Matching moments and matrix computations

Jörg Liesen
Technical University of Berlin

and

Zdeněk Strakoš
Charles University in Prague and Czech Academy of Sciences

http://www.karlin.mff.cuni.cz/˜strakos

SC2011 in honor of Claude Brezinski and Sebastiano Seatzu
Saardinia, October 2011

CG $\equiv$ matrix form of the Gauss-Christoffel Q.

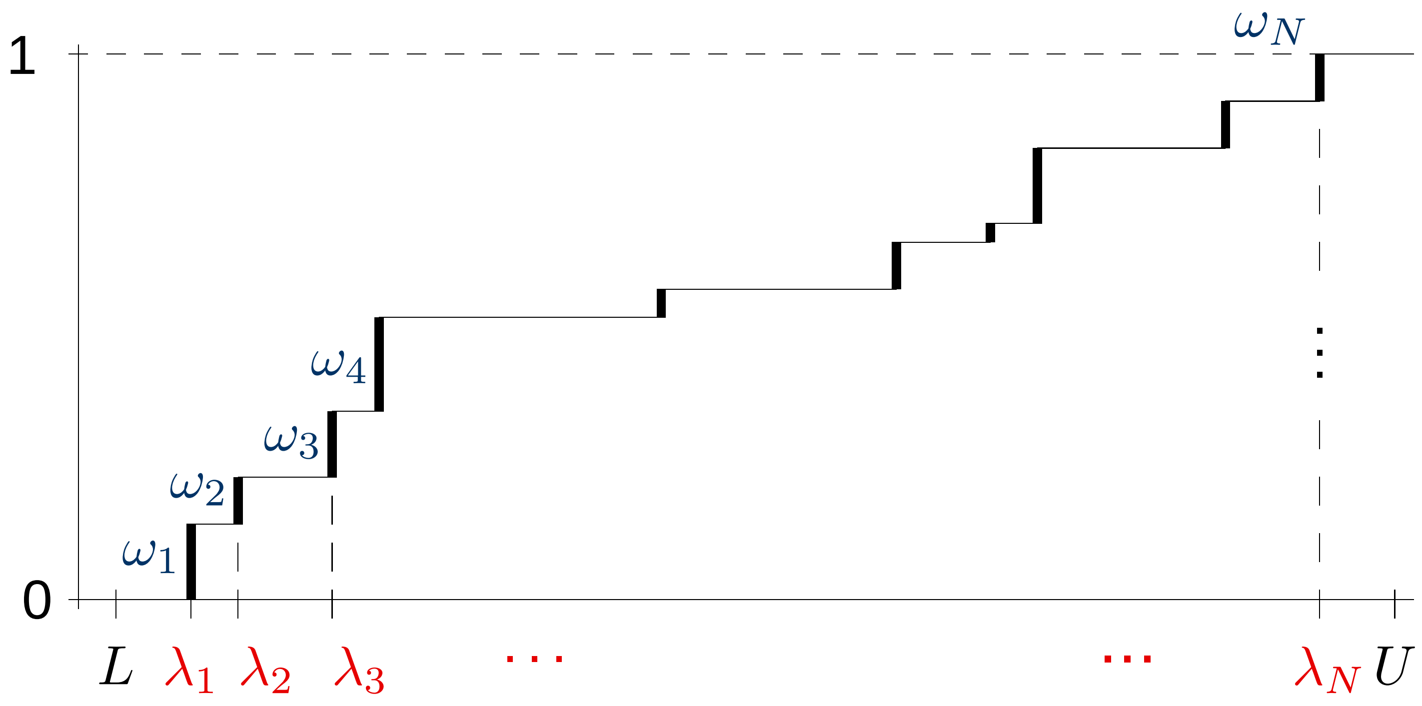
$$\begin{tikzcd}
Ax = b\,,\ x_0 \arrow[r, leftrightarrow] & \omega(\lambda), \quad \displaystyle\int_\zeta^\xi (\lambda)^{-1}\, d\omega(\lambda) \\
T_n\, y_n \;=\; \|r_0\|\, e_1 \arrow[u] \arrow[r, leftrightarrow] & \omega^{(n)}(\lambda), \quad \displaystyle\sum_{i=1}^{n} \omega_i^{(n)} \left(\theta_i^{(n)}\right)^{-1} \arrow[u]
\end{tikzcd}$$

$$x_n \;=\; x_0 + W_n\, y_n$$

$$\boxed{\omega^{(n)}(\lambda) \longrightarrow \omega(\lambda)}$$

Distribution function $\omega(\lambda)$

λ_i, s_i are the eigenpairs of A , $\omega_i = |(s_i, w_1)|^2$, $w_1 = r_0/\|r_0\|$



Hestenes and Stiefel (1952)

CG and Gauss-Christoffel quadrature errors

$$\int_L^U \lambda^{-1}\, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} \left(\theta_i^{(n)}\right)^{-1} \;+\; R_n(f)$$

$$\frac{\|x - x_0\|_{\mathbf{A}}^2}{\|r_0\|^2} \;=\; n\text{-th Gauss quadrature} \;+\; \frac{\|x - x_n\|_{\mathbf{A}}^2}{\|r_0\|^2}$$

