Analysis of Krylov subspace methods: Moments, error estimators, numerical stability and unexpected consequences

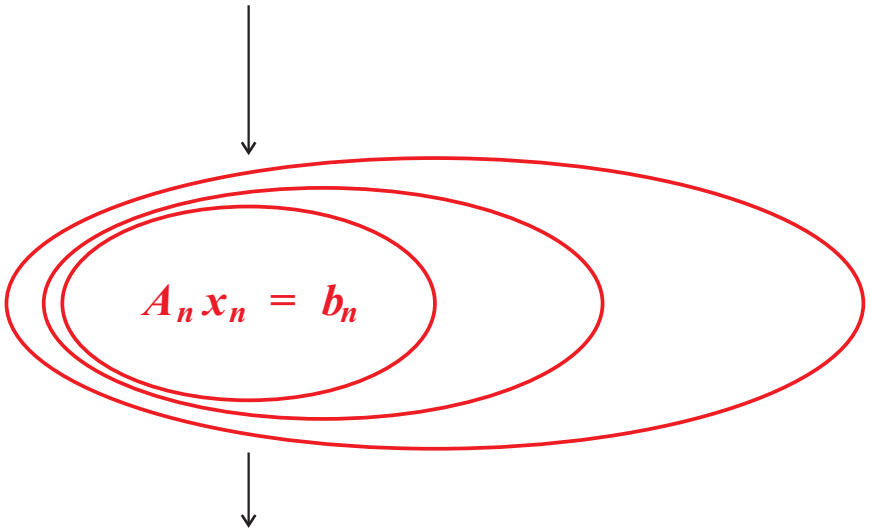
Zdeněk Strakoš
Academy of Sciences and Charles University, Prague
http://www.cs.cas.cz/˜strakos

A joint work with
Dianne P. O'Leary, Chris C. Paige and Petr Tichý

New trends in scientific computing, CIRM, Luminy, February 2009.

Projections on nested subspaces

$$A\,x \;=\; b, \quad A \in R^{N\times N}$$



x_n approximates the solution x
using the subspace of small dimension.

Projection processes

$$x_n \in x_0 + \mathcal{S}_n\,, \quad r_n \equiv b - Ax_n \in r_0 + A\mathcal{S}_n\,,$$

where the constraints needed to determine x_n are given by

$$r_n \perp \mathcal{C}_n\,, \quad \mathcal{C}_n^{\perp} \oplus A\mathcal{S}_n = \mathcal{R}^N\,,$$

$\mathcal{S}_n$ is the search space, $\mathcal{C}_n$ is the constraint space.

$$r_0 = r_0\,|_{A\mathcal{S}_n} + r_0\,|_{\mathcal{C}_n^{\perp}} \equiv r_0\,|_{A\mathcal{S}_n} + r_n\,, \quad r_n \in \mathcal{C}_n^{\perp}\,,$$

the projection should be called orthogonal if $\mathcal{C}_n = A\mathcal{S}_n$,
and it should be called oblique otherwise.
Illustrations using conjugate gradients and GMRES will be given in the next few slides.

Krylov subspace methods

$$\mathcal{S}_n \equiv \mathcal{K}_n \equiv \mathcal{K}_n(A, r_0) \equiv span\,\{r_0, Ar_0, \cdots, A^{n-1}r_0\}.$$

Krylov subspaces accumulate the dominant information of A with respect to r_0. Unlike in the power method for computing the single dominant eigenspace, here all the information accumulated along the way is used,

see Parlett (1980), Example 12.1.1.

The idea of projections using Krylov subspaces is in a fundamental way linked with the problem of moments.

Conjugate gradients (CG)

$$\|x - x_n\|_A \;=\; \min_{u \,\in\, x_0 + \mathcal{K}_n(A,r_0)} \|x - u\|_A$$

with the formulation via the Lanczos process, $w_1 = r_0/\|r_0\|$,

$$A\,W_n \;=\; W_n\,T_n \;+\; \delta_{n+1} w_{n+1} e_n^T\,, \quad T_n \;=\; W_n^T(A)\,A\,W_n(A)\,,$$

