Numerical Linear Algebra Before the Last Paradigm Shift*

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> October 5, 2005 Berkeley

*Thomas Kuhn, *The Structure of Scientific Revolutions*, The University of Chicago Press, Chicago, 1970.

"The state of numerical mathematics stayed pretty much the same as Gauss left it until World War II."

- Herman Goldstine, 1972

2



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— Herman Goldstine, 1972

3

Size of Numerical ODE Literature

Bibliographies of Hairer, Petzold, Wanner, Werner, et al.



Frobenius norm matrices adjustment of observations survey adjustments Gaussian elimination geodesy matrix factoring

Frobenius norm

 $\|A\|_F$

1911 Frobenius



Ferdinand Frobenius 1849 – 1917

Sitzungsberichte der Koniglich Prußischen Akademie der Wissenschaften zu Berlin, 241 – 248 (1911) Let r_1, \ldots, r_n be the characteristic roots of a matrix of the form

$$R = \sum r_{i,j} x_i y_j$$

I define the Spur

$$\chi(R) = \sum r_{i,i} = \sum r_i$$

and the Spannung

$$\vartheta(R) = \chi(R \, \bar{R}') = \|R\|_F^2$$

1911 Frobenius



Ferdinand Frobenius 1849 – 1917

Sitzungsberichte der Koniglich Prußischen Akademie der Wissenschaften zu Berlin, 241 – 248, 654–665 (1911) The Spannung

$$\vartheta(R) = \|R\|_F^2$$

obeys the Schwartz inequality

$$\sqrt{artheta(P\!-\!Q)} \leq \sqrt{artheta(P)} \!+\! \sqrt{artheta(Q)}$$

and also

 $\vartheta(PQ) < \vartheta(P) \vartheta(Q)$

1929 von Neumann's Hilbert spaces



John von Neumann 1903 – 1957

Allgemeine Eigenwerttheorie Hermitescher Funktionaloperatoren, *Mathematische Annalen*, 102:49–131 (1929) Von Neumann was mostly interested in unbounded operators.

1932 Banach's Banach spaces



The norme |U| of a linear operator U(x) is the smallest number M satisfying

 $|U(x)| \leq M \, |x|$

Stefan Banach 1892 – 1945

Théorie des Opérations linéaires, Warsaw (1932)

for all x

1934 Wedderburn



His extensive bibliography is the source for references to Peano, Schur and the earlier Frobenius paper.

He chose the absolute value

 $|\cdot| = ||\cdot||_F$

Joseph Wedderburn 1892 – 1945

Lectures on Matrices, American Mathematical Society, New York (1934)

1937 von Neumann, again



John von Neumann 1903 – 1957

Some Matrix-Inequalities and Metrization of Matric-Space, *Tomsk Univ. Rev.* (1937)

Let φ be a symmetric gauge function.

For a matrix X, form XX^* and its proper values $\omega_1, \ldots, \omega_n$, and define

$$|X|_{\varphi} = \varphi(\omega_1^{1/2}, \dots, \omega_n^{1/2})$$

1943 Hotelling



Harold Hotelling 1895 – 1973

Some New Methods in Matrix Calculation, *The Annals of Mathematical Statistics*, 14:1–34 (1943) "The norm of the matrix \boldsymbol{A}

$$N(A) = \|A\|_F$$

is what Wedderburn defines as the absolute value."

1946 MacDuffee



"Notation for matrices is far from agreed."