With $x_0 = 0$,

$$b^* A^{-1} b \;=\; \sum_{j=0}^{n-1} \gamma_j \|r_j\|^2 \;+\; r_n^* A^{-1} r_n \,.$$

CG : model reduction matching $2n$ moments;

Golub, Meurant, Reichel, Boley, Gutknecht, Saylor, Smolarski, ... ,
Meurant and S (2006), Golub and Meurant (2010), S and Tichý (2011)

Outline

1. CG convergence bounds based on Chebyshev polynomials
2. Sensitivity of the Gauss-Christoffel quadrature
3. PDE discretizations and matrix computations

1 Beauty of Chebyshev polynomials

- Flanders and Shortley, Numerical determination of fundamental modes (1950)
- Lanczos, Chebyshev polynomials in the solution of large scale linear systems (1953)
- Stiefel, Kernel polynomials in linear algebra and their numerical applications (1958)
- Rutishauser, Theory of gradient methods (1959)

For the state of the art demonstration of the beauty of Chebyshev polynomials we refer to the work of Nick Trefethen and his collaborators.

1 Linear bounds for the nonlinear method?

$$\begin{aligned}
\|x - x_n\|_A &= \min_{\substack{p(0)=1\\ \deg(p)\le n}} \|A^{1/2} p(A)(x - x_0)\| \\
&= \min_{\substack{p(0)=1\\ \deg(p)\le n}} \|Y p(\Lambda) Y^* A^{1/2}(x - x_0)\| \\
&\le \left(\min_{\substack{p(0)=1\\ \deg(p)\le n}} \max_{1\le j\le N} |p(\lambda_j)| \right) \|x - x_0\|_A
\end{aligned}$$

Using the shifted Chebyshev polynomials on the interval $[\lambda_1, \lambda_N]$,

$$\|x - x_n\|_A \le 2 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^n \|x - x_0\|_A .$$

1 Minimization property and the bound

This bound has a remarkably wiggling history:

- Markov (1890)
- Flanders and Shortley (1950)
- Lanczos (1953), Kincaid (1947), Young (1954, ...)
- Stiefel (1958), Rutishauser (1959)
- Meinardus (1963), Kaniel (1966)
- Daniel (1967a, 1967b)
- Luenberger (1969)

It represents nothing but the bound for the Chebyshev method,
Liesen and S (2012?)

1 Composite bounds considering large outliers?

This bound should not be used in connection with the behaviour of CG unless $\kappa(A) = \lambda_N / \lambda_1$ is really small or unless the (very special) distribution of eigenvalues makes it relevant.

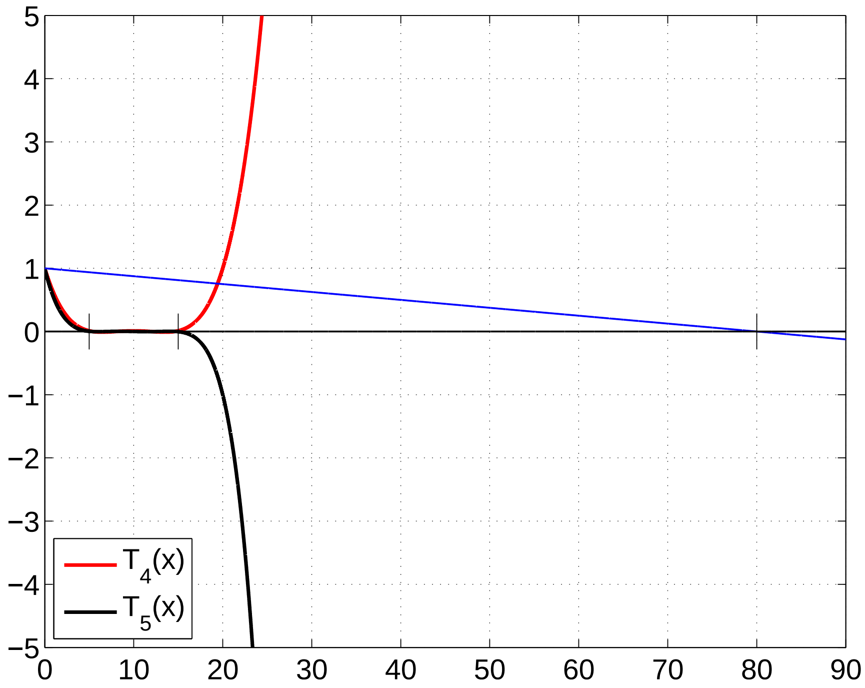
In particular, one should be very careful while using it as a part of a composite bound in the presence of the large outlying eigenvalues

$$\min_{\substack{p(0)=1 \\ \deg(p) \le n-s}} \max_{1 \le j \le N} |\, q_s(\lambda_j)\, p(\lambda_j) \,| \;\le\; \max_{1 \le j \le N} |q_s(\lambda_j)| \left| \frac{T_{n-s}(\lambda_j)|}{T_{n-s}(0)} \right|$$

$$<\; \max_{1 \le j \le N-s} \left| \frac{T_{n-s}(\lambda_j)}{T_{n-s}(0)} \right| .$$

This Chebyshev method bound on the interval $[\lambda_1, \lambda_{N-s}]$ is then valid after s initial steps.

