Modified Moments for Indefinite Weight Functions
(a Tribute to a Fruitful Collaboration with Gene H. Golub)

Martin H. Gutknecht

Seminar for Applied Mathematics
ETH Zurich

Remembering Gene Golub Around the World

Leuven, February 29, 2008

My education in numerical analysis at ETH Zurich

My teachers of numerical analysis:

- Eduard Stiefel [1909–1978] (first, basic NA course, 1964)
- Peter Läuchli [b. 1928] (ALGOL, 1965)
- Hans-Rudolf Schwarz [b. 1930] (numerical linear algebra, 1966)
- Heinz Rutishauser [1917–1970] (follow-up numerical analysis course; “selected chapters of NM” [several courses]; computer hands-on training)
- Peter Henrici [1923–1987] (computational complex analysis [many courses])

The best of all worlds?

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What did I learn?

- Gauss elimination, simplex alg., interpolation, quadrature, conjugate gradients, ODEs, FDM for PDEs, ...
- qd algorithm [often], LR algorithm, continued fractions, ...
- many topics in computational complex analysis, e.g., numerical conformal mapping

What did I miss to learn? (numerical linear algebra only)

- QR algorithm
- nonsymmetric eigenvalue problems
- SVD (theory, algorithms, applications)
- Lanczos algorithm (sym., nonsym.)
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Gene's first two talks at ETH Zurich (probably)

- 4 June 1971: "Some modified eigenvalue problems"
- 28 Nov. 1974: "The block Lanczos algorithm"

Gene was one of many famous visitors Peter Henrici attracted.

Fall 1974: GHG on sabbatical at ETH Zurich.
I had just finished editing the *"Lectures of Numerical Mathematics"* of Heinz Rutishauser (1917–1970).

GHG proposed that I apply for a postdoc position at UBC.
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Met

- Paul Van Dooren (postdoc)
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- Joe Oliger, Robert Schreiber (NA profs)
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My collaboration with Gene on modified moments

After 1980 Gene was a frequent visitor at ETH Zurich.
Either at Applied Math. (Henrici) or CS (Gander).

In Feb./Mar. 1988, for the first time, we started to work together.

Aim: **Compute the recurrence coefficients of a set of orthogonal polynomials (for some unknown measure) from modified moments — even when their was no positive weight function.**

Previous work: Chebyshev 1859, Sack/Donovan '72, Wheeler '74, Gautschi '70, '78/'84, '82, '86.

Ultimate aim: **Use this for adapting the parameters of the Chebyshev iteration (or a similar method) for the iterative solution of large linear systems.**

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My new background:

In 1983/84 I had given a course on **Padé Approximation** (Gragg, Baker/Graves-Morris).

In 1985, while at IBM Yorktown, I had started to work seriously on **iterative methods for linear systems**.

In 1986 I had given a course on **Rational Interpolation** (Werner, Cuyt).

I knew some of **Gautschi's work on modified moments**.

I was working on a paper on the **rational interpolation table (Newton-Padé table) and corresponding continued fractions**. (Included the Padé table and P-fractions as a special case.)

As was typical for Gene, he quickly and nicely explained me the problem and gave me a number of references:

Given a sequence of polynomials $\{\tau_n\}$ (with $\partial\tau_n = n$) and their

- **modified moments** $\nu_n := \int \tau_n(z)d\lambda(z) := \underbrace{\langle \mathbf{r}_0, \tau_n(\mathbf{A})\mathbf{r}_0\rangle}_{\langle \mathbf{r}_0, \mathbf{r}_n\rangle}$

or their

- **Gramian** $N := [\nu_{m,n}]_{m,n=0}^{\infty}$,
  where $\nu_{m,n} := \int \tau_m(z)\tau_n(z)d\lambda(z)$,

find the recurrence coefficients $\{\alpha_n\}, \{\beta_n\}$ of the (possibly formally) orthogonal polynomials (FOPs) $\{\pi_n\}$ associated with the unknown, possibly indefinite measure λ.

"Classical case": $\tau_n = z^n$, **moments** $:= \mu_n := \int z^n d\lambda(z)$, λ positive measure.

"Classical case" $\{\mu_n\}_0^{2\overline{m}+1} \rightsquigarrow \{\alpha_n\}_0^{\overline{m}}, \{\beta_n\}_0^{\overline{m}}$:
Chebyshev algorithm [Chebyshev (1859)]

"Generic modified case" $\{\nu_n\}_0^{2\overline{m}+1} \rightsquigarrow \{\alpha_n\}_0^{\overline{m}}, \{\beta_n\}_0^{\overline{m}}$:
modified Chebyshev algorithm
[Sack/Donovan '72, Wheeler '74, Gautschi]

Our aim was to do the "nongeneric modified case".
Needed techniques similar to those for recurrences in Padé tables with blocks (Arne Magnus, Gragg, Draux) or in the Newton-Padé table with blocks (Claessens, Werner, G.).

Fairly quickly, I came up with a solution.

Using more matrix notation than previous authors we also obtained a nicer treatment of the generic case.

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The Chebyshev and the modified Chebyshev algorithms are based on recurrences for the matrix elements of the lower triangular matrix

$$S :\equiv [\sigma_{m,n}], \qquad \sigma_{m,n} = \int \tau_m(z)\pi_n(z)d\lambda(z).$$

In its first column we have the given moments μ_n or the modified moments ν_m, resp.