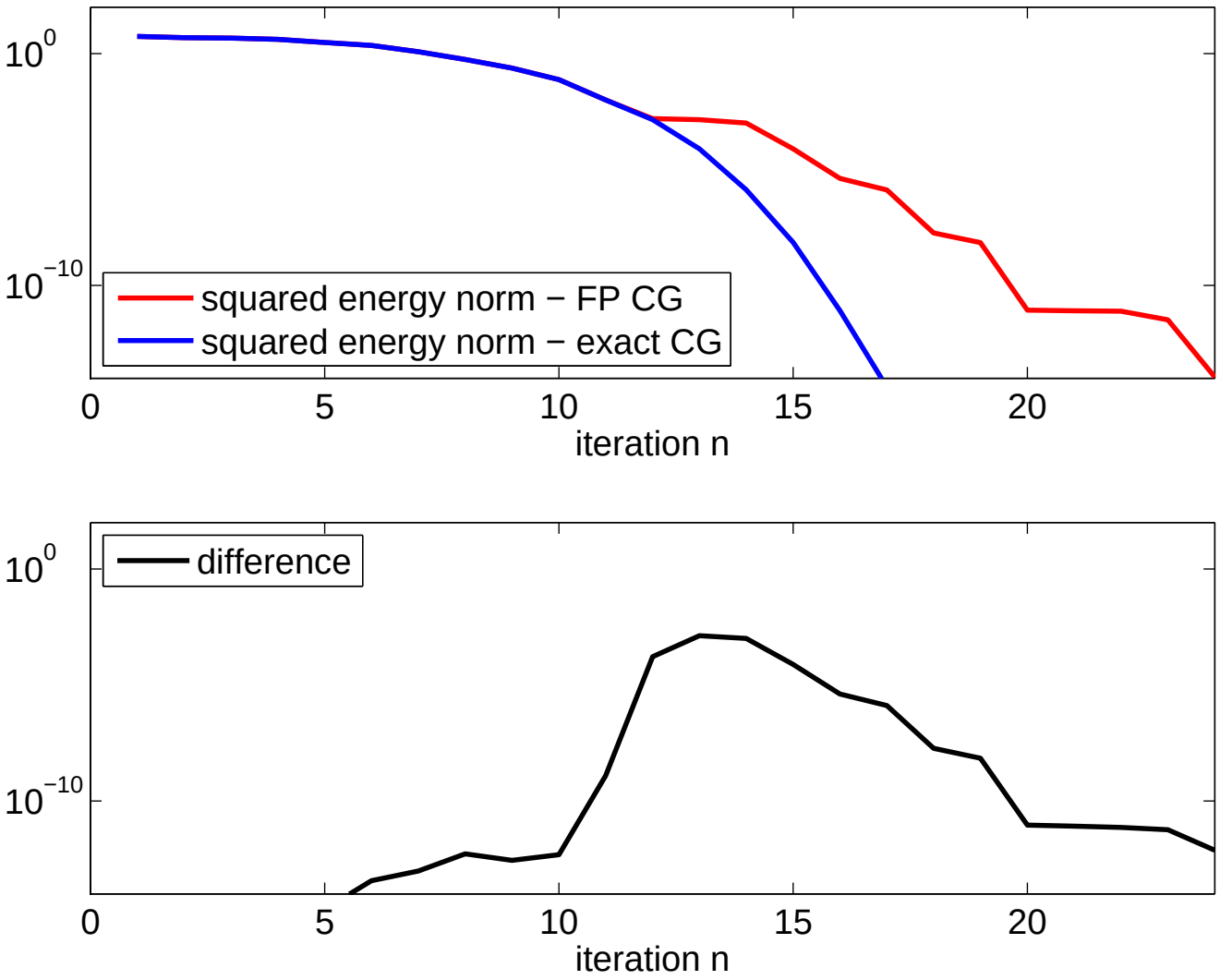
and the CG approximation given by

$$T_n\,y_n \;=\; \|r_0\| e_1\,, \quad x_n \;=\; x_0 \;+\; W_n\,y_n\,.$$

In terms of projection processes

$$\mathcal{S}_n = \mathcal{C}_n \equiv \mathcal{K}_n(A, r_0) = \mathcal{R}(W_n)\,, \quad r_n = (-1)^n w_{n+1}\|r_n\| \perp \mathcal{R}(W_n) = \mathcal{C}_n\,.$$

Motivation I: CG in finite precision arithmetic



Motivation I: CG in finite precision arithmetic

A is diagonal positive definite, see S (1991), Greenbaum, S (1992),

$$\lambda_i \;=\; \lambda_1 \,+\, \frac{i-1}{N-1}\,(\lambda_N - \lambda_1)\,\gamma^{N-i}\,, \quad i = 2, \ldots, N-1,$$

In the experiment we take $\lambda_1 = 0.1$, $\lambda_N = 100$, $N = 24$, $\gamma = 0.55$.

Initial residual has been generated randomly.

Motivation I: Observations

- Rounding errors can cause large delays.
- They may cause an irregular staircase-like behaviour.
- Local decrease of error says nothing about the total error.
- Stopping criteria must be based on global information.
- It must be justified by rigorous rounding error analysis.

Golub and S (1994), S and Tichý (2002, 2005),
Meurant and S (Acta Numerica, 2006)

Comput. Methods Appl. Mech. Engrg. (2003).

Error estimation in numerical PDE

Three reasons for including the algebraic errors into the a-posteriori error estimates:

- We need to estimate $|||p - p_h^{(n)}|||$, not $|||p - p_h|||$.
- It can make computations efficient by stopping the iterations after the algebraic error drops to the level not affecting significantly the total error.
- The mesh refinement can in the presence of singularity pass the difficulty from discretisation to computation. Are there practical examples, when the discretisation error is small while the algebraic error due to roundoff is large?

S and Liesen (2005), Jiránek, Vohralík and S (2008).

Generalized minimal residuals (GMRES)

$$\|b - A\,x_n\| \;=\; \min_{u \,\in\, x_0 + \mathcal{K}_n(A,r_0)} \|b - A\,u\|$$

with the formulation via the Arnoldi process

$$A\,W_n \;=\; W_{n+1}\,H_{n+1,n}\,, \quad H_{n+1,n} \;=\; W_{n+1}^T(A)\,A\,W_n(A)\,,$$