1 The polynomial $q_s(\lambda)$ has desired roots



The Chebyshev polynomials $T_4(\lambda), T_5(\lambda)$, and the polynomial $q_1(\lambda)$, $q_1(0) = 1$ having the single root at the large outlying eigenvalue.

1 Quote (2009, ...): the desired accuracy ϵ

Theorem. After

$$k = s + \left\lceil \frac{\ln(2/\epsilon)}{2} \sqrt{\frac{\lambda_{N-s}}{\lambda_1}} \right\rceil$$

iteration steps the CG will produce the approximate solution x_n satisfying

$$\|x - x_n\|_A \le \epsilon \, \|x - x_0\|_A \, .$$

This recently republished and used statement is in finite precision arithmetic not true at all.

1 Mathematical model of FP CG

CG in finite precision arithmetic can be seen as the exact arithmetic CG for the problem with the slightly modified distribution function with larger support, i.e., with single eigenvalues replaced by tight clusters.

Paige (1971-80), Greenbaum (1989),
Parlett (1990), S (1991), Greenbaum and S (1992), Notay (1993), ... ,
Druskin, Knizhnermann, Zemke, Wülling, Meurant, ...
Recent review and update in Meurant and S, Acta Numerica (2006).

Fundamental consequence:

In FP computations, the composite convergence bounds eliminating in exact arithmetic large outlying eigenvalues at the cost of one iteration per eigenvalue do not, in general, work.

1 Axelsson (1976), quote Jennings (1977)

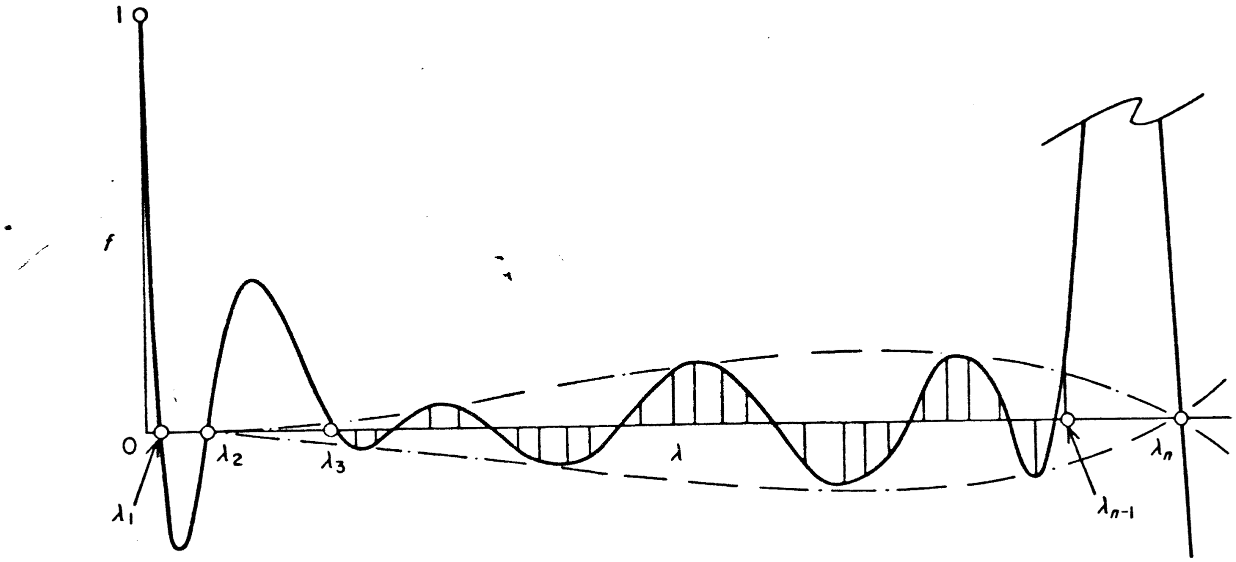
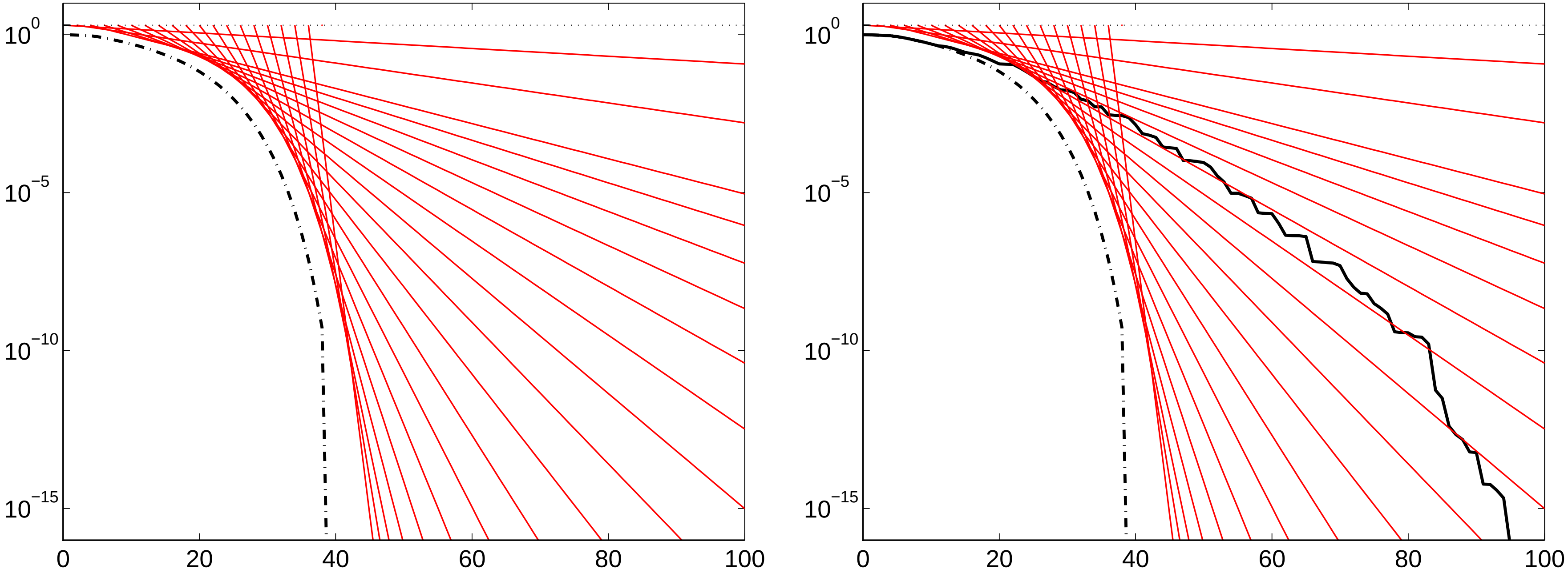