Cyrus MacDuffee 1895 – 1961

The Theory of Matrices, New York (1946)

1947 von Neumann and Goldstine



norm

$$N(A) = \|A\|_F$$

upper bound

$$|A| = \max_{|x|=1} |Ax| = ||A||_2$$

lower bound

$$|A|_\ell = \min_{|x|=1} |Ax|$$

von Neumann 1903 – 1957 and Goldstine 1913 – 2004

Numerical Inverting of Matrices of High Order, *Bulletin of the American Mathematical Society*, 53:1021–1099 (1947)

1948 Turing



norm

 $N(A) = \|A\|_F$

maximum expansion

$$B(A) = \|A\|_2$$

maximum coefficient

$$M(A) = \max_{i,j} |a_{i,j}|$$

Alan Turing 1912 – 1954

Rounding-off Errors in Matrix Processes, The Quarterly Journal of Mechanics and Applied Mathematics, 1:287–308 (1948)

1953 Householder



norm

 $N(A) = \|A\|_F$

maximum

 $M(A) = \|A\|_2$

bound

Alston Householder 1904 – 1993

Principles of Numerical Analysis, McGraw-Hill, New York (1953)

$$b(A) = \max_{i,j} |a_{i,j}|$$

1956, 1959 Bodewig



norm

$$N(A) = \|A\|_F$$

maximum expansion or bound

 $|A| = ||A||_2$

maximum coefficient

$$m(A) = \max_{i,j} |a_{i,j}|$$

E(wald?) Bodewig

Matrix Calculus, North-Holland, Amsterdam (1956, 1959)

1963 Wilkinson



James Wilkinson 1919 – 1986

Rounding Errors in Algebraic Processes, Prentice Hall, Amsterdam (1963)

Euclidean or Schur norm

 $\|A\|_E = \|A\|_F$

Question: Who introduced || • || notation?

Possible Answer:

Maybe Bauer or Stoer in the 1960's.

1964 Householder, again



Euclidean length of a matrix

 $au^{1/2}(A^H A) = \|A\|_F$

Alston Householder 1904 – 1993

The Theory of Matrices in Numerical Analysis, Blaisdell, New York (1964)

1970 Rutishauser



the so-called Schur norm

 $||A||_2 = ||A||_F$

Heinz Rutishauser 1918 – 1970

Lectures on Numerical Mathematics, Birkhäuser, Boston (1990), posthumous

1973 Stewart



the Frobenius norm

 $\|A\|_F$

Pete Stewart

Introduction to Matrix Computations, Academic Press, New York (1973) Historical Pitfalls, Illustrated by $\|\cdot\|_F$

1. Anachronism:

"Historical description means understanding things as people understood them <u>then</u>."

2. Chronology:

"Chronology is not the same thing as history. History is processed chronological data."

Kenneth May (1915 - 1977)

"Historiography: A Perspective for Computer Scientists," in *A History of Computing in the 20th Century*, edited by Metropolis, Howlett, Rota, 1980.

$\|\cdot\|_F$ Chronology

1887	Peano	used value of $\ \cdot\ _F$
1909	Schur	used value of $\ \cdot\ _{F}$
1911	Frobenius	Spannung $\vartheta(\cdot) = \ \cdot\ _F^2$ with sum and product rules
1929	von Neumann	Hilbert spaces
1932	Banach	Banach space operator ·
1934	Wedderburn	absolute value $ \cdot = \cdot _F$
1937	von Neumann	matrix space metrization $ \cdot _{arphi}$
1943	Hotelling	norm $N(\cdot) = \ \cdot\ _F$
1946	MacDuffee	"notation is far from agreed"

$\|\cdot\|_F$ Chronology, continued

1947	von Neumann and Goldstine	norm $N(\cdot) = \ \cdot\ _F$ and upper bound $ \cdot = \ \cdot\ _2$
1948	Turing	$N(\cdot), B(\cdot), M(\cdot)$
1953	Householder	$N(\cdot), M(\cdot), b(\cdot)$
1954	Givens	$N(\cdot)$
1959	Bodewig	$N(\cdot), \cdot , m(\cdot)$
1963	Wilkinson	Euclidean, Schur norm $\ \cdot\ _E$
1964	Householder	Euclidean length $ au^{1/2}(\cdot^H \cdot)$
1970	Rutishauser	Schur norm $\ \cdot\ _2 = \ \cdot\ _F$
1973	Stewart	Frobenius norm $\ \cdot\ _F$

$\|\cdot\|_F$ History

- 1. Value $\|\cdot\|_F$ was used by early matrix researchers, and by Frobenius especially. The real story is how it came to be named after Frobenius.
- 2. Hotelling deliberately ignored Wedderburn and chose norm $N(\cdot)$; perhaps to avoid Germanisms?
- 3. Von Neumann and Goldstine knew the proper notation (operator norms existed in functional analysis) but they deferred to Hotelling. Their choice led others to adopt $N(\cdot)$ for many years.
- 4. Attempt to use *Schur norm* $\|\cdot\|_E$ was supplanted by *Frobenius norm* $\|\cdot\|_F$ in the 1970's.

