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The University of Manchester

Rehabilitating Correlations, Avoiding Inversion, and Extracting Roots

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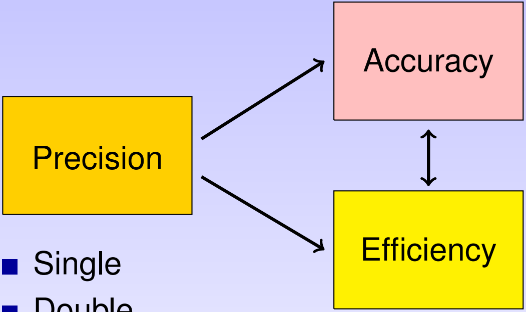
The Actuarial Profession
March 20, 2013, London



- Estimates
- Guarantees

- Single
- Double
- Quad
- Variable

- Speed
- Parallelism
- Energy efficiency

Outline

1. Rehabilitating Correlations
2. Matrix Inversion
3. Matrix Roots

Correlation Matrix

An $n \times n$ symmetric matrix A is a **correlation matrix** if

- It has ones on the diagonal.
- All its eigenvalues are nonnegative.

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Is this a correlation matrix?

$$\begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}.$$

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Is this a correlation matrix?

$$\begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}.$$

Spectrum: $-0.4142, 1.0000, 2.4142.$

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 1400×1400 at the moment, but this will probably grow to 6500×6500.”

How to Proceed

- $\times$ Make ad hoc modifications to matrix: e.g., shift negative e'vals up to zero then diagonally scale.

- $\surd$ Plug the gaps in the missing data, then compute an exact correlation matrix.

- $\surd$ Compute the **nearest correlation matrix** in the weighted Frobenius norm ($\|A\|^2 = \sum_{i,j} w_i w_j a_{ij}^2$).
  Given approx correlation matrix A find correlation matrix C to minimize $\|A - C\|$.
  - Constraint set is a closed, convex set, so unique minimizer.

Development

Derived theory and algorithm:

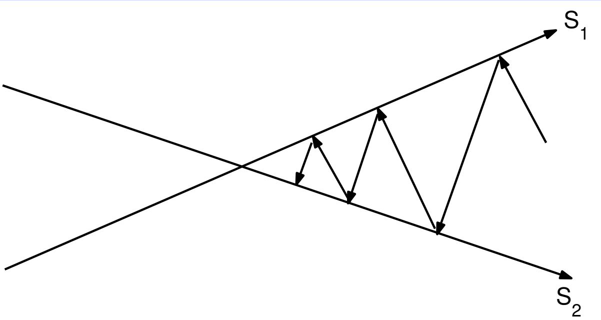
N. J. Higham, Computing the Nearest Correlation Matrix—A Problem from Finance, IMA J. Numer. Anal. 22, 329–343, 2002.

Extensions in:

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

Alternating Projections Algorithm

von Neumann (1933): for subspaces.
Dykstra (1983): corrections for closed convex sets.



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

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)

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:

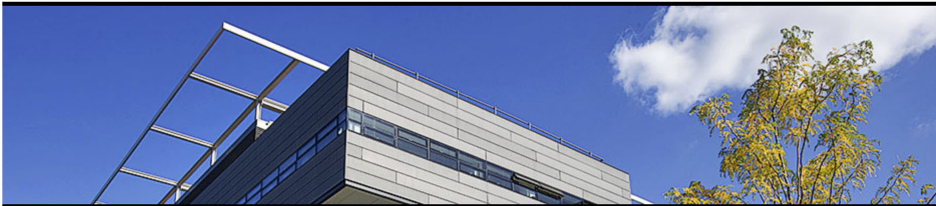
> *I am trying to do [statistical task] and SAS issues an error and reports that my correlation matrix is not positive definite. What is going on and how can I complete [the task]?*

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.