FIG. 4. A Chebyshev polynomial modified by a simple third order auxiliary polynomial having zeros at λ_1, λ_2 and λ_n.

p. 72: ... it may be inferred that rounding errors ... affects the convergence rate when large outlying eigenvalues are present.

1 The composite bounds completely fail



Composite bounds with varying number of outliers:
Exact CG (left) and FP CG (right),
Gergelits (2011).

2 CG and Gauss-Christoffel quadrature errors

$$\int_L^U \lambda^{-1}\, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} \left(\theta_i^{(n)}\right)^{-1} \;+\; R_n(f)$$

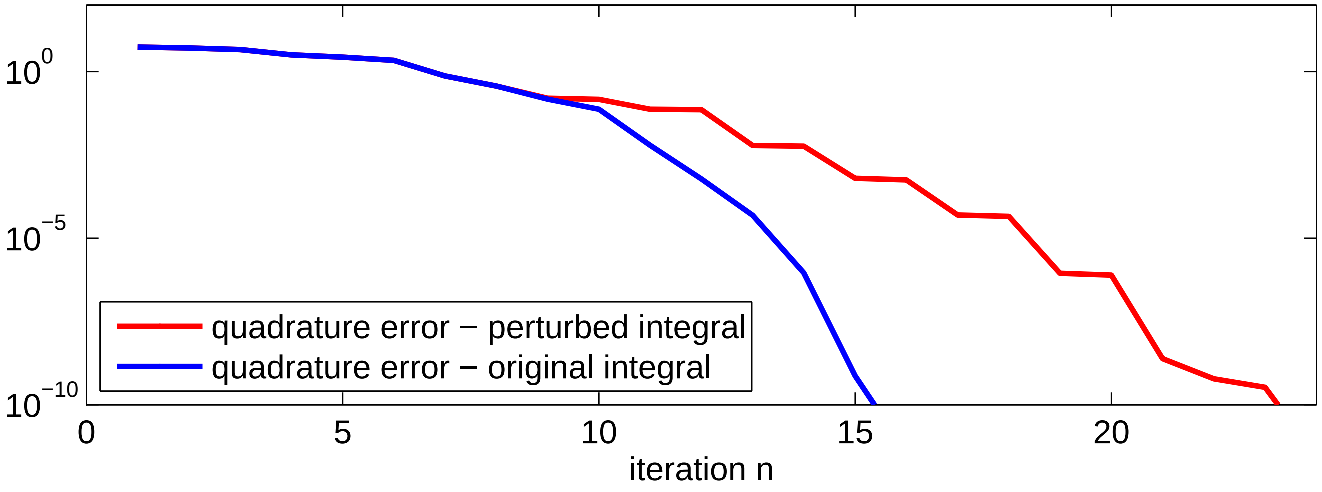
$$\frac{\|x - x_0\|_{\mathbf{A}}^2}{\|r_0\|^2} \;=\; n\text{-th Gauss quadrature} \;+\; \frac{\|x - x_n\|_{\mathbf{A}}^2}{\|r_0\|^2}$$