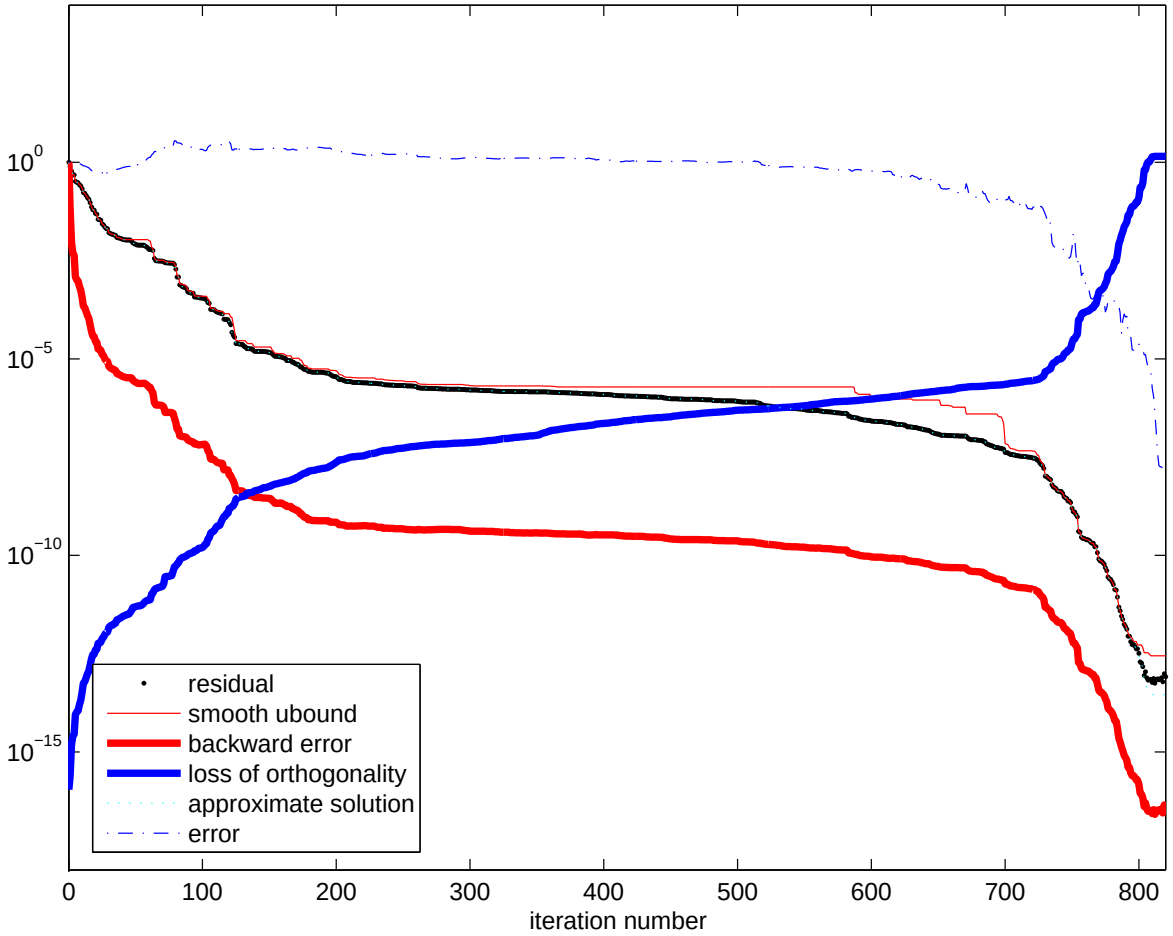
and the GMRES approximation given by

$$y_n \;=\; \arg\min_u \; \|\,\|r_0\|e_1 - \;H_{n+1,n}\,u\|\,, \quad x_n \;=\; x_0 \;+\; W_n\,y_n\,.$$

In terms of projection processes

$$\mathcal{S}_n \equiv \mathcal{K}_n(A,r_0) = \mathcal{R}(W_n)\,,\; \mathcal{C}_n \equiv A\,\mathcal{K}_n(A,r_0) = \mathcal{R}(AW_n)\,, \quad r_n \perp \mathcal{C}_n\,.$$

Motivation II: MGS GMRES in finite precision



Sherman2 from Matrix market, problem rhs.

Motivation II: Observations

- Despite the loss of orthogonality, the modified Gram-Schmidt implementation is as accurate as the Householder reflections-based implementation.
- There is no delay due to rounding errors.
- Loss of orthogonality seems inversely proportional to the normwise backward error.
- Full loss of orthogonality means that the normwise backward error is proportional to machine precision.

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2. Convergence of CG in the presence of close eigenvalues
3. Gauss-Christoffel quadrature can be sensitive to small perturbations of the distribution function
4. Sensitivity of Jacobi matrices to spectral data
5. Back to CG in finite precision arithmetic
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From Gauss-Christoffel quadrature to conjugate gradients and back

1. Gauss-Christoffel quadrature, moments and CG

1 : Matching moments

Consider a non-decreasing distribution function $\omega(\lambda)$, $\lambda \geq 0$ with the moments

$$\xi_k = \int_0^\infty \lambda^k \, d\omega(\lambda) \,, \quad k = 0, 1, \ldots \,.$$

Find the distribution function $\omega^{(n)}(\lambda)$ with n points of increase $\lambda_i^{(n)}$ which matches the first $2n$ moments for the distribution function $\omega(\lambda)$,

$$\int_0^\infty \lambda^k \, d\omega^{(n)}(\lambda) \equiv \sum_{i=1}^{n} \omega_i^{(n)} (\lambda_i^{(n)})^k = \xi_k, \quad k = 0, 1, \ldots, 2n-1 \,.$$

1 : Gauss-Christoffel quadrature

Clearly,

$$\int_0^\infty \lambda^k \, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} (\lambda_i^{(n)})^k \,, \quad k = 0, 1, \ldots, 2n-1$$

represents the n-point Gauss-Christoffel quadrature, see

C. F. Gauss, *Methodus nova integralium valores per approximationem inveniendi,* (1814)

C. G. J. Jacobi, *Uber Gauss' neue Methode, die Werthe der Integrale näherungsweise zu finden,* (1826)

With no loss of generality we assume $\xi_0 = 1$.

1 : Stieltjes recurrence

Let $p_1(\lambda) \equiv 1, p_2(\lambda), \ldots, p_{n+1}(\lambda)$ be the first $n+1$ orthonormal polynomials corresponding to the distribution function $\omega(\lambda)$.