← The Lanczos Tapes

SIAM Conference on Computational Science and Engineering 2013 Preview →

The Nearest Correlation Matrix

Posted on February 13, 2013

A correlation matrix is a symmetric matrix with unit diagonal and nonnegative eigenvalues. In 2000 I was approached by a London fund management company who wanted to find the nearest correlation matrix (NCM) in the Frobenius norm to an *almost correlation matrix*: a symmetric matrix having a significant number of (small) negative eigenvalues. This problem arises when the data from which the correlations are constructed is asynchronous or incomplete, or when models are stress-tested by artificially adjusting individual correlations. Solving the NCM problem (or obtaining a true correlation matrix some other way) is important in order to avoid subsequent calculations breaking down due to negative variances or volatilities, for example.

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Original NCM Problem

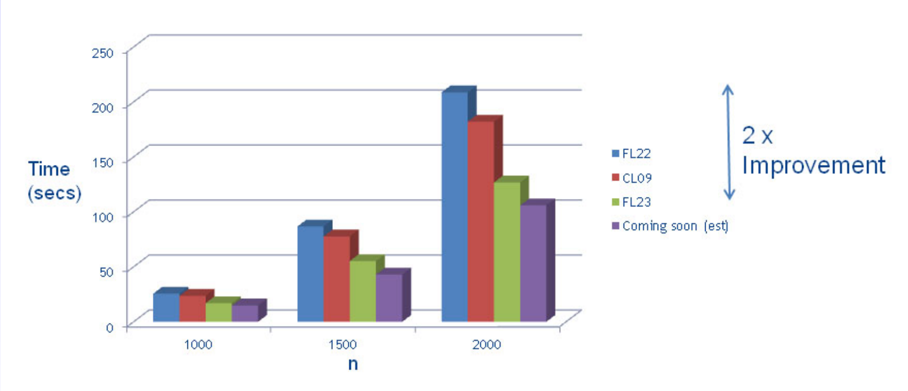
- Alternating Projections Method
  - MATLAB: Craig Lucas, near_cor.
  - MATLAB: Erlend Ringstad, validcorr.
  - MATLAB: Nick Higham, randcorr (see below).
  - R: Jens Oehlschlaegel and R Matrix package authors, nearPD.
  - SAS: Rick Wicklin, NearestCorr.

- Newton Method
  - MATLAB: Defeng Sun, various codes.
  - NAG Library (Fortran/SMP, C, NAG Toolbox for MATLAB, .NET, Java, Excel, R):
    - g02aaf (Fortran), g02aac (C), g02aa.m (MATLAB), g02aa (R),
    - g02abf (Fortran), g02abc (C), g02ab.m (MATLAB), g02ab (R): allows for weighted Frobenius norm based on two-side scaling and lower bounds on the eigenvalues.
    - g02ajf (Fortran), g02ajf.m (MATLAB) to appear in Mark 24: allows for componentwise weighted Frobenius norm and lower bounds on the eigenvalues.

Alternating Projections vs Newton

Matrix	tol	Code	Time (s)	Iters
1. Random (100)	1e-10	g02aa	0.023	4
		nearcorr	0.052	15
2. Random (500)	1e-10	g02aa	0.48	4
		nearcorr	3.01	26
3. Real-life (1399)	1e-4	g02aa	6.8	5
		nearcorr	100.6	68

Performance of NAG Codes



Factor Model (1)

$$\xi = \underbrace{X}_{n\times k}\underbrace{\eta}_{k\times 1} + \underbrace{F}_{n\times n}\underbrace{\varepsilon}_{n\times 1}, \qquad \eta_i, \varepsilon_i \in N(0,1),$$

where $\mathrm{var}(\xi_i) \equiv 1$, $F = \mathrm{diag}(f_{ii})$. Implies

$$\sum_{j=1}^{k} x_{ij}^2 \le 1, \qquad i = 1\colon n.$$

- "Multifactor normal copula model".
- Collateralized debt obligations (CDOs).
- Multivariate time series.

