Contributions to Numerical Analysis in the 1950ies

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http://www.scsc.ethz.ch/∼mhg/talks/sam50.ps
http://www.scsc.ethz.ch/∼mhg/talks/cg.ps

IAM's Contributions to Numerical Analysis

Most important contributors:

- **Eduard Stiefel** (1909–1978)
- **Heinz Rutishauser** (1918–1970)

Further contributors:

- **Urs Hochstrasser**
- **Max Engeli**
- **Theo Ginsburg**
- **Peter Läuchli**
- **Hans-Rudolf Schwarz**

There was a close cooperation with the TH Munich
(*Fritz L. Bauer, Roland Bulirsch, Klaus Samelson, Josef Stoer*).

Peter Henrici (1923–1987) joined ETH in 1962,
the SAM in 1970.

Ambros P. Speiser was responsible for building up the
ERMETH.

IAM's Contributions to Numerical Analysis

Two seminal discoveries:

- conjugate gradient (CG) method for solving linear systems [ES]
- QD algorithm and LR algorithm [HR]

Other important contributions:

- stability of numerical methods for ODEs [HR]
- preconditioning CG by Chebyshev iteration [HR]
- CG for least squares [PL]
- Chebyshev approximation (L^∞-norm; connection between the simplex and the Remes algorithms [ES]
- contributions to interpolation and quadrature [ES + HR]
- Algorithms based on Jacobi rotation patters, including bulge chasing [HR + HRS]
- contributions to Bauer's simultaneous iteration method [HR]
- ALGOL implementations for the *Handbook Series Linear Algebra* [HR, HRS, TG]
- foundation of Springer's *Numerische Mathematik* [ES] and of the *Mitteilungen aus dem Institut für Angewandte Mathematik*

IAM's Contributions to Computer Science

Fundamental work in Computer Science:

- operation of Zuse Z4 computer [ES, APS, HR, ...]
- construction and operation of ERMETH [ES, HR, APS, AS, ...]
- concept of a compiler [HR]
- major contributions to ALGOL58 and ALGOL60 [HR]
- first compiler for ALGOL58 [HRS]
- symbolic language SYMBAL [ME]
- an axiomatic theory of roundoff arithmetics [HR]

This is not discussed further here.

Accounts of the Early Work at the IAM

Numerous short articles in journals and newspapers by A.P. Speiser, H. Rutishauser, A. Schai, E. Stiefel, J.R. Stock,... .

H.R. Schwarz: **The Early Years of Computing in Switzerland**,
Annals History of Computing, Vol. 3, No. 2, April 1981, pp. 121–132.

M.H. Gutknecht: **The pioneer days of scientific computing in Switzerland**,
In: *A History of Scientific Computing* (S.G. Nash, ed.), pp. 301–313. ACM Press, New York, and Addison-Wesley, Reading, Mass., 1990.

The Conjugate Gradient (CG) Method

- Discovered independently by **Eduard Stiefel** (Stiefel, 1952) and by **Magnus Hestenes** (Hestenes, 1951), the latter in cooperation with his coworkers J.B. Rosser, G. Forsythe, and L. Paige.
- Worked out in detail in Hestenes and Stiefel (1952) after the authors met at the *Symposium on Simultaneous Linear Equations and the Determination of Eigenvalues*, August 23-25, 1951, held at the *Institute of Numerical Analysis (INA) of the US National Bureau of Standards (NBS)* at Los Angeles.
- Stiefel spent six months at the INA.
- Numerical experiments by R. Hayes, U. Hochstrasser, and M. Stein.
- Further papers include Stiefel (1955) and Hestenes (1956).
- For detailed history see Golub and O'Leary (1989).
- Magnus Hestenes (1906-1991) and others extended CG to the nonlinear case, *i.e.*, convex minimization.

- Today CG is the preferred iterative method for large, sparse, symmetric positive definite (spd) linear systems.
- CG of limited popularity in the 1950ies and 1960ies.
- Susceptible to roundoff effects.
- Became popular in the 1970ies when problems became bigger and better preconditioners were made available (Reid, 1971).
- *Preconditioning:* system is replaced by an equivalent one whose matrix is more suitable for CG, but need not be explicitly given.
  Preconditioner may consist itself of a few steps of an iterative method.
- Preconditioning (by Chebyshev iteration) introduced in **Heinz Rutishausers** *Theory of Gradient Methods* (today called **Krylov space methods**) published in Engeli, Ginsburg, Rutishauser and Stiefel (1959).
- Today we have a variety of preconditioning techniques (SOR, SSOR, incomplete Cholesky factorizations, sparse approximate inverses, ...; one may include multigrid and domain decomposition).

The Biconjugate Gradient (BiCG) Method

- CG method closely related to the *method of minimized iterations* of **Cornelius Lanczos** (Lanczos, 1952), today called the **biconjugate gradient (**BiCG**) method**, which is not restricted to symmetric matrices.
- Before, Cornelius Lanczos (1893 - 1974) had introduced an intimately related method for computing eigenvalues (Lanczos, 1950), today called the **Lanczos algorithm**.
- Based on biorthogonality (duality) instead of orthogonality. $\rightsquigarrow$ biorthogonalization (BiO) algorithm
- Explained and discussed in Rutishauser (1953).
- BiCG has been hardly used (in the west) till $\sim$1980.
- Revived by Fletcher (1976).
- It can break down (rarely);
  a problem fixed $\sim$1990 with **look-ahead steps**.
- Also susceptible to roundoff effects.
- BiCG is very efficient w.r.t. both computing time and memory requirements (compared to other methods for non-symmetric systems).
- It is the basis of a family of even more efficient algorithms called Lanczos-type product methods (LTPMs).
  It includes, *e.g.*, BiCGStab.