Then, writing $P_n(\lambda) = (p_1(\lambda), \ldots, p_n(\lambda))^T$,

$$\lambda\, P_n(\lambda) \;=\; T_n\, P_n(\lambda) \;+\; \delta_{n+1}\, p_{n+1}(\lambda)\, e_n$$

represents the Stieltjes recurrence, with the Jacobi matrix

$$T_n \equiv \begin{pmatrix} \gamma_1 & \delta_2 & & \\ \delta_2 & \gamma_2 & \ddots & \\ & \ddots & \ddots & \delta_n \\ & & \delta_n & \gamma_n \end{pmatrix}, \quad \delta_l > 0\,.$$

1 : Algebraic connection - Lanczos

Algebraically, T_n represents the result of the Lanczos process applied to T_n with the starting vector e_1. Therefore $p_1(\lambda) \equiv 1, p_2(\lambda), \ldots, p_n(\lambda)$ are orthonormal with respect to the innerproduct

$$(p_s, p_t) \equiv \sum_{i=1}^{n} |(z_i^{(n)}, e_1)|^2 \, p_s(\theta_i^{(n)}) \, p_t(\theta_i^{(n)}) \,,$$

where $z_i^{(n)}$ is the orthonormal eigenvector of T_n corresponding to the eigenvalue $\theta_i^{(n)}$, and $p_{n+1}(\lambda)$ has the roots $\theta_i^{(n)}, i = 1, \ldots, n$.

Consequently,

$$\omega_i^n = |(z_i^{(n)}, e^1)|^2, \quad \lambda_i^{(n)} = \theta_i^{(n)},$$

Golub and Welsh (1969), ... , Meurant and S (2006).

1 : Vector moment problem in CG

Given $Ax = b$ with an SPD $A \in \mathcal{R}^{N\times N}$, $r_0 = b - Ax_0$, $w_1 = r_0/\|r_0\|$. Assume, for simplicity of notation, $\dim(\mathcal{K}_n(A, r_0)) = n$. Find a linear SPD operator A_n on $\mathcal{K}_n(A, r_0)$ such that

$$
\begin{aligned}
A_n\, w_1 &= A\, w_1\,, \\
A_n\,(A\, w_1) \equiv A_n^2\, w_1 &= A^2 w_1\,, \\
&\vdots \\
A_n\,(A^{n-2} w_1) \equiv A_n^{n-1}\, w_1 &= A^{n-1} w_1\,, \\
A_n\,(A^{n-1} w_1) \equiv A_n^{n}\, w_1 &= Q_n\,(A^n w_1)\,,
\end{aligned}
$$

where Q_n projects onto $\mathcal{K}_n$ orthogonally to $\mathcal{C}_n \equiv \mathcal{K}_n$.

Vorobyev (1958 R., 1965 E.), Brezinski (1997), S (2008)

1 : Scalar and vector moment problems

With the spectral decomposition of A and A_n we get the scalar formulation for matching the $2n$ scalar moments given above.

Vorobyev (1958 R.), Chapter III,

with references to Lanczos (1950, 1952), Hestenes and Stiefel (1952), Ljusternik (1956 R., *Solution of problems in linear algebra by the method of continued fractions*), see also Stiefel (1958), Rutishauser (1954, 1959), ...

Extensions to the non-Hermitian Lanzczos and Arnoldi algorithms given in S (2008).

1 : Matching moments model reduction

Estimation of errors in iterative methods, numerical approximation of the scattering amplitude, application in sciences $c^* A^{-1} b$

Dahlquist, Golub and Nash (1978), . . . , Golub and Meurant (1994), . . . , Meurant, S (2006);
Gordon (1968), . . .
Fischer and Freund (1992), Freund and Hochbruck (1993), . . . , Saylor and Smolarski (2001), Golub, Stoll and Wathen (2009), S and Tichý (2009)

Model reduction in approximation of large scale dynamical systems, in terms of the transfer function $T(s) = c^*(sE - A)^{-1}b\,,\ s \in \mathcal{C}_A \subset \mathcal{C}$

Gragg and Lindquist (1983), Villemagne and Skelton (1987), Gallivan, Grimme and Van Dooren (1994), . . . , Bai (2002), Freund (2003), Antoulas (2005), . . . , Guercin and Willcox (2008).

1 : CG $\equiv$ matrix formulation of the Gauss Q

$$
\begin{array}{ccc}
Ax = b\,,\; x_0 & \longleftrightarrow & \displaystyle\int_{\zeta}^{\xi} (\lambda)^{-1}\, d\omega(\lambda) \\
\uparrow & & \uparrow \\
T_n\, y_n \;=\; \|r_0\|\, e_1 & \longleftrightarrow & \displaystyle\sum_{i=1}^{n} \omega_i^{(n)} \left(\theta_i^{(n)}\right)^{-1}
\end{array}
$$

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

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

1 : Interplay between analysis and algebra

The benefits are not always used in the conjugate gradients literature, nor in the computational orthogonal polynomials and Gauss-Christoffel quadrature literature. For the direction from analysis to algebra, it offers an additional insight into CG. For the other direction, the algebraic formulation simplifies some old, and opens some new, questions on quadrature.

Numerical stability analysis of the Lanczos recurrences and of the conjugate gradient method due to

Paige, Parlett, Scott, Simon, Greenbaum, Grcar, Meurant, S, Notay, Druskin, Knizhnermann, Zemke, Wülling

and others is not used in the literature on computation of the Gauss-Christoffel quadrature at all.

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Exact arithmetic !