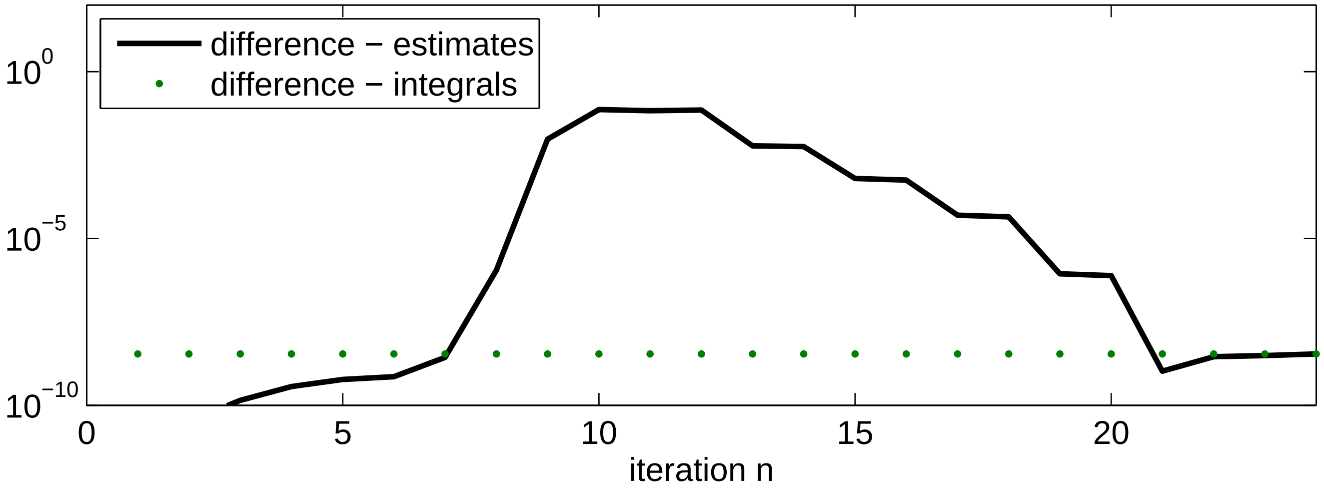
Consider two slightly different distribution functions with

$$I_\omega \;=\; \int_L^U \lambda^{-1}\, d\omega(\lambda) \;\approx\; I_\omega^n$$

$$I_{\tilde{\omega}} \;=\; \int_L^U \lambda^{-1}\, d\tilde{\omega}(\lambda) \;\approx\; I_{\tilde{\omega}}^n$$

2 Sensitivity of the Gauss-Christoffel Q.





2 : A point going back to 1814

1. Gauss-Christoffel quadrature for a small number of quadrature nodes can be highly sensitive to small changes in the distribution function that enlarge its support.

   In particular, the difference between the corresponding quadrature approximations (using the same number of quadrature nodes) can be many orders of magnitude larger than the difference between the integrals being approximated.

2. This sensitivity in Gauss-Christoffel quadrature can be observed for discontinuous, continuous, and even analytic distribution functions, and for analytic integrands uncorrelated with changes in the distribution functions, with no singularity close to the interval of integration.

2 Theorem - O'Leary, S, Tichý (2007)

Consider distribution functions $\omega(\lambda)$ and $\tilde{\omega}(\lambda)$ on $[L, U]$. Let $p_n(\lambda) = (\lambda - \lambda_1) \dots (\lambda - \lambda_n)$ and $\tilde{p}_n(\lambda) = (\lambda - \tilde{\lambda}_1) \dots (\lambda - \tilde{\lambda}_n)$ be the nth orthogonal polynomials corresponding to ω and $\tilde{\omega}$ respectively, with $\hat{p}_s(\lambda) = (\lambda - \xi_1) \dots (\lambda - \xi_s)$ their least common multiple.
If f'' is continuous on $[L, U]$, then the difference $\Delta^n_{\omega,\tilde{\omega}}$ between the approximation I^n_ω to I_ω and the approximation $I^n_{\tilde{\omega}}$ to $I_{\tilde{\omega}}$, obtained from the n-point Gauss-Christoffel quadrature, is bounded as

$$\begin{aligned} |\Delta^n_{\omega,\tilde{\omega}}| \; &\leq \; \left| \int_L^U \hat{p}_s(\lambda) f[\xi_1, \dots, \xi_s, \lambda] \, d\omega(\lambda) \; - \; \int_L^U \hat{p}_s(\lambda) f[\xi_1, \dots, \xi_s, \lambda] \, d\tilde{\omega}(\lambda) \right| \\ &+ \; \left| \int_L^U f(\lambda) \, d\omega(\lambda) \; - \; \int_L^U f(\lambda) \, d\tilde{\omega}(\lambda) \right| . \end{aligned}$$

3 Take very simple model boundary value problem

$$-\Delta u \;=\; 16\eta_1\eta_2(1-\eta_1)(1-\eta_2)$$

on the unit square with zero Dirichlet boundary conditions. Galerkin finite element method (FEM) discretization with linear basis functions on the regular triangular grid with the mesh size $h = 1/(m+1)$, where m is the number of inner nodes in each direction. Discrete (piecewise linear) solution

$$u_h \;=\; \sum_{j=1}^{N} \zeta_j \, \phi_j(\eta_1, \eta_2)\,.$$

Computational error

$$\underbrace{u - u_h^{(n)}}_{\text{total error}} \;=\; \underbrace{u - u_h}_{\text{discretisation error}} \;+\; \underbrace{u_h - u_h^{(n)}}_{\text{algebraic error}}\;.$$

3 Local discretization and global computation

Discrete (piecewise linear) solution

$$u_h \;=\; \sum_{j=1}^{N} \zeta_j \, \phi_j(\eta_1, \eta_2)\,.$$

- If ζ_j is known exactly, then $u_h^{(n)} = u_h$, and the global information is approximated as the linear combination of the local basis functions.

