theory and can converge to an incorrect answer.
- Algorithm based on **spectral projected gradient method** (**Borsdorf, H & Raydan, 2011).**
  - Respects the constraints, exploits their convexity, and converges to a feasible stationary point.
  - NAG routine `g02aef` (Mark 23, 2012).

# Impact of Manchester NLA Research

- **Matrix condition number estimation**:
  LAPACK, `A\b`, most libraries, HP48G calculator.
- **Quadratic eigenvalue problem solver**:
  `polyeig`, LAPACK, NAG.
- $e^A$, $\log A$, $\cos A$, $A^{1/2}$, $A^t$, and their Fréchet derivatives.

# Knowledge Transfer Partnership #1

- University of Manchester and NAG (2010–2013) funded by EPSRC, NAG and TSB.
- Academics: Nick Higham and Françoise Tisseur.
- Developing suite of NAG Library codes for matrix functions.
- Extensive set of new codes included in Mark 23 (2012).
- Improvements to existing state of the art: **faster and more accurate**.

*My work also supported by €**2M** ERC Advanced Grant.*

WEDNESDAY, 16 JANUARY 2013

# Matrix Functions in Parallel

Last year I wrote a blog post about NAG's work on parallelising the computation of the matrix square root. More recently, as part of our Matrix Functions Knowledge Transfer Partnership with the University of Manchester, we've been investigating parallel implementations of the Schur-Parlett algorithm [1].

Most algorithms for computing functions of matrices are tailored for a specific function, such as the matrix exponential or the matrix square root. The Schur-Parlett algorithm is much more general; it will work for any "well behaved" function (this general term can be given a more mathematically precise meaning). For a function such as

$$f(A) = e^A + \sin 2A - \cosh 4A,$$



PRODUCTS & SERVICES

- Numerical Libraries
- Compilers
- GPU Software & Consulting
- HPC Applications Support
- HPC Technology Consulting
- Software Engineering Services
- Training
- Partner Program
- Research & Development

# Knowledge Transfer Partnership #2

- **TSB call for KTP Proposals in Multicore and Parallel Computing** (summer 2011).
- University of Manchester and NAG (2012–2013), funded by NAG and TSB.
- Academics: Jack Dongarra, Nick Higham and David Silvester.
- Developing, tuning and integrating the **Parallel Linear Algebra for Scalable Multicore Architectures** (PLASMA) library to support NAG products.

# Other Links

- The MathWorks (MATLAB).
- Arup (Oasys).
- Others at early stage.

# Manchester Industry Workshops

- 1-day workshops with 3–4 problems presented by industry.
- Tackled by academics and PhD students in small groups.
- Lead to MSc projects, KTPs, consultancy, . . .

# From Algorithms to Software

- Try to practice **reproducible research**.
- My work made freely available in MATLAB form from my website, MATLAB Central File Exchange.
- Regular requests to provide codes for *even the simplest* algorithms.
- Many users want high quality, fully documented software. But
  - not usually funded by grants,
  - attracts little academic credit.

# Other World-Leading UK Numerical Analysis Software

Includes, e.g.,

- The HSL Mathematical Software Library (STFC RAL).
- Very large-scale nonlinear optimization (Edinburgh).
- Chebfun (Oxford).

# References I



R. Borsdorf, N. J. Higham, and M. Raydan.
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