

How Rutishauser may have found the qd and LR algorithms, the fore-runners of QR

Martin H. Gutknecht and Beresford N. Parlett

¹Seminar for Applied Mathematics
ETH Zurich

²Department of Mathematics
University of California
Berkeley

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Rutishauser's qd algorithm: early papers

- Rutishauser (1954a, ZAMP): Der Quotienten–Differenzen–Algorithmus
- Rutishauser (1954b, ZAMP): Anwendungen des Quotienten–Differenzen–Algorithmus
- Rutishauser (1954c, Arch.Math.): Ein infinitesimales Analogon zum Quotienten–Differenzen–Algorithmus
- Rutishauser (1955a, ZAMP): Bestimmung der Eigenwerte und Eigenvektoren einer Matrix mit Hilfe des Quotienten–Differenzen–Algorithmus
- Rutishauser (1957a, Mitt. IAM, ETH): Der Quotienten–Differenzen–Algorithmus
- Henrici (1958, NBS book): The Quotient-Difference Algorithm

Eduard Stiefel's suggestion (~ 1953)

Stiefel's suggestion to Rutishauser: Given \mathbf{A} , \mathbf{x}_0 , \mathbf{y}_0 , use the **Schwarz constants** (= **moments** = **Markov parameters**)

$$s_k \equiv \mathbf{y}_0^T \mathbf{A}^k \mathbf{x}_0 \quad (k = 0, 1, 2, \dots) \quad (1)$$

to find the eigenvalues of \mathbf{A} .

Daniel Bernoulli (1732), J. König (1884):

$$\frac{s_{\nu+1}}{s_\nu} \longrightarrow \lambda_1 \quad \text{as } \nu \longrightarrow \infty \quad \text{if } |\lambda_1| > |\lambda_2| \geq |\lambda_2| \geq \dots$$

Note: It turned out that for the other eigenvalues, Stiefel's proposal was a bad idea, since the dependence of the EVals from the moments is highly ill-conditioned (**Gautschi (1968)**).

Moments and their generating function

Given: $N \times N$ matrix \mathbf{A} and $\mathbf{x}_0, \mathbf{y}_0 \in \mathbb{R}^N$, let

$$f(z) := \left\langle \mathbf{y}_0, (z\mathbf{I} - \mathbf{A})^{-1} \mathbf{x}_0 \right\rangle = \left\langle \mathbf{y}_0, \frac{1}{z} (\mathbf{I} - \frac{1}{z}\mathbf{A})^{-1} \mathbf{x}_0 \right\rangle \quad (2)$$

f is a rational function of type $(N-1, N)$, so $f(\infty) = 0$.

The poles of f are eigenvalues of \mathbf{A} .

f can be expanded into a power series in z^{-1} :

$$f(z) = \sum_{k=0}^{\infty} \frac{s_k}{z^{k+1}} = \frac{s_0}{z} + \frac{s_1}{z^2} + \frac{s_2}{z^3} + \dots \quad (3)$$

where

$$s_k = \mathbf{y}_0^T \mathbf{A}^k \mathbf{x}_0$$

So, f is the **generating function** of the moments.

Alternative formulations of the problem

Clearly, there are several equivalent problems:

- Find eigenvalues of \mathbf{A} .
- Find poles of generating (rational) function f .
- Find zeros of the denominator polynomial of f (Bernoulli).

In theory, the problem had been solved before by

- Hadamard (1892) (his PhD thesis!),
- de Montessus de Ballore (1902/1905),
- Aitken (1926/1931).

But none of them had an efficient algorithm.

Rutishauser cites Hadamard and Aitken, but never de Montessus de Ballore, who proved the convergence of Padé approximants with fixed denominator degree.