2 : A particular larger problem

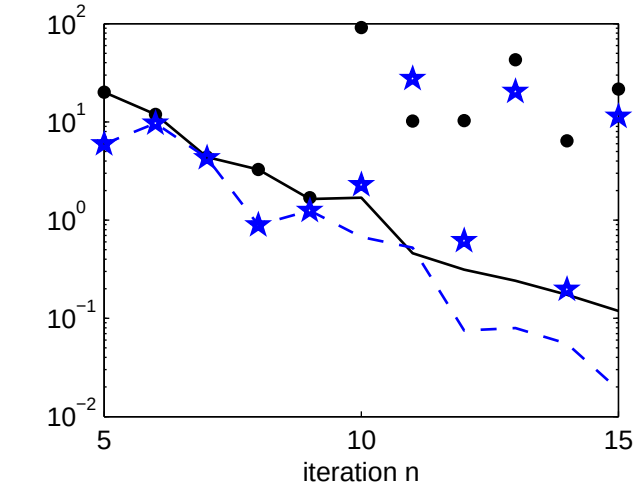
$\hat{A} \in \mathbb{R}^{2N \times 2N}$ diagonal SPD, $\hat{w}_1 \in \mathbb{R}^{2N}$, obtained by replacing each eigenvalue of A by a pair of very close eigenvalues of $\hat{A}$ sharing the weight of the original eigenvalue. In terms of the distribution functions, $\hat{\omega}(\lambda)$ has doubled points of increase but it is very close to $\omega(\lambda)$.

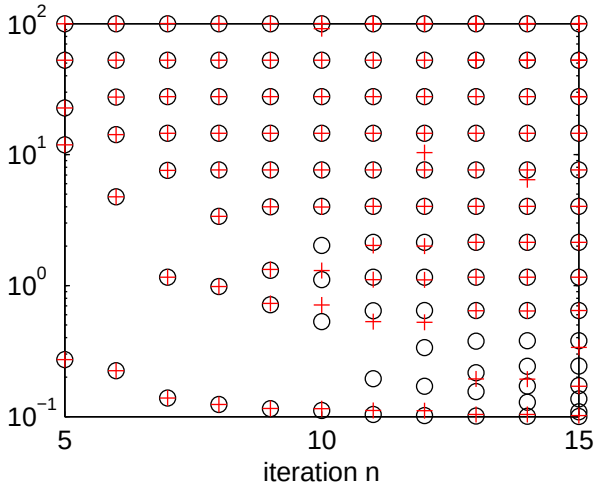
$$\hat{A}, \hat{w}_1 \quad \longrightarrow \quad \hat{T}_n \quad \longrightarrow \quad \hat{T}_{2N} = \hat{W}_{2N}^T \hat{A} \hat{W}_{2N}$$

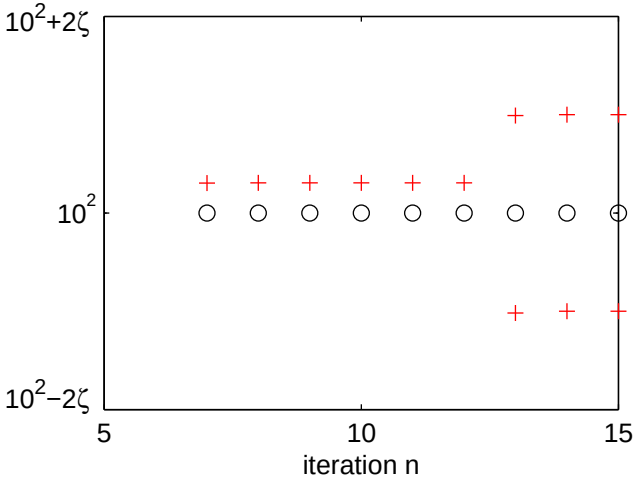
$\hat{T}_{2N}$ has all its eigenvalues close to those of A.

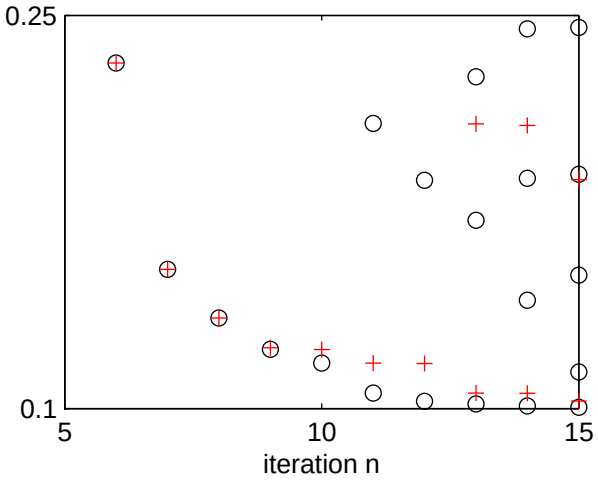
However, $\hat{T}_n$ can be for $n \leq N$ very different from T_n.

2 : Lanczos results for A, w_1 and $\hat{A}, \hat{w}_1$:

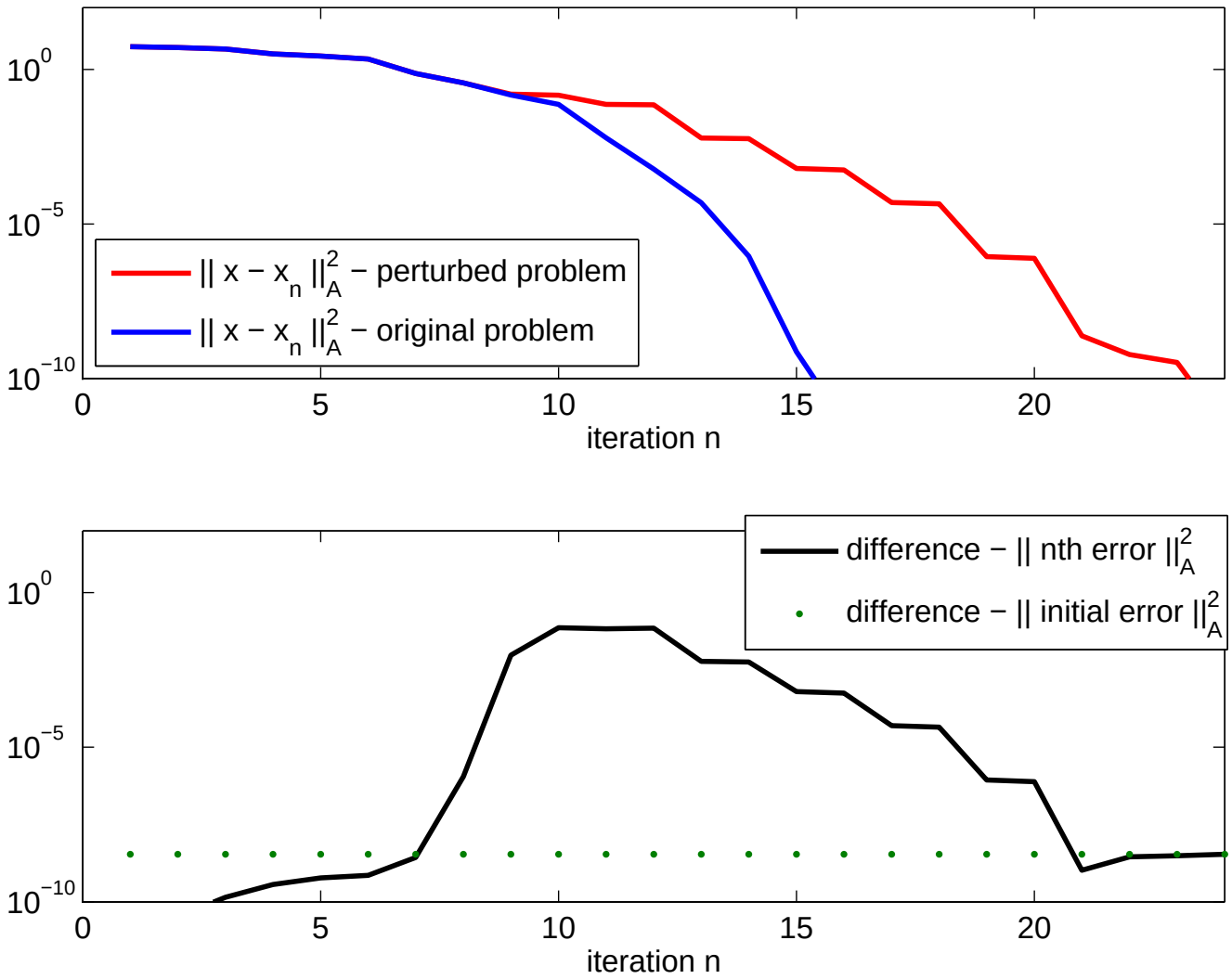








2 : CG results for A, w_1 and $\hat{A}, \hat{w}_1$:



2 : Ritz values in the presence of close eig-s

In the presence of very close eigenvalues, a Ritz value in the exact Lanczos or CG method initially converges to the cluster as fast as if the cluster were replaced by a single eigenvalue with the combined weight.

Within a few further steps it converges very fast to one of the eigenvalues, with another Ritz value converging simultaneously to approximate the rest of the cluster. In the presence of more than two eigenvalues in a cluster, the story repeats until all eigenvalues in a cluster are approximated by individual Ritz values.

The ’additional’ Ritz values in the clusters are, however missing in the other part of the spectrum, and the convergence of CG is delayed, in comparison to the single eigenvalues case, by the number of steps needed to provide the ’missing’ Ritz values.

2 : Consequences

- Replacing single eigenvalues by clusters can cause large delays.
- The presence of close eigenvalues causes an irregular staircase-like behaviour.
- Local decrease of error says nothing about the total error.
- Stopping criteria must be based on the global information.

2 : Published explanations

The fact that the presence of close eigenvalues affects the convergence of Ritz values and therefore the rate of convergence of the conjugate gradient method is well known; see the beautiful explanation given by

van der Sluis and van der Vorst (1986, 1987).

It is closely related to the convergence of the Rayleigh quotient in the power method and to the so-called ‘misconvergence phenomenon’ in the Lanczos method, see

O’Leary, Stewart and Vandergraft (1979),
Parlett, Simon and Stringer (1982).

2 : Caution

Kratzer, Parter and Steuerwalt, *Block splittings for the conjugate gradient method*, Computers and Fluids 11, (1983), pp. 255-279. The statement on p. 261, second paragraph, in our notation says:

> The convergence of CG for A, w_1 and $\hat{A}$, $\hat{w}_1$ ought to be similar; at least $\|\hat{x} - \hat{x}_N\|_{\hat{A}}$ should be small.

Similar statements can be found in several later papers and some books. The arguments are based on relating the CG minimizing polynomial to the minimal polynomial of A. For some distribution of eigenvalues of A, however, its minimal polynomial (normalized to one at zero) can have extremely large gradients and therefore it can be very large at points even very close to its roots (here at the eigenvalues of $\hat{A}$).

Recall the the essence of CG is matching moments!

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3 : CG and Gauss-Ch. quadrature errors

At any iteration step n, CG represents the matrix formulation of the n-point Gauss quadrature of the R-S integral determined by A and r_0,