- Influence of the Inversion Paper can be seen in the number of people who adopted N(·) because von Neumann did.
- Why did von Neumann defer to Hotelling in using this eccentric notation?

"... as simple as possible, but not simpler." 27

Matrices

1759 Lagrange



Joseph-Louis Lagrange 1736 – 1813 Quadratic form of x_1 , x_2 , x_3

$$\begin{split} f &= 5x_1^2 + 20x_1x_2 + 19x_2^2 \\ &+ 10x_1x_3 + 22x_2x_3 + 6x_3^2 \end{split}$$

Substitute

$$x_1 = \frac{u_1}{2} - \frac{1}{2} \left(\frac{20}{5} x_2 + \frac{10}{5} x_3 \right)$$

to get

$$f = 5\frac{u_1^2}{1} - x_2^2 + 2x_2x_3 + x_3^2$$

1759 Lagrange



Joseph-Louis Lagrange 1736 – 1813 Quadratic form is

$$f = x^t A x$$

where $A = U^t DU$. Linear substitution u = Ux gives

 $f = u^t D u$

Lagrange used the weighted sum of squares to identify local extrema.

1801 Gauss



J. C. F. Gauss 1777 – 1855

Disquisitiones arithmeticae, Leipzig, art. no. 266 (1801)

Studied quadratic forms of 2 and 3 variables.

"It is sufficient to draw this broad field to the attention of geometers." *There is ample material for the exercise of their genius.*"

* geometer = mathematician

1852 – 1882 Matrix Algebra



SylvesterCayleyEisensteinLaguerreFrobenius1814 - 18971821 - 18951823 - 18521834 - 18861849 - 1917

Invented by several people more or less independently to represent the linear substitutions that were used to study quadratic and bilinear forms.

T. Hawkins, "Another look at Cayley and the theory of matrices," *Archives Internationales d'Histoire des Sciences*, 27(100):82–112 (1977).

1857, 1907 Not Cholesky's Factorization 32



Restated Jacobi's result "known to Lagrange and Gauss" using "matrix calculus of Frobenius."

A quadratic form

$$S = \sum_{i,k=1}^n \alpha_{i,k} x_i x_k$$

Toeplitz 1881 – 1940 Jacobi 1804 – 1851

Toeplitz, "Die Jacobische Transformation der quadratischen Formen von unendlichvielen Veränderlichen," *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen*, 101–109 (1907). could be expressed as $S^{-1} = U^\prime U$ or $S = U^{-1}U^{\prime-1}$

1857, 1907 Not Cholesky's Factorization 33



Toeplitz 1881 – 1940 Jacobi 1804 – 1851

Toeplitz, "Die Jacobische Transformation der quadratischen Formen von unendlichvielen Veränderlichen," *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen*, 101–109 (1907). Restated Jacobi's result "known to Lagrange and Gauss" using "matrix calculus of Frobenius."



Linear Algebra Timeline



Computational

"The state of numerical mathematics stayed pretty much the same as Gauss left it until World War II."