Hadamard's theorem (1892)

Given the power series of f in z^{-1} of (3), let $H_0^{(\nu)} \equiv 1$, and define the *Hankel determinants*

$$H_k^{(\nu)} = \begin{vmatrix} s_\nu & s_{\nu+1} & \cdots & s_{\nu+k-1} \\ s_{\nu+1} & s_{\nu+2} & \cdots & s_{\nu+k} \\ \vdots & \vdots & \ddots & \vdots \\ s_{\nu+k-1} & s_{\nu+k} & \cdots & s_{\nu+2k-2} \end{vmatrix} \quad \begin{array}{l} (k = 1, 2, \dots; \\ \nu = 0, 1, \dots) \end{array}$$

THEOREM

[Hadamard (1892)] If $|\lambda_{k+1}| < \Lambda < |\lambda_k|$, then, as $\nu \rightarrow \infty$,

$$H_k^{(\nu)} = \text{const} \cdot (\lambda_1 \cdots \lambda_k)^\nu \left[1 + \mathcal{O} \left(\frac{\Lambda}{|\lambda_k|} \right)^\nu \right]$$

For a simpler proof see [Henrici \(1958\)](#) or [Henrici \(1974\)](#).

COROLLARY

If f has N simple poles, then

- 1 $H_k^{(\nu)} \neq 0$ ($k = 1, \dots, N$) for large enough ν ,
and $H_{N+1}^{(\nu)} = 0$ ($\forall \nu$).
- 2 If $|\lambda_k| > |\lambda_{k+1}|$ then

$$\frac{H_k^{(\nu+1)}}{H_k^{(\nu)}} \longrightarrow \lambda_1 \lambda_2 \cdots \lambda_k \quad \text{as } \nu \longrightarrow \infty. \quad (4)$$

- 3 If $|\lambda_{k-1}| > |\lambda_k| > |\lambda_{k+1}|$ then

$$q_k^{(\nu)} \equiv \frac{H_k^{(\nu+1)}}{H_k^{(\nu)}} \cdot \frac{H_{k-1}^{(\nu)}}{H_{k-1}^{(\nu+1)}} \longrightarrow \lambda_k \quad \text{as } \nu \longrightarrow \infty. \quad (5)$$

Computing, for fixed ν , the Hankel determinants $H_1^{(\nu)}, \dots, H_N^{(\nu)}$ (if nonzero) requires the LU decomposition of the matrix $H_N^{(\nu)}$.

Aitken (1926, 1931) used what is now called “*Jacobi identity*” (“theorem of compound determinants”)

$$\left(H_k^{(\nu)}\right)^2 = H_k^{(\nu-1)}H_k^{(\nu+1)} + H_{k+1}^{(\nu-1)}H_{k-1}^{(\nu+1)}. \quad (6)$$

It had also been known to Hadamard, but Aitken used it to build up — from the left or from the top — the table

$$\begin{array}{cccccc} 1 & & & & & \\ 1 & H_1^{(0)} & & & & \\ 1 & H_1^{(1)} & H_2^{(0)} & & & \\ 1 & H_1^{(2)} & H_2^{(1)} & H_3^{(0)} & & \\ 1 & H_1^{(3)} & H_2^{(2)} & H_3^{(1)} & H_4^{(0)} & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{array}$$

Rutishauser's qd algorithm (QD-Algorithmus)

Rutishauser (1954a) knew Aitken's work and refers to (4),

$$\boxed{\frac{H_k^{(\nu+1)}}{H_k^{(\nu)}} \longrightarrow \lambda_1 \lambda_2 \cdots \lambda_k} \quad \text{as } \nu \longrightarrow \infty$$

as the key to computing non-dominant poles.

But instead of computing the $H_k^{(\nu)}$ -table, he headed directly for recurrences for

$$\boxed{q_k^{(\nu)} := \frac{H_k^{(\nu+1)}}{H_k^{(\nu)}} \cdot \frac{H_{k-1}^{(\nu)}}{H_{k-1}^{(\nu+1)}}} \quad \text{and} \quad \boxed{e_k^{(\nu)} := \frac{H_{k+1}^{(\nu)}}{H_k^{(\nu)}} \cdot \frac{H_{k-1}^{(\nu+1)}}{H_k^{(\nu+1)}}} \quad (7)$$

In Rutishauser (1954a) he derives the formulas needed for $q_2^{(\nu)}$, and then states recursions for general k .

qd table (QD-Schema):