- Apart from trivial cases, ζ_j , which supplies the global information, is not known exactly.

3 Energy norm of the error

Theorem

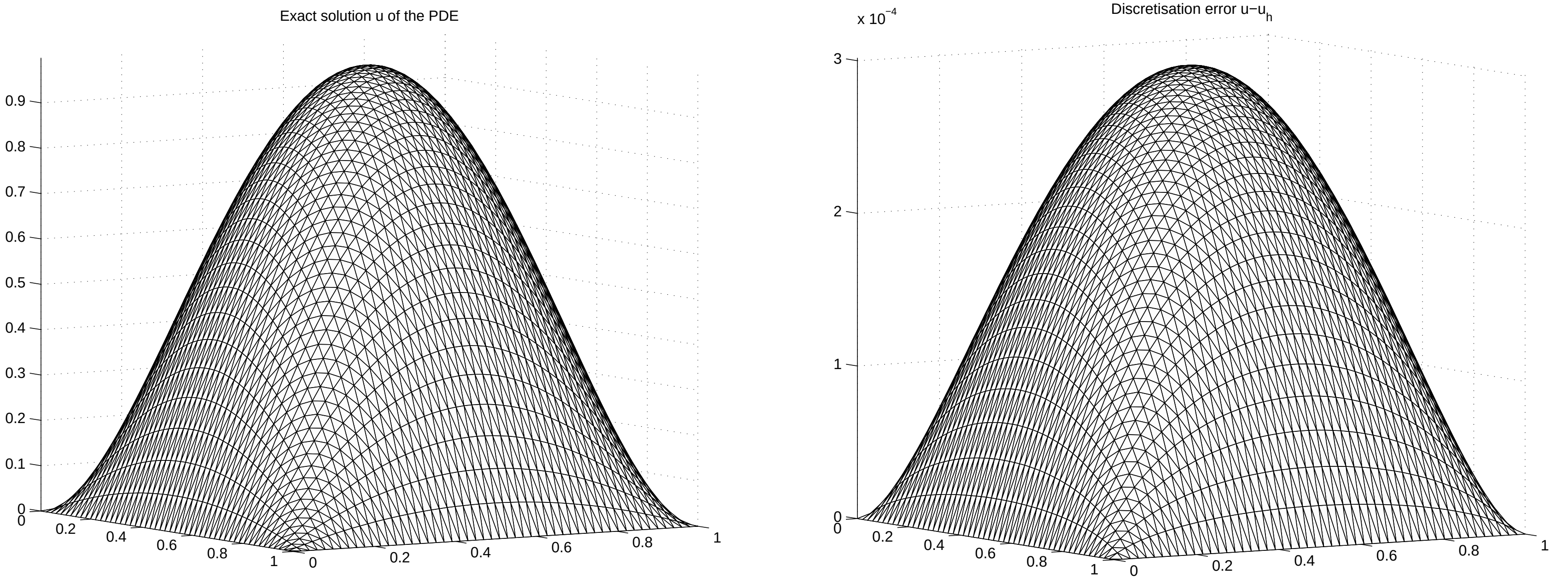
Up to a small inaccuracy proportional to machine precision,

$$\begin{aligned} \|\nabla(u - u_h^{(n)})\|^2 &= \|\nabla(u - u_h)\|^2 + \|\nabla(u_h - u_h^{(n)})\|^2 \\ &= \|\nabla(u - u_h)\|^2 + \|x - x_n\|_A^2 \,. \end{aligned}$$

