Functions of Matrices: From Cayley and Sylvester to MATLAB

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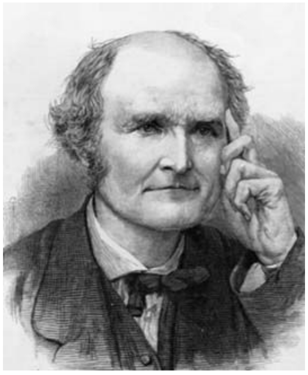

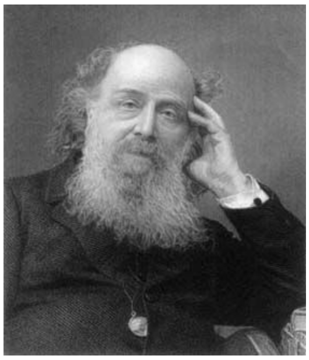

Figure 1: Arthur Cayley (1821–1895), FRS and James Joseph Sylvester (1814–1897), FRS.

Matrix theory was developed by Cayley [3], Sylvester [9], and others starting in the 1850s. In Cayley's first paper on the subject, *A Memoir on the Theory of Matrices* [2, 1858] he investigated one of the most intriguing matrix functions: the square root. An early example of the effective practical use of matrix functions is in the book *Elementary Matrices and Some Applications to Dynamics and Differential Equations* [4, 1938] by aerospace engineers Frazer, Duncan, and Collar, which emphasizes the important role of the matrix exponential in solving differential equations. This book was "the first to employ matrices as an engineering tool" [1, 1987].

Applications of functions of matrices are ubiquitous, some examples being Monte-Carlo simulations in theoretical particle physics, Procrustes problems in factor and shape analysis, dynamical systems, Markov models, and algebraic Riccati equations in control theory. Spurred by the applications, interest in the theory and computation of matrix functions is growing. Numerical software packages such as Maple, Mathematica and MATLAB all have the ability to evaluate a variety of different matrix functions.

The matrix exponential is the most-studied matrix function (apart from the inverse, which is so special that it is treated separately). Some formulas for it are given in Figure 2. Many methods have been proposed for computing e^A, but most of them are impractical, because of their computational cost or their unstable behaviour in finite precision arithmetic. A classic paper *Nineteen Dubious Ways to Compute the Exponential of a Matrix* [8, 2003] surveys the least dubious of the available e^A methods.

So what is currently the best method for computing e^A? For general $n \times n$ matrices A,

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Figure 2: Some formulas for e^A for an $n \times n$ matrix A.

$I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \cdots$	$\lim_{s\to\infty} (I + A/s)^s$	$(e^{A/2^s})^{2^s}, \quad s \in \mathbb{Z}$
Cauchy $\frac{1}{2\pi i}\int_\Gamma e^z(zI - A)^{-1}\,dz$	Jordan $Z\mathrm{diag}(e^{J_k})Z^{-1}$	Sylvester $\sum_{i=1}^{n} f[\lambda_1, \ldots, \lambda_i] \prod_{j=1}^{i-1}(A - \lambda_j I)$

the answer is the scaling and squaring method. It uses the relation $e^A = (e^{A/2^s})^{2^s}$, with s an integer chosen large enough that A/s has elements of order 1, which ensures that its exponential is easily approximated. An approximation $e^{A/2^s} \approx r_m(A/2^s)$ is employed, where r_m is a special form of rational approximation known as a Padé approximant, with m the degree of the numerator and denominator polynomials.

While writing my forthcoming book *Functions of Matrices: Theory and Computation* [7, 2008] I realized that the standard implementation of the scaling and squaring method was not of optimal efficiency. By optimizing the parameters s and m, via error analysis and some high precision computation, I was able to derive a more efficient scaling and squaring algorithm [6, 2005], which has subsequently been adopted in MATLAB and other packages. The new algorithm turns out to be both *more efficient and more accurate* than the old—an example of the very rare phenomenon in numerical analysis that faster implies more accurate (or vice versa). More commonly, faster implies *less* accurate, and a considerable body of work has built up exploring the tradeoff between the twin aims of speed and accuracy; see, for example, [5, 2002].

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[The] availability of `expm(A)` *in early versions of MATLAB quite possibly contributed to the system's technical and commercial success.*

— CLEVE B. MOLER and CHARLES F. VAN LOAN [8]