From its diagonal and its first codiagonal one can compute the recurrence coefficients $\{\alpha_n\}, \{\beta_n\}$ of the FOPs π_n.

Everything can be read off the matrix identity

$$SG = T^{\mathsf{T}} S,$$

where G and T are the Hessenberg (or, often tridiagonal) matrices that contain the recurrence coefficients of the π_n and τ_n, resp.

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But Gene knew of a number of related problems, such as the one where a leading principle submatrix of the Gramian

$$N := [\nu_{m,n}]_{m,n=0}^{\infty} \qquad \text{with} \quad \nu_{m,n} := \int \tau_m(z)\tau_n(z)d\lambda(z),$$

is given instead of the modified moments.

We decided to cover several such related problems too. Finally, everything fit together wonderfully.

At Varga's 60th birthday conference in Kent, I gave on March 31, 1989, a talk on the paper.

The paper was sent in in July 1989 and appeared in

Numer. Math. 57, pp. 607–624 (1990).

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So, finally, I vaguely understood the Lanczos–Padé connection, and suggested that I will also look into the Lanczos breakdown problem. Gene encouraged me to do that; he did not suggest that this rather technical problem should become a joint project.

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The details were not yet clear to me, but it was clear from the work of Rutishauser (qd booklet), Gragg (1972, 1974), and others that the Lanczos algorithm, (formal) orthogonal polynomials, the qd algorithm, and the here treated Chebyshev algorithm are all closely related.

Gene advised me to also look up the work of Parlett and his student Taylor. Their approach was completely different.

Before end of May 1989 I had figured out how the recurrences for the nonnormal Padé table (Struble, Arne Magnus, Gragg, Draux) can be translated into a nongeneric Lanczos algorithm that can overcome exact breakdowns.

I thought that near-breakdowns should be treated like exact breakdowns: i.e., by replacing an unstable problem by a nearby stable problem.

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Gene's pointer to the Lanczos algorithm (cont'd)

I met Gene again in Tromsø, June 5–10, 1988, at a Supercomputing Conference.

Told him before dinner that I had found a "nongeneric" Lanczos algorithm. After dinner "everybody" knew it.

Gene's pointer to the Lanczos algorithm (cont'd)

I wanted to cover nongeneric versions of "everything":

- the nonsymmetric three-term Lanczos algorithm
- the nonsymmetric two-term Lanczos algorithm
- the biconjugate gradient method
- the corresponding recurrences for the formal orthogonal polynomials
- the corresponding P-fractions (continued fractions)
- the LU decomposition of the corresponding Hessenberg matrices
- the qd algorithm

Gene's pointer to the Lanczos algorithm (cont'd)

In Fall 1989 I had well over 100 pages, when Dan Boley contacted me, telling me that he was working with Golub, Elhay, and Kautsky on a paper in which they wanted to apply Lanczos to the problem of error correcting codes, and that he too had developed a version of Lanczos that overcame exact breakdowns.

I quickly submitted the first part of my work (with the 3-term formulas) entitled

> *A completed theory of the unsymmetric Lanczos process and related algorithms, Part I*

to SIMAX, where it was received on Dec. 11, 1989.

Although it was accepted after a minor revision done quickly, it took more than two years to get it published in April 1992.

So, when revising it, I dedicated it to Gene on the occasion of his 60th birthday.

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> *The unsymmetric Lanczos algorithm and their relations to formal orthogonal polynomials, Padé approximation, continued fractions, and the qd algorithm*

at the Joint Mathematics Meeting in Phoenix on Jan. 14, 1989.

I gave extended versions of the same talk another 10 times, incl. at the

> *(First) Copper Mountain Conference on Iterative Methods, April 2–5, 1990*

where a thick paper was distributed as part of a five-volume proceedings. The talk was on the generic case, but the last slide was on the nongeneric one.

The invitation to the Copper Mountain meeting showed a figure of mine with a nonnormal Padé table.

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(a) Invitation to Copper Mtn. Conf.

(b) Last slide of talk

Gene's pointer to the Lanczos algorithm (cont'd)

A revised and extended version of the Copper Mtn. paper was ultimately published in

Acta Numerica 6, 271–397 (1997).

Of course, it was Gene who suggested that I publish this there.

Look-ahead Lanczos

A related talk on the nongeneric case I gave first twice in South Africa in July 1989 and then at the

Householder Symp. IX, Tylosand, June 18–22, 1990.

At this meeting Roland Freund introduced QMR, and Henk van der Vorst introduced (Bi)CGStab.

Roland and I agreed to join forces, and in the sequel he developed with Noël Nachtigal a Fortran 77 program for the look-ahead Lanczos algorithm, which in contrast to my previous work handled near-breakdowns more appropriately. After all, the linear algebra approach of Parlett and Taylor had proven to be more successful — but it missed all the nice connections to the FOPs and the other classical topics.

By 1990 the topic had become very poplar; a number of other people started to publish on this topic (Parlett, Boley / Elhay / Golub / G., Brezinski / Redivo Zaglia / Sadok, Bank / Chan, ...).

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Summary

Gene had an enourmous

- memory for the literature in our field
- ability to find (or recall) new problems and applications
- memory for names and faces
- ability to make connections (both in math and among people)
- capability to socialize
- capability to motivate others (in part. young) people to follow up on an idea

That made him the natural leader of a whole scientific community.