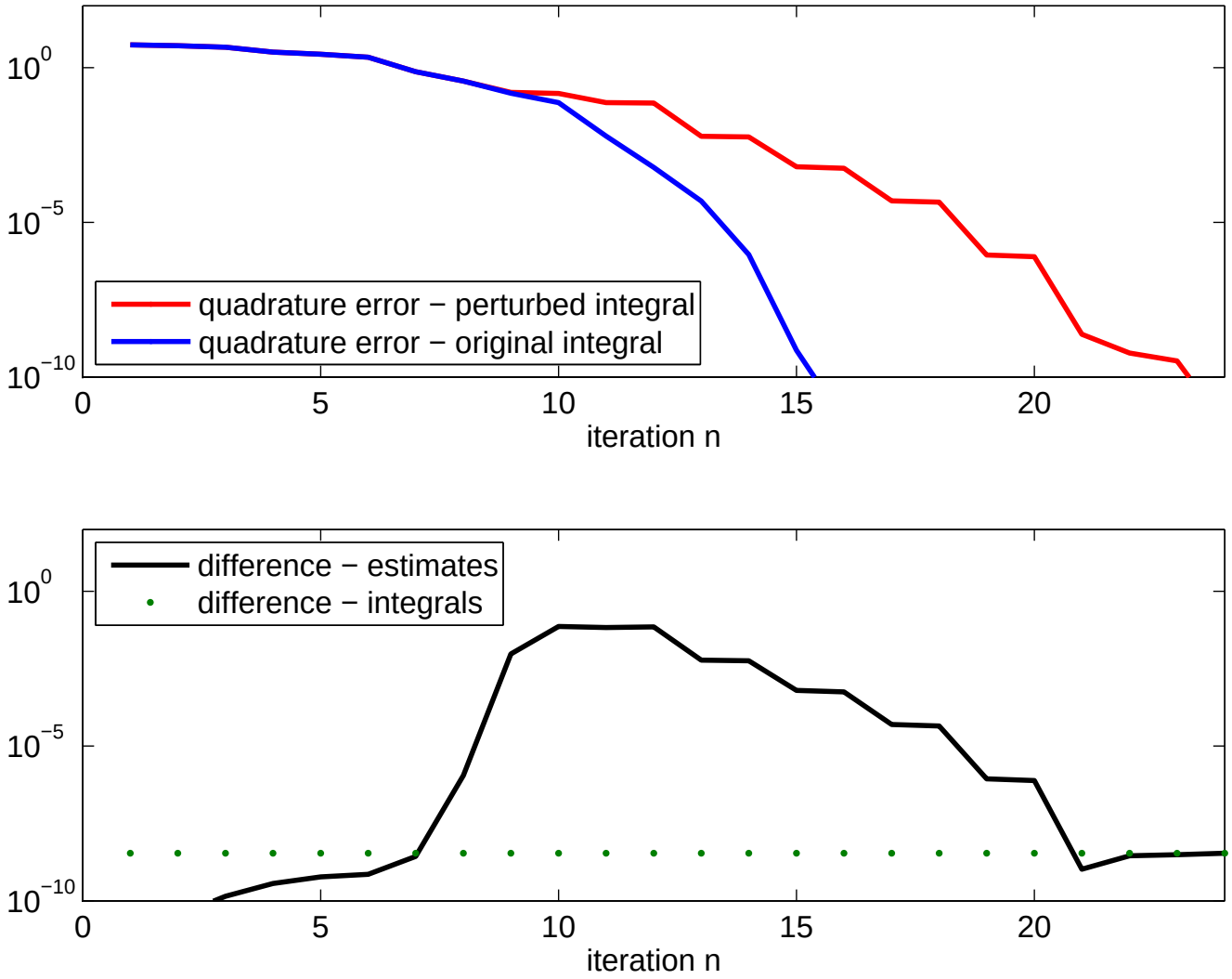
$$\int_{\zeta}^{\xi} f(\lambda)\, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} f(\theta_i^{(n)}) \;+\; R_n(f)\,.$$

For $f(\lambda) \equiv \lambda^{-1}$ the formula takes the form

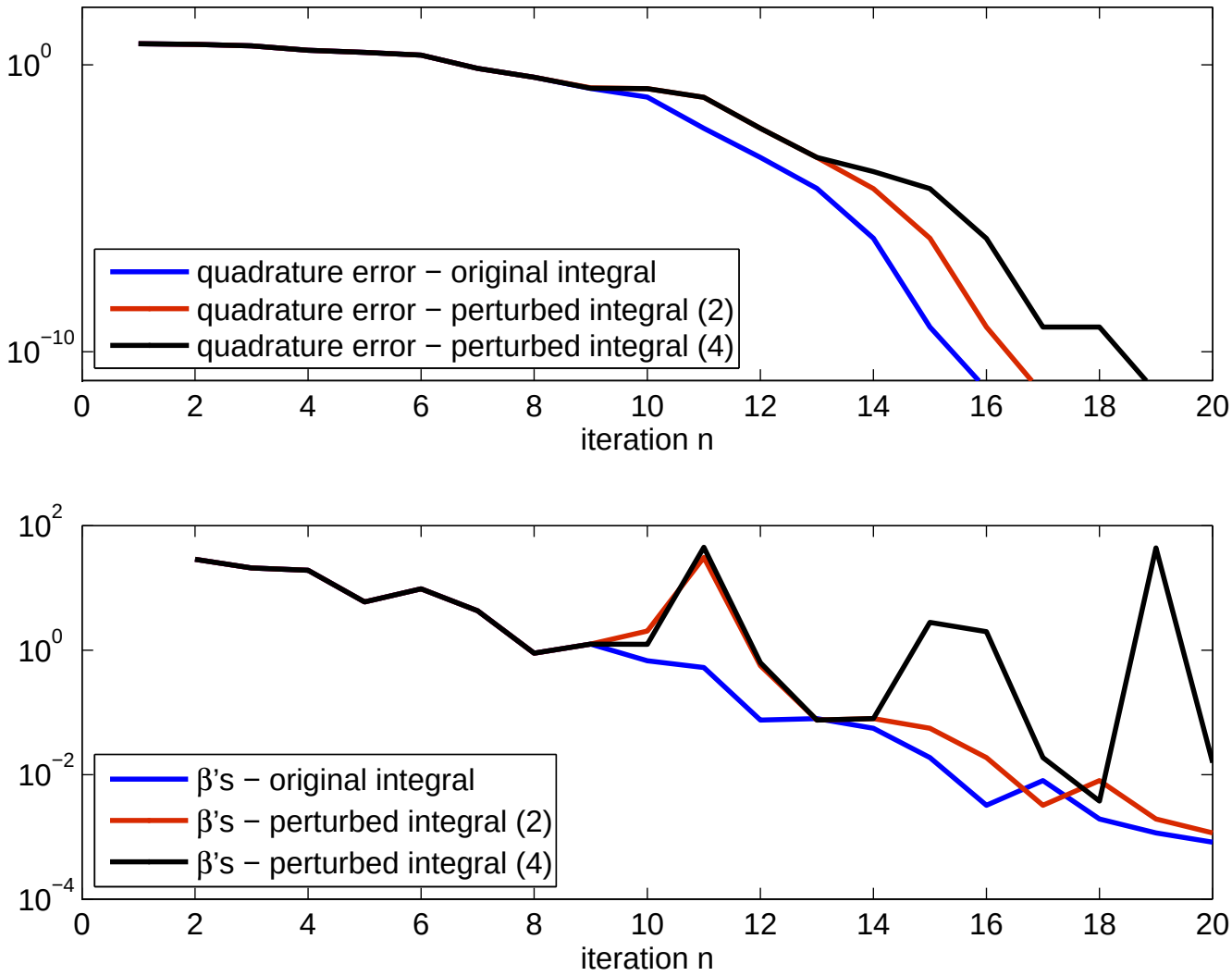
$$\frac{\|x - x_0\|_{\mathbf{A}}^2}{\|r_0\|^2} \;=\; n\text{-th Gauss quadrature} \;+\; \frac{\|x - x_n\|_{\mathbf{A}}^2}{\|r_0\|^2}\,.$$