Factor Model (2)

Yields correlation matrix of form

$$C(X) = D + XX^T = D + \sum_{j=1}^{k} x_j x_j^T,$$

$$D = \mathrm{diag}(I - XX^T), \qquad X = [x_1, \dots, x_k].$$

$C(X)$ has k **factor correlation matrix structure**.

$$C(X) = \begin{bmatrix} 1 & y_1^T y_2 & \dots & y_1^T y_n \\ y_1^T y_2 & 1 & \dots & \vdots \\ \vdots & & \ddots & y_{n-1}^T y_n \\ y_1^T y_n & \dots & y_{n-1}^T y_n & 1 \end{bmatrix}, \quad y_i \in \mathbb{R}^k.$$

Factor Structure

Nearest correlation matrix **with factor structure**.

- *Principal factors method* (Andersen et al., 2003) has no convergence theory and can converge to an incorrect answer.

Factor Structure

Nearest correlation matrix **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, 2010**).
  - Respects the constraints, exploits their convexity, and converges to a feasible stationary point.
  - NAG routine **`g02aef`** (Mark 23, 2012).

Variations

- Specific rank or bound on correlations.
- Block structure.
- Bounds on individual correlations.
- *Other requirements?*

Outline

1 Rehabilitating Correlations

2 Matrix Inversion

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Avoiding Inversion

Fundamental Tenet of Numerical Analysis

Don't invert matrices.

Avoiding Inversion

Fundamental Tenet of Numerical Analysis

Don't invert matrices.

- $Ax = b$: use Gaussian elimination (with pivoting), not $x = A^{-1}b$.
- $x^T A^{-1} y = x^T(A^{-1}y)$.
- $(A^{-1})_{ii} = e_i^T A^{-1} e_i$.
- $\mathrm{trace}(A^{-1}) \approx m^{-1} \sum_{k=1}^{m} v_k^T A^{-1} v_k$, $v_k \sim \mathrm{uniform}\{-1, 1\}$. (Bekas et al., 2007)

How to Invert (1)

- Use a condition estimator to warn when A is nearly singular.

```
>> A = hilb(16);
>> X = inv(A);
Warning: Matrix is close to singular or
badly scaled. Results may be inaccurate.
RCOND =  9.721674e-19.
```

How to Invert (2)

- To compute **variance–covariance matrix** $(X^TX)^{-1}$ of least squares estimator, use QR factorization $X = QR$ ($(X^TX)^{-1} = R^{-1}R^{-T}$) and *do not* explicitly form X^TX.

- Quality of computed inverse $\widehat{Y} \approx A^{-1}$ measured by

$$\frac{\|\widehat{Y}A - I\|}{\|\widehat{Y}\|\,\|A\|} \quad \textit{or} \quad \frac{\|A\widehat{Y} - I\|}{\|\widehat{Y}\|\,\|A\|}$$

but not both.

Computing the Sample Variance

Sample variance of $x_1, \dots, x_n$:

$$s_n^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2, \text{ where } \bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i. \qquad (1)$$

Can compute using one-pass formula:

$$s_n^2 = \frac{1}{n-1}\left(\sum_{i=1}^{n} x_i^2 - \frac{1}{n}\left(\sum_{i=1}^{n} x_i\right)^2\right). \qquad (2)$$

Computing the Sample Variance

Sample variance of $x_1, \dots, x_n$:

$$s_n^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2, \text{ where } \bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i. \qquad (1)$$

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For $x = (10000, 10001, 10002)$ using 8-digit arithmetic,
(1) gives: 1.0, (2) gives 0.0.

(2) can even give negative results in floating point arithmetic!

Casio fx-992VB

Note:
The sample standard deviation σ_{n-1} is defined as

Nota:
La desviación estándar de muestra σ_{n-1} se define como

$$\sqrt{\frac{\Sigma x^2 - \frac{(\Sigma x)^2}{n}}{n-1}}$$

the population standard deviation σ_n is defined as

la desviación estándar de población σ_n se define como

$$\sqrt{\frac{\Sigma x^2 - \frac{(\Sigma x)^2}{n}}{n}}$$

Spreadsheets in the Cloud

Standard deviation of $x = [n,\ n+1,\ n+2]^T$.

n	Exact	Google Sheet
10^7	1	1
10^8	1	0

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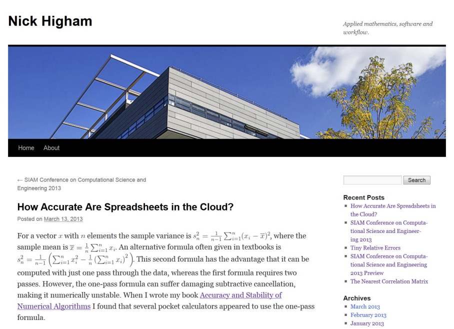
Nick Higham

Applied mathematics, software and workflow.