- Herman Goldstine, 1972



Technology of XIX and Early XX Century

Adjustment of Observations
Errors of Observation







Adrien-Marie Legendre 1752 – 1833 Johann Carl Friedrich Gauss 1777 – 1855 Pierre-Simon Laplace 1749 – 1827 Adjustment of Observations

Statistical theory showed

optimal estimation problems $\begin{cases} minimizing quadratic quadratic functions \end{cases}$

Legendre: la méthode des moindres quarrés

Nouvelle méthodes pour la détermination des orbites des comètes, Paris (1805)

Gauss: developed probabilistic justification Theoria Motus Corporum Coelestium in Sectionibus Conicus Solem Ambientium, Hamburg (1809)

Observations Needing Adjustment

case 1. Over-determined observations

$$\min_{x} \|b - Ax\|_2$$

solved by $A^tAx = c$ with $c = A^tb$

case 2. <u>Under</u>-determined observations

$$\min_{Ax = b} \|x\|_2$$

solved by $AA^tu = b$ where $x = A^tu$

Both resulted in *normal equations*

Observations Needing Adjustment

case 1. Over-determined observations

$$\min_{x} \|b - Ax\|_2$$

found in Astronomy

case 2. Under-determined observations

$$\min_{Ax = b} \|x\|_2$$

found in Geodesy

Both resulted in normal equations

Aside: Astronomical Calculations

Trophy Calculations:

- Fitting orbit of Ceres

 (over-determined obser-vations) Gauss
- 2. Triangulating distance to Cygni Bessel

3. . . .

Nievergelt, "A tutorial history of least squares with applications to astronomy and geodesy," in *Numerical Analysis: Historical Developments in the 20th Century*, edited by Brezinski and Wuytack, North Holland, 2001.





Aside: Astronomical Calculations

Trophy Calculations:

Fitting orbit of Ceres

 (over-determi ser Little Used in Little Used in the XIX Century

 The XIX Century distance to Cygni — Bessel

3. . .

Nievergelt, "A tutorial history of least squares with applications to astronomy and geodesy," in *Numerical Analysis: Historical Developments in the 20th Century*, edited by Brezinski and Wuytack, North Holland, 2001. **Recurring Work:**

- 1. Ephemerides
- Nautical
 Almanacs
- 3. Reducingobservationsto celestialcoordinates

Grier, *When Computers Were Human*, Princeton, 2005.

Observations Needing Adjustment

case 1. Over-determined observations Little Used in Little Vsed in the XIX Century $\min_{x} \|b - Ax\|_2$ Solved by $A^tAx = c$ with $c = A^tb$

case 2. <u>Under</u>-determined observations

$$\min_{Ax = b} \|x\|_2$$

solved by $AA^tu = b$ where $x = A^tu$

Both resulted in *normal equations*

Technology of XIX and Early XX Century

44

Survey Adjustments

















Angle Adjustment Problem Addressed by

case 2. <u>Under</u>-determined observations

$\min_{Ax = b} \|x\|_2$

53

solved by $AA^tu = b$ where $x = A^tu$

- Unknowns x were adjustments to all (or most of) the measured angles
- Constraints Ax = b called *conditions*
 - 1. angle conditions (2 kinds)
 - 2. side conditions

1. "Angle Equation" Conditions



2. "Side Equation" Condition (Sine Laws)



 $\sin(\overline{OAB} + \epsilon_1)$ $\times \sin(\overline{OBC} + \epsilon_2)$ $\times \sin(\overline{OCA} + \epsilon_3)$ $\sin(\overline{OBA} + \epsilon_4)$ $\times \sin(\overline{OCB} + \epsilon_5)$ $\times \sin(\overline{OAC} + \epsilon_6)$ OAB = measured angle $\epsilon_1 = adjustment$

55

2. Side Equation Condition



 $\ln \sin \overline{OAB} + \epsilon_1 \cot \overline{OAB} + \ln \sin \overline{OBC} + \epsilon_2 \cot \overline{OBC} + \ln \sin \overline{OCA} + \epsilon_3 \cot \overline{OCA} = *$

 $\ln \sin \overline{OBA} + \epsilon_4 \cot \overline{OBA} + \\ \ln \sin \overline{OCB} + \epsilon_5 \cot \overline{OCB} + \\ \ln \sin \overline{OAC} + \epsilon_6 \cot \overline{OAC}$

* Equality is only to first order in the angle corrections.