	$q_1^{(0)}$							
0		$e_1^{(0)}$	\times	$q_2^{(0)}$				
	$q_1^{(1)}$		\times					
0		$e_1^{(1)}$			$e_2^{(0)}$			
	$q_1^{(2)}$			$q_2^{(1)}$		\dots		
0		$e_1^{(2)}$			$e_2^{(1)}$		$e_{N-1}^{(0)}$	
	$q_1^{(3)}$		$+$	$q_2^{(2)}$		\dots		$q_N^{(0)}$
0		$e_1^{(3)}$			$e_2^{(2)}$		$e_{N-1}^{(1)}$	0
	$q_1^{(4)}$			$q_2^{(3)}$		\dots		$q_N^{(1)}$
0		$e_1^{(4)}$			$e_2^{(3)}$		$e_{N-1}^{(2)}$	0
	\vdots			\vdots			\vdots	
\vdots		\vdots		\vdots			\vdots	\vdots

$$e_1^{(0)} \cdot q_2^{(0)} = q_1^{(1)} \cdot e_1^{(1)}$$

$$q_2^{(1)} + e_2^{(1)} = e_1^{(2)} + q_2^{(2)}$$

Rhombus rules (called so by [Stiefel, 1955](#)) of **qd algorithm**:

For building up the table columnwise from left to right:

$$\left. \begin{aligned} e_k^{(\nu)} &:= e_{k-1}^{(\nu+1)} + q_k^{(\nu+1)} - q_k^{(\nu)} \\ q_{k+1}^{(\nu)} &:= q_k^{(\nu+1)} \frac{e_k^{(\nu+1)}}{e_k^{(\nu)}} \end{aligned} \right\} \quad (k = 1, 2, \dots) \quad (8)$$

For building up the table row-wise, from top to bottom:

$$\left. \begin{aligned} q_k^{(\nu+1)} &:= q_k^{(\nu)} + e_k^{(\nu)} - e_{k-1}^{(\nu+1)} \\ e_k^{(\nu+1)} &:= e_k^{(\nu)} \frac{q_k^{(\nu+1)}}{q_{k+1}^{(\nu)}} \end{aligned} \right\} \quad (k = 1, 2, \dots) \quad (9)$$

Recursions (9) are the basis of the **progressive qd algorithm** (the *relevant* version).

In Rutishauser (1954a) the correctness of the rhombus rules follows later from the connections to continued fractions (probably Stiefel's argument).

Originally, Rutishauser derived them probably from Hadamard's "Jacobi identity"

$$\left(H_k^{(\nu)}\right)^2 = H_k^{(\nu-1)} H_k^{(\nu+1)} + H_{k+1}^{(\nu-1)} H_{k-1}^{(\nu+1)}.$$

Henrici (1958), who was in contact with Rutishauser, pointed out that one rhombus rule (+) can be derived by combining two applications of this formula, the other (\times) just by using the definitions (9) of $q_k^{(\nu)}$ and $e_k^{(\nu)}$.

The details have been worked out in Parlett (1996), a TR entitled "What Hadamard missed".

From power series to a continued fractions

By a standard operation the given power series (3) in z^{-1} of f ,

$$f(z) = \sum_{k=0}^{\infty} \frac{s_k}{z^{k+1}} = \frac{s_0}{z} + \frac{s_1}{z^2} + \frac{s_2}{z^3} + \dots$$

can be turned into a continued fraction (which typically converges in a much larger region). We may also write

$$f(z) = \frac{s_0}{z} + \frac{s_1}{z^2} + \dots + \frac{s_{\nu-1}}{z^{\nu}} + \frac{f_{\nu}(z)}{z^{\nu}}. \quad (10)$$

and expand the remainder $f_{\nu}(z)$ of the power series into a continued fractions.

In each case, two different types of continued fractions can be used. So we get two whole series of continued fractions.

It turns out that their coefficients are related by the rhombus rules.