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How Accurate Are Spreadsheets in the Cloud?

Posted on March 13, 2013

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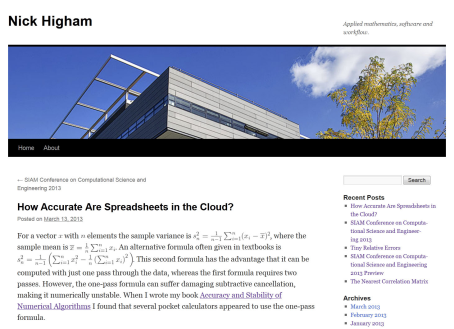

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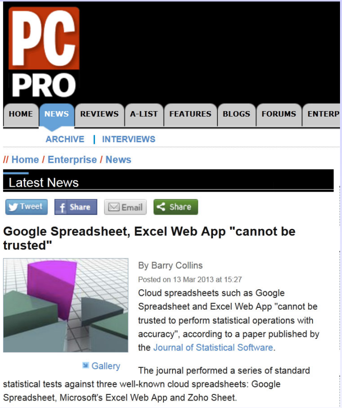

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Google Spreadsheet, Excel Web App "cannot be trusted"

By Barry Collins

Posted on 13 Mar 2013 at 15:27

Cloud spreadsheets such as Google Spreadsheet and Excel Web App "cannot be trusted to perform statistical operations with accuracy", according to a paper published by the Journal of Statistical Software.

Gallery

The journal performed a series of standard statistical tests against three well-known cloud spreadsheets: Google Spreadsheet, Microsoft's Excel Web App and Zoho Sheet.

McCullough & Yalta (2013)

Outline

1 Rehabilitating Correlations

2 Matrix Inversion

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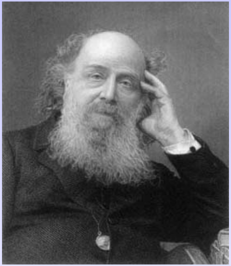
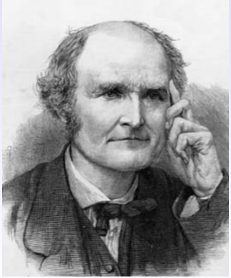
Cayley and Sylvester



- Term **"matrix"** coined in 1850 by James Joseph Sylvester, FRS (1814–1897).

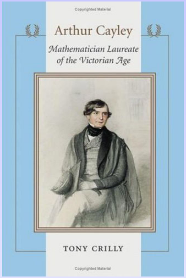


- **Matrix algebra** developed by Arthur Cayley, FRS (1821–1895).
  Memoir on the Theory of Matrices (1858).

Cayley and Sylvester on Matrix Functions

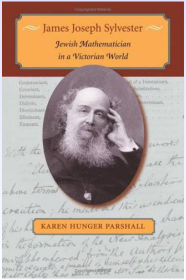
- Cayley considered matrix square roots in his 1858 memoir.

  Tony Crilly, *Arthur Cayley: Mathematician Laureate of the Victorian Age*, 2006.



- Sylvester (1883) gave first definition of $f(A)$ for general f.

  Karen Hunger Parshall, *James Joseph Sylvester. Jewish Mathematician in a Victorian World*, 2006.



Matrix Roots in Markov Models

- Let vectors v_{2011}, v_{2010} represent risks, credit ratings or stock prices in 2011 and 2010.
- Assume a Markov model $v_{2011} = P v_{2010}$, where P is a transition probability matrix.
- $P^{1/2}$ enables predictions to be made at 6-monthly intervals.