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in einem Dreiecksnetze.

Gaussian Elimination

1823, 1828 Gauss



J. C. F. Gauss 1777 – 1855

Theoria combinationes observationum erroribus minimis obnoxiae: Pars prior and Supplementum, Göttingen, 1823 and 1828. case 2. <u>Under</u>-determined observations

 $\min_{Ax = b} \|x\|_2$

solved by $AA^tu = b$ where $x = A^tu$.

1823, 1828 Gauss



J. C. F. Gauss 1777 – 1855

Theoria combinationes observationum erroribus minimis obnoxiae: Pars prior and Supplementum, Göttingen, 1823 and 1828. Normal equations:

Stewart, "Gauss, Statistics, and Gaussian Elimination," in *Computing Science and Statistics: Computationally Intensive Statistical Methods*, edited by Sall and Lehman, Fairfax Station, 1994

1823, 1828 Gaussian Elimination



J. C. F. Gauss 1777 – 1855

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$$egin{aligned} [bb,1]&=[bb]-rac{[ab]^2}{[aa]}\ [bc,1]&=[bc]-rac{[ab][ac]}{[aa]}\ etc.\ [cc,2]&=[cc]-rac{[ac]^2}{[aa]}-rac{[bc,1]^2}{[bb,1]}\ [cd,2]&=[cd]-rac{[ac][ad]}{[aa]}-\dots\ etc.\ etc.\ \end{aligned}$$



Normal equations:

Dana P. Bartlett

General Principles of the Method of Least Squares with Applications, third edition, Boston, 1915.

1915 Dana Bartlett



1st reduced normal equations:

 $[bb,1]=[bb]-rac{[ab][ab]}{[aa]}$

 $[bc,1] = [bc] - rac{[ab][ac]}{[ac]}$

where

Dana P. Bartlett

General Principles of the Method of Least Squares with Applications, third edition, Boston, 1915.

Linear Algebra Timeline



- Gauss invented a notation to organize elimination that was used for 100 years.
- During most of its existence, Gaussian elimination was used to solve normal equations.

 Von Neumann and Goldstine studied the rounding errors of

$$A^{-1} = A^t (AA^t)^{-1}$$

This essentially was the main use for Gaussian elimination for 150 years.

• Their results stimulated a search for new algorithms (QR, SVD) that eventually replaced the normal equations in 1965.

Big Science, XIX Century Edition

Geodesy

Surveying Continents



Southeast Alaska 1929

- 1. Surveyors
 - gather baseline and angle data
- 2. Computers (original usage)(a) form underdetermined angle adjustment eqns
 - (b) form and solve normal equations
- 3. Cartographers
 - use adjusted triangulations to draw maps

Surveying Continents



Old C&GS Office with third floor computing rooms Washington

1. Surveyors

- gather baseline and angle data
- 2. Computers (original usage)
 - (a) form underdetermined angle adjustment eqns
 - (b) form and solve normal equations
- 3. Cartographers
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U. S. Coast and Geodetic Survey (C&GS) 70

Oldest American Scientific Agency



Benjamin Peirce 3rd Superintendent (served 1867 – 74)



Charles Schott Assistant in charge of the Computing Division (served 1848 – 99)



Myrrick Doolittle 1830 – 1911 Computer (served 1873 – ??)

The Numerical Linear Algebra



Doolittle's Example

Doolittle, "Method employed in the solution of normal equations and the adjustment of a triangularization," in *Report of the Superintendent of the U. S. Coast and Geodetic Survey (showing the progress of the work during the fiscal year ending with June, 1878),* Government Printing Office, 1881. Selection of Conditions:

- 2 unknowns for each station off the baseline
- What is the rank of the matrix of conditions?
- *n* as big as 41 or 52!
- Solution of Normal Equations:
 - 3-digit hand arithmetic!
 - Crelle's 3-digit tables
 - were used for \times and \div

circa 1875 *Ill-Conditioned*



Peter Guthrie Tait 1831 – 1901

"Cosmical Astronomy," Good Words, 19–23 (1875).