Using zero Dirichlet boundary conditions,

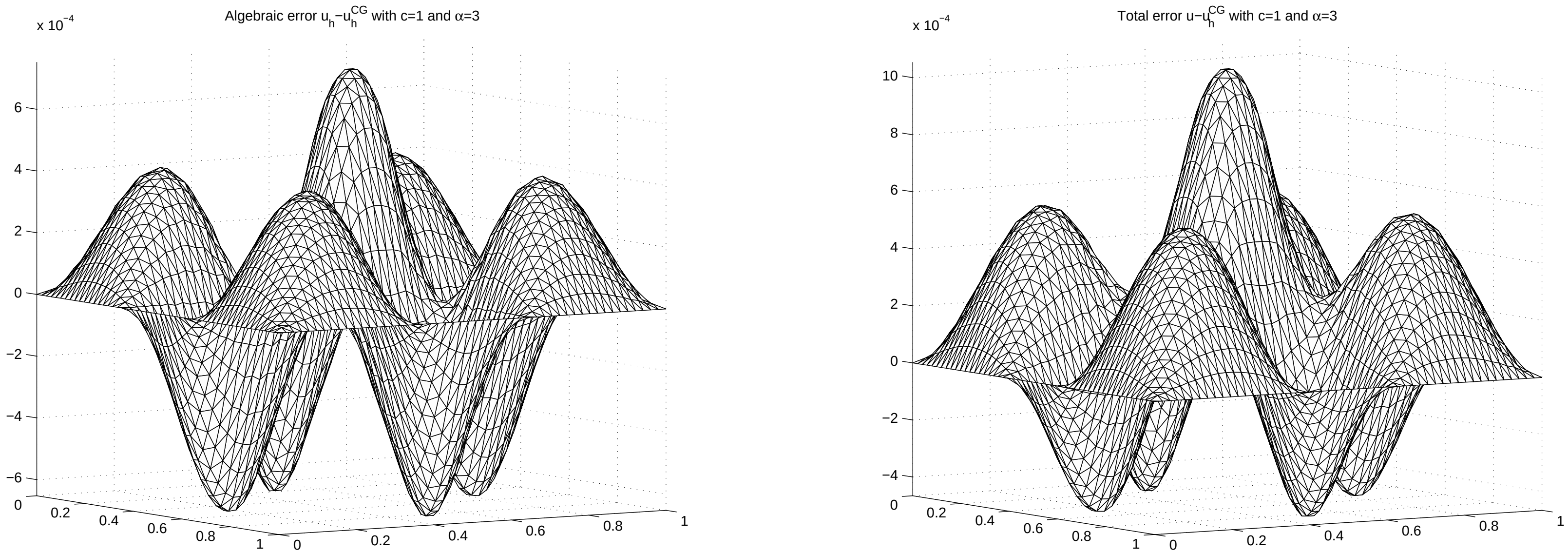
$$\|\nabla(u - u_h)\|^2 = \|\nabla u\|^2 - \|\nabla u_h\|^2 \,.$$

3 Solution and the discretization error



Exact solution u of the Poisson model problem (left)
and the MATLAB `trisurf` plot of the discretization error $u - u_h$ (right).

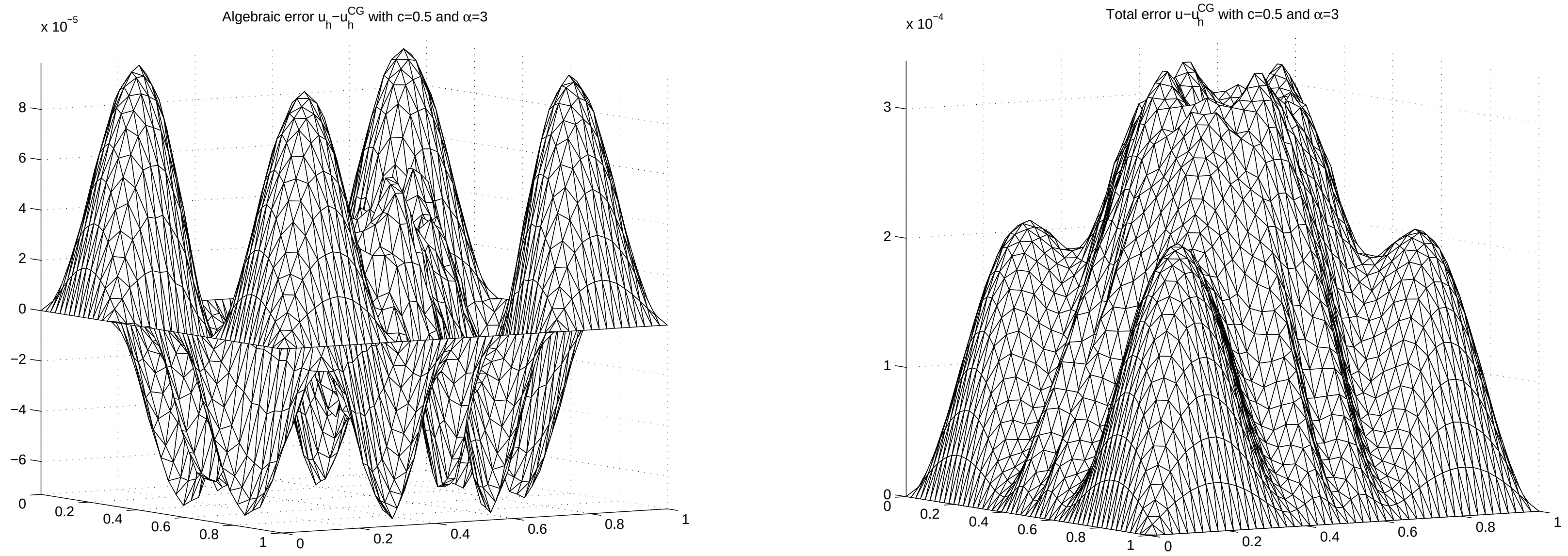
3 Algebraic and total errors



Algebraic error $u_h - u_h^{(n)}$ (left) and the MATLAB `trisurf` plot of the total error $u - u_h^{(n)}$ (right)

$$\begin{aligned} \|\nabla(u - u_h^{(n)})\|^2 &= \|\nabla(u - u_h)\|^2 + \|x - x_n\|_A^2 \\ &= 5.8444e-03 + 1.4503e-05\,. \end{aligned}$$