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- $P^{1/2}$ enables predictions to be made at 6-monthly intervals.

$P^{1/2}$ is matrix X such that $X^2 = P$. What are $P^{2/3}$, $P^{0.9}$?

$$\boxed{P^s = \exp(s \log P)}\,.$$

Problem: $\log P$, $P^{1/k}$ may have wrong sign patterns $\Rightarrow$ “regularize”.

Chronic Disease Example

- Estimated 6-month transition matrix.
- Four AIDS-free states and 1 AIDS state.
- 2077 observations (Charitos et al., 2008).

$$P = \begin{bmatrix} 0.8149 & 0.0738 & 0.0586 & 0.0407 & 0.0120 \\ 0.5622 & 0.1752 & 0.1314 & 0.1169 & 0.0143 \\ 0.3606 & 0.1860 & 0.1521 & 0.2198 & 0.0815 \\ 0.1676 & 0.0636 & 0.1444 & 0.4652 & 0.1592 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Want to estimate the **1-month transition matrix**.

$$\Lambda(P) = \{1, 0.9644, 0.4980, 0.1493, -0.0043\}.$$

- **H & Lin** (2011).
- **Lin** (2011, for survey of regularization methods.

MATLAB: Arbitrary Powers

```
>> A = [1 1e-8; 0 1]
A =
   1.0000e+000   1.0000e-008
             0   1.0000e+000

>> A^0.1
ans =
     1     0
     0     1

>> expm(0.1*logm(A))
ans =
   1.0000e+000   1.0000e-009
             0   1.0000e+000
```

MATLAB Arbitrary Power

- New **Schur algorithm** (**H & Lin, 2011, 2013**) reliably computes A^p for any real p.
- New backward-error based **inverse scaling and squaring alg** for matrix logarithm (**Al-Mohy, H & Relton, 2012**)—faster and more accurate.
- Alternative Newton-based algorithms available for $A^{1/q}$ with q an integer, e.g., for

$$X_{k+1} = \frac{1}{q}\big[(q+1)X_k - X_k^{q+1}A\big], \qquad X_0 = A,$$

$X_k \to A^{-1/q}$.

Knowledge Transfer Partnership

- University of Manchester and NAG (2010–2013) funded by EPSRC, NAG and TSB.
- Developing suite of NAG Library codes for matrix functions.
- Extensive set of new codes included in Mark 23 (2012), Mark 24 (2013).
- Improvements to existing state of the art: **faster and more accurate**.

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

WEDNESDAY, 11 JULY 2012

The Matrix Square Root, Blocking and Parallelism

NAG recently embarked on a 'Knowledge Transfer Partnership' with the University of Manchester to introduce matrix function capabilities into the NAG Library. As part of this collaboration, Nick Higham (University of Manchester), Rui Ralha (University of Minho, Portugal) and I have been investigating how blocking can be used to speed up the computation of matrix square roots.

There is plenty of interesting mathematical theory concerning matrix square roots, but for now we'll just use the definition that a matrix X is a square root of A if $X^2=A$. Matrix roots have applications in finance and population modelling, where transition matrices are used to describe the evolution of a system from over a certain time interval, t. The square root of a transition matrix can be used to describe the evolution for the interval $t/2$. The matrix square root also forms a key part of the algorithms used to compute other matrix functions.

To find a square root of a matrix, we start by computing a Schur decomposition. The square root U of the resulting upper triangular matrix T can then be found via a simple recurrence over the elements U_{ij} and T_{ij}:

$$U_{ii} = \sqrt{T_{ii}},$$

$$U_{ii}U_{ij} + U_{ij}U_{jj} = T_{ij} - \sum_{k=i+1}^{j-1} U_{ik}U_{kj}.$$

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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

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

Final Remarks

- Fast moving developments in numerical linear algebra algorithms.
- Numerical reliability is essential.
- Partnership with NAG enables rapid inclusion of our algorithms in the NAG Library.

Keen to hear about your matrix problems.

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