"The danger of selecting such condition equations that the solution will be somewhat unstable is difficult to avoid."

Wright and Hayford, "The Adjustment of Observations by the Method of Least Squares with Applications to Geodetic Work," Van Nostrand, New York, 1906.

"The difficulty of determining the sun's distance lies in the measurement of the angles, and in what is called the *illconditioned* form of triangle."

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Pertinent to the Inversion Paper

- Von Neumann and Goldstine's error bounds were considered unrealistically large when tested on small problems solved by *post*-WWII technology (10-digit mechanical calculators) ...
- ... but the concerns about Gaussian elimination were based on experience from *pre*-WWII calculations (3-digit paper and pencil) for which the pessimistic bounds probably were realistic.

Another Story: Regression and Correlation 74



Karl Pearson 1857 – 1936 Statistics replaced geodesy as the main use for linear algebra after WWI

- continental surveys were complete
- data analysis was important for agriculture and government

Karl Pearson led in the computational developments and published *Tracts for Computers*, essentially the first numerical analysis textbooks

Grier, *When Computers Were Human*, Princeton, 2005.

Question: actuaries also used computing; did they use linear algebra?

Linear Algebra Timeline



 Von Neumann and Goldstine deferred to Hotelling in matters of numerical linear algebra because, as a leader of the American statistical community, he represented a profession with considerable computing expertise.

Numerical Linear Algebra Algorithms Correspond to Matrix Factorizations

A = LU

Who invented the paradigm?

Stewart, "The Decompositional Approach to Matrix Computation," Computing in Science and Engineering, 2(1):50–59 (2000).

1823, 1828 Gaussian Elimination



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Before matrices; no paradigm.

1924 Cholesky Factorization



 $\min_{Ax = b} \|x\|_2$

 $AA^t u = b$ where $x = A^t u$. Cholesky's insight was that many matrices have the same normal equations. He chose one that was easy to solve.

 $LL^t = AA^t$

Andre-Louis Cholesky 1875 – 1918

Benoit, "Note sur une méthode ...," *Bulletin géodésique*, 67–77 (1924).

Real breakthrough was the inner product formulas for *L*. No matrices in the paper, hence no paradigm.

1907 "Toeplitz" Factorization?



Toeplitz 1881 – 1940 Jacobi 1804 – 1851

Toeplitz, "Die Jacobische Transformation der quadratischen Formen von unendlichvielen Veränderlichen," *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen*, 101–109 (1907). Restated Jacobi's result "known to Lagrange and Gauss" using "matrix calculus of Frobenius."

A quadratic form

$$S = \sum_{i,k=1}^n \alpha_{i,k} x_i x_k$$

could be factored as

$$S^{-1} = U'U$$

or
$$S=U^{-1}U^{\prime-1}$$

but U is given by determinants

80

1938 "Banachiewicz" Factorization?



Tadeusz Banachiewicz 1882 – 1954

Astronomer and polymath who calculated first orbit of Pluto.

Expressed calculations using "Cracovian" matrix multiplication. Had a Cholesky-like method.

Inspired Jensen to do the same for Cayleyan matrix multiplication.

Many papers in Academy of Science of Poland were widely cited.

1938 Dwyer Square-Root Factorization? 82

Paul Dwyer

Dwyer, "A matrix presentation of least squares and correlation theory with matrix justification of improved methods of solution," *The Annals of Mathematical Statistics*, 5:82–89 (1944). Michigan statistician.

Developed matrix formulation of least squares, normal equations, and symmetric factorization.

Primary source in the United States for what was later

named "Cholesky's algorithm."

Triangular Factoring

Citation Patterns Among Earliest Authors



- All other authors were interested in normal equations.
- Von Neumann and Goldstine were the first to describe factoring of nonsymmetric matrices. They originated the *LDU* form.

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*Thomas Kuhn, *The Structure of Scientific Revolutions*, The University of Chicago Press, Chicago, 1970.