Continued fractions: J -fractions and S -fractions

$$f_\nu(z) := \sum_{k=0}^{\infty} \frac{s_{\nu+k}}{z^{k+1}} = z^\nu \left(f(z) - \sum_{k=0}^{\nu-1} \frac{s_k}{z^{k+1}} \right) \quad (11)$$

can be expanded both into a **Jacobi fraction** or **J-fraction**

$$f_\nu(z) = \cfrac{s_\nu}{z - q_1^{(\nu)}} - \cfrac{e_1^{(\nu)} q_1^{(\nu)}}{z - q_2^{(\nu)} - e_1^{(\nu)}} - \cfrac{e_2^{(\nu)} q_2^{(\nu)}}{z - q_3^{(\nu)} - e_2^{(\nu)}} - \dots \quad (12)$$

and into a formal **Stieltjes fraction** or **S-fraction**

$$f_\nu(z) = \cfrac{s_\nu}{z} - \cfrac{q_1^{(\nu)}}{1} - \cfrac{e_1^{(\nu)}}{z} - \cfrac{q_2^{(\nu)}}{1} - \cfrac{e_2^{(\nu)}}{z} - \dots \quad (13)$$

The J -fraction is the so-called *even part* of the S -fraction obtained by merging two successive terms into one.

Continued fractions: J-fractions and S-fractions

The *odd part* of the S-fraction is another formal J-fraction, obtained by merging the two differently chosen successive terms into one,

$$f_\nu(z) = \frac{s_\nu}{z} \left\{ 1 + \left| \frac{q_1^{(\nu)}}{z - q_1^{(\nu)} - e_1^{(\nu)}} \right| - \left| \frac{e_1^{(\nu)} q_2^{(\nu)}}{z - q_2^{(\nu)} - e_2^{(\nu)}} \right| - \left| \frac{e_2^{(\nu)} q_3^{(\nu)}}{z - q_3^{(\nu)} - e_3^{(\nu)}} \right| - \dots \right\}. \quad (14)$$

By comparing this J-fraction with the one for

$$f_{\nu+1}(z) = z f_\nu(z) - s_\nu, \quad (15)$$

one recovers Rutishauser's *rhombus rules* of the qd algorithm.

This is the nicest derivation of the qd algorithm, but not the original one.

Rutishauser (1954a) indicates that it may have been suggested to him by Stiefel.

Continued fractions, Padé approximations, FOPs

The “*partial sums*” = *convergents* = *approximants* of the continued fractions are confluent rational interpolants of f .

They are *Padé approximants* (at ∞) associated with the moments $s_{k+\nu}$ ($k = 0, 1, \dots$; ν fixed) of the function $f_\nu(z)$ defined by

$$f(z) = \frac{s_0}{z} + \frac{s_1}{z^2} + \dots + \frac{s_{\nu-1}}{z^\nu} + \frac{f_\nu(z)}{z^\nu}.$$

For fixed ν , the denominators of the convergents (= Padé approximants) are (formal) orthogonal polynomials $p_k^{(\nu)}(z)$.

They can be arranged in a table that he called **p-table**. (Analogous to the Padé table.)

Continued fractions, Padé approximations, FOPs (cont'd)

Rutishauser realized that they are also the *Lanczos polynomials* of the (nonsymmetric) Lanczos algorithm (Lanczos, 1950) for \mathbf{A} started with the pair $(\mathbf{y}_0, \mathbf{A}^\nu \mathbf{x}_0)$.

Rutishauser never mentions Padé approximants, but he had no need, since they are just the convergents of the J-fractions and S-fractions.

For him, actually only the FOPs in the denominator matter.

Later, 1966–74, Householder, Gragg, and Stewart stress the connection to Padé approximants in several papers.

N.B.: Hadamard's theorem (1892) \sim de Montessus de Ballore's theorem (1902/1905).

Associated polynomials: recurrences

The p-table can be built up from the initial column $p_0^{(\nu)} \equiv 1$ by the left-to-right recurrence

$$p_k^{(\nu)}(z) := zp_{k-1}^{(\nu+1)}(z) - q_k^{(\nu)} p_{k-1}^{(\nu)}(z). \quad (16)$$

Rutishauser (1954a) derived also a top-to-bottom recurrence

$$p_k^{(\nu+1)}(z) := p_k^{(\nu)}(z) - e_k^{(\nu)} p_{k-1}^{(\nu+1)}(z). \quad (17)$$

and the diagonal 3-term recurrence (with $e_0^{(\nu)} \equiv 0$, $p_0^{(\nu)} \equiv 1$)

$$p_{k+1}^{(\nu)}(z) := [z - q_{k+1}^{(\nu)} - e_k^{(\nu)}] p_k^{(\nu)}(z) + e_k^{(\nu)} q_k^{(\nu)} p_{k-1}^{(\nu)}(z) \quad (18)$$

Further relations and applications

So, in addition to introducing and investigating the qd algorithm [Rutishauser \(1954a\)](#) [rec. 5 Aug. 1953] [\(1954b\)](#) [rec. 18 Sep. 1953], [\(1955a\)](#) [rec. 19 July 1954]) explained many connections to other topics and gave many applications; e.g., in [\(1954a\)](#):

- the connection to continued fractions,
- the connection to the Lanczos BIO algorithm,
- the connection to the CG algorithm,
- computing partial fraction decompositions of rational fcts.