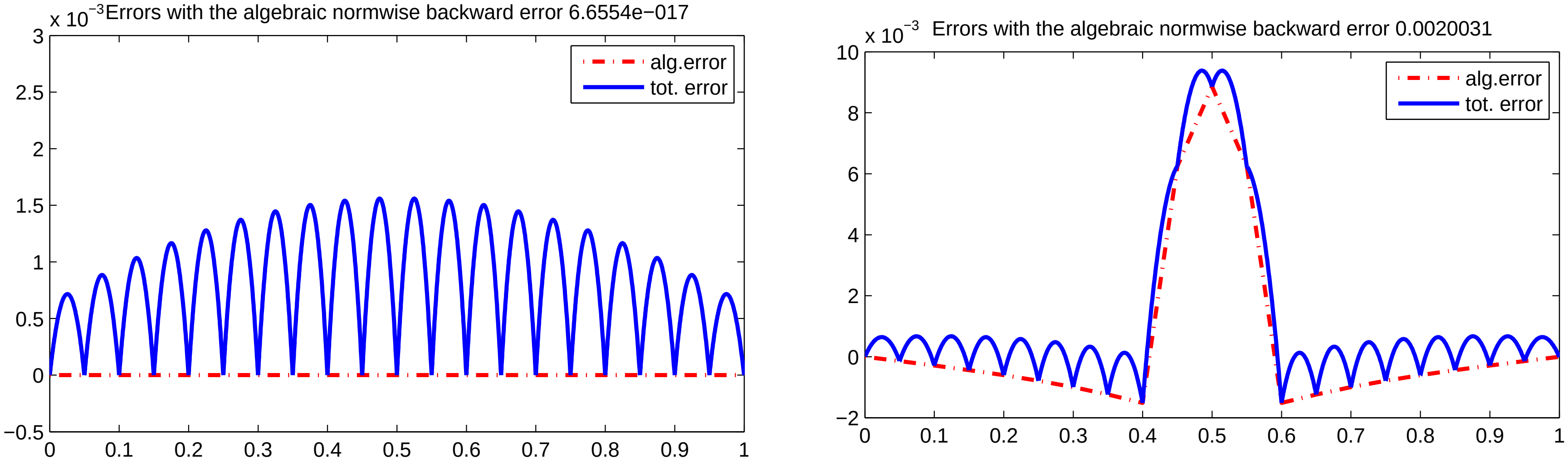
3 Algebraic and total errors



Algebraic error $u_h - u_h^{(n)}$ (left) and the MATLAB `trisurf` plot of the total error $u - u_h^{(n)}$ (right)

$$\begin{aligned} \|\nabla(u - u_h^{(n)})\|^2 &= \|\nabla(u - u_h)\|^2 + \|x - x_n\|_A^2 \\ &= 5.8444e-03 + 5.6043e-07\,. \end{aligned}$$

3 One can see 1D analogy



The discretization error (left),
the algebraic and the total error (right),
Papež (2011).

3 Adaptivity?

We need *a-posteriori* error bounds which are:

- Locally efficient,
- fully computable (no hidden constants),
- and allow to compare the contribution of the discretization error and the algebraic error to the total error.

Conclusions

- History is important for the presence and future.
- An example: Thinking in term of matching moments can be useful.

- Many Thanks and Congratulations!

Ideas and people I

- Euclid (300BC), Hippassus from Metapontum (before 400BC), ... ,
- Bhascara II (1150), Brouncker and Wallis (1655-56): Three term recurences (for numbers)
- Euler (1737, 1748), ... , Brezinski (1991), Khrushchev (2008)
- Gauss (1814), Jacobi (1826), Christoffel (1858, 1857), ... , Chebyshev (1855, 1859), Markov (1884), Stieltjes (1884, 1893-94): Orthogonal polynomials, quadrature, analytic theory of continued fractions, problem of moments, minimal partial realization, Riemann-Stieltjes integral
  Gautschi (1981, 2004), Brezinski (1991), Van Assche (1993), Kjeldsen (1993),
- Hilbert (1906, 1912), ... , Von Neumann (1927, 1932), Wintner (1929) resolution of unity, integral representation of operator functions in quantum mechanics

Ideas and people II

- Krylov (1931), Lanczos (1950, 1952, 1952c), Hestenes and Stiefel (1952), Rutishauser (1953), Henrici (1958), Stiefel (1958), Rutishauser (1959), ... , Vorobyev (1958, 1965), Golub and Welsh (1968), ... , Laurie (1991 - 2001), ...
- Gordon (1968), Schlesinger and Schwartz (1966), Reinhard (1979), ... , Horáček (1983-...), Simon (2007)
- Paige (1971), Reid (1971), Greenbaum (1989), ...
- Magnus (1962a,b), Gragg (1974), Kalman (1979), Gragg, Lindquist (1983), Gallivan, Grimme, Van Dooren (1994), ...

⟶ Euler, Christoffel, Chebyshev (Markov), Stieltjes !

Thank you for your kind patience