Connected Areas and Problems

- CG and BiCG
- the **minimal** or **conjugate residual** (CR) **method**
- the **Lanczos algorithm**
- **orthonal polynomials**
- **Gauss quadrature**
- the **moment problem**
- **fast Hankel solvers**
- **Padé approximation** (*i.e.*, maximum order rational interpolation at one point)
- the **model reduction problem** of systems theory (scalar or SISO case)
- **continued fractions**, in particular **Jacobi fractions** and **Stieltjes fractions**
- the **quotient-difference** (QD) **algorithm**
- the LR and QR **algorithms** for tridiagonal matrices
- the **Toda flow**
- the ϵ**-algorithm** for convergence acceleration

Most but not all of these connections were known to Stiefel and Rutishauser.

- Due to **Heinz Rutishauser**; described in 3 ZAMP papers (1954, 1954, 1955); reprinted in revised form in Rutishauser (1957).

- Given the **Schwarz constants** or **moments**

$$\mu_k :\equiv \langle \tilde{\mathbf{y}}, \mathbf{A}^k \mathbf{y} \rangle, \quad k = 0, 1, 2, \ldots, 2N-1,$$

  of an $N \times N$ matrix $\mathbf{A}$ and two N-vectors $\mathbf{y}$, $\tilde{\mathbf{y}}$, the QD algorithm normally allows us to compute the eigenvalues of $\mathbf{A}$.

- This problem was posed by Stiefel in a discussion about the Lanczos algorithm.
  "Auf diese Anregung hin entwickelte der Verfasser einen Algorithmus, der die gestellte Aufgabe löst".

- Starting point is the generating function of the moments,

$$F(z) :\equiv \sum_{k=0}^{\infty} \frac{\mu_k}{z^{k+1}},$$

  which satisfies

$$F(z) = \langle \tilde{\mathbf{y}}, (z\mathbf{I} - \mathbf{A})^{-1} \mathbf{y} \rangle.$$

  Hence, F is a rational function of order at most N, and its poles are eigenvalues of $\mathbf{A}$.

- The QD algorithm generalizes results of Aitken and Hadamard and turns them into an effective algorithm.

- However, the problem posed by Stiefel is very ill-conditioned; see Gautschi (1986). Consequently, the QD algorithm is unstable; it can even break down if $\mathbf{A}$ is not spd.
- As intermediate results, the BICG **recurrence coefficients** are produced.
- They are also the coefficients of a **continued fraction** (formally a Stieltjes fraction) that represents F:

$$F(z) = \frac{\mu_0|}{|z} - \frac{q_1|}{|1} - \frac{e_1|}{|\zeta} - \frac{q_2|}{|1} - \frac{e_2|}{|\zeta} - \cdots .$$

- The **progressive form** of the QD algorithm starts from those coefficients.
- It can be understood as a way to construct analogue continued fractions for the tails

$$z^\ell \left(F(z) - \sum_{k=0}^{\ell-1} \frac{\mu_k}{z^{k+1}} \right) = \sum_{k'=0}^{\infty} \frac{\mu_{k'+\ell}}{z^{k'+1}},$$

- It also allows us to compute the poles of a rational function (and thus the zeros of a polynomial).
- For symmetric positive definite matrices and $\tilde{\mathbf{y}} = \mathbf{y}$, the progressive QD algorithm is stable (Rutishauser, 1963).
- To speed up convergence, spectral shifts and deflations are needed.

- The **differential form** DQD of Rutishauser (1976) is more accurate and was rediscovered by Fernando and Parlett (1994).
  Its shifted version has become a competitive method for the tridiagonal spd eigenvalue problem.

- Beresford Parlett hopes it will lead to an accurate and efficient method for the nonsymmetric tridiagonal eigenvalue problem.

- The QD algorithm is equivalent to the LR **algorithm** for tridiagonal matrices: given $\mathbf{T}_0$ compute

  $$\mathbf{T}_n =: \mathbf{L}_n\mathbf{R}_n\,, \quad \mathbf{T}_{n+1} := \mathbf{R}_n\mathbf{L}_n\,, \quad n = 0, 1, 2, \ldots.$$

  All matrices $\mathbf{T}_n$ are similar, *i.e.*, have same eigenvalues. Normally, $\mathbf{T}_n$ approaches a triangular matrix exhibiting the eigenvalues in the diagonal.
  Of course, the process can break down if $\mathbf{T}_0$ is not spd.

- The LR **algorithm** for general matrices (Rutishauser, 1957) works analogously: given $\mathbf{A}_0$ compute

  $$\mathbf{A}_n =: \mathbf{L}_n\mathbf{R}_n\,, \quad \mathbf{A}_{n+1} := \mathbf{R}_n\mathbf{L}_n\,, \quad n = 0, 1, 2, \ldots.$$

- The QR **algorithm** of Francis (1961/62) is based on the same idea, but uses the QR factorization, which is stable:

  $$\mathbf{A}_n =: \mathbf{Q}_n\mathbf{R}_n\,, \quad \mathbf{A}_{n+1} := \mathbf{R}_n\mathbf{Q}_n\,, \quad n = 0, 1, 2, \ldots.$$

  Ever since the standard algorithm for the tridiagonal eigenvalue problem when all eigenvalues are sought.

- The **infinitesimal analog** of the QD algorithm (Rutishauser, 1954; Rutishauser, 1957) describes the **Toda flow** (Toda, 1970).

- The connections between this self-similar flow, the QD algorithm, the QR algorithm, and the ϵ-algorithm have recently attracted new interest;
  see Watkins and Elsner (1990) and Nagai, Tokihiro and Satsuma (1998), and references given there.

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