In [\(1954b\)](#):

- summation of badly converging series,
- solving algebraic equations = computing zeros of polynomials,
- quadratic convergence by using *shifts / double shifts*.

In (1955a):

- computing EVals by *combining Lanczos' B1O alg. and the progressive qd algorithm*,
- computing EVecs (several new algorithms are suggested),
- EVals and EVecs of infinite matrices.

Still missing:

- *tridiagonal matrices* (except for computing shifts),
- *LU decomposition* of these tridiagonal matrices,
- *LR algorithm*.

So, the qd algorithm consists of performing the step

$$\mathbf{T}_n^{(\nu)} = \mathbf{L}_n^{(\nu)} \mathbf{R}_n^{(\nu)} \rightsquigarrow \mathbf{R}_n^{(\nu)} \mathbf{L}_n^{(\nu)} = \mathbf{T}_n^{(\nu+1)}$$

called **LR transformation**, which is a similarity transformation:

$$\mathbf{T}_n^{(\nu+1)} = \mathbf{R}_n^{(\nu)} \mathbf{T}_n^{(\nu)} \left(\mathbf{R}_n^{(\nu)} \right)^{-1}.$$

The likely motivation:

- Diagonals (“rows”) of qd-table correspond to J-fractions, FOPS (Lanczos polynomials), and tridiagonal matrices.
- Rhombus rules lead us from one diagonal to the next.
- They are matched by construction with J- and S-fractions.
- There are corresponding rules for the polynomials.
- **Hence, there must be a rule for transforming one tridiagonal matrix into the next.**

The LR algorithm

LR algorithm: succession of LR transformations (LR steps).

Convergence of $\mathbf{e}_k^{(\nu)} \rightarrow 0$ ($k = 1, \dots, n$) as $\nu \rightarrow \infty$ means:

Convergence of $\mathbf{L}_n^{(\nu)}$ to diagonal matrix as $\nu \rightarrow \infty$,

Convergence of $\mathbf{T}_n^{(\nu)}$ to upper bidiagonal matrix as $\nu \rightarrow \infty$,

The diagonals of $\mathbf{T}_n^{(\nu)}$ and $\mathbf{R}_n^{(\nu)}$ ultimately contain eigenvalues of \mathbf{A} ,

Generalization to full matrices is immediate, but unimportant.

The LR algorithm: publications

The first two publications on the LR algorithm were in French, two two-page notes in the *Comptes Rendus*: Rutishauser (1955e) [séance du 3 janvier 1955], Rutishauser/Bauer (1955) [séance du 25 avril 1955].

1956 Rutishauser produced a mimeographed 51-page ETH research report in English, entitled “Report on the Solution of Eigenvalue Problems with the LR–transformation”. Two years later it got properly published in a National Bureau of Standards (NBS) book series (Rutishauser, 1958a).

In the same issue: Henrici’s review paper on the qd algorithm, and Stiefel’s paper on kernel polynomials in NLA.

In 1957, Rutishauser included a 5-page appendix on the LR transformation in the (German) booklet that compiled and updated most of his previous work on qd (Rutishauser, 1957a).

Conclusions

The discovery of the qd and the LR algorithms probably evolved in the following steps:

- Generalizing Aitken's work \rightsquigarrow qd table / algorithm.
- Considering the corresponding p-table (gen. Lanczos' work) and finding the diagonal 3-term recurrence for this table.
- Making the connection to continued fractions and Lanczos polynomials (and as well to many other topics).
- Making the connection to tridiagonal matrices.
- Noticing their extremely simple LU decomposition.
- Noticing that

qd algorithm = LR algorithm for tridiagonal matrices

- Generalizing the LR algorithm to full matrices.