This was a base for the CG error estimation (see above), survey in Meurant and S (2006).

3 : Sensitivity of the Gauss-Ch. Quadrature



3 : Simplified problem

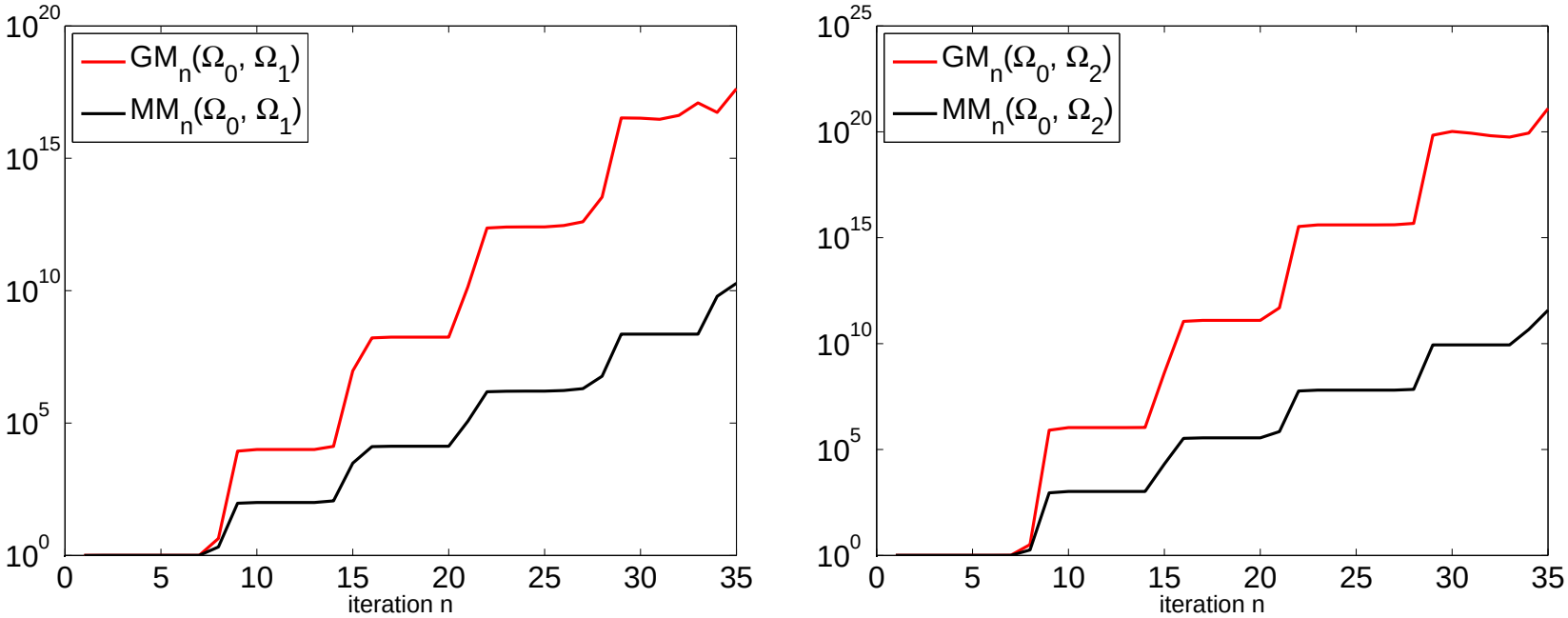


3 : Theorem - O'Leary, S, Tichý (2007)

Consider distribution functions $\omega(x)$ and $\tilde{\omega}(x)$ on $[a,b]$. Let $p_n(x) = (x-x_1)\dots(x-x_n)$ and $\tilde{p}_n(x) = (x-\tilde{x}_1)\dots(x-\tilde{x}_n)$ be the nth orthogonal polynomials corresponding to ω and $\tilde{\omega}$ respectively, with $\hat{p}_s(x) = (x-\xi_1)\dots(x-\xi_s)$ their least common multiple.
If f'' is continuous on $[a,b]$, 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 k-point Gauss-Christoffel quadrature, is bounded as

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

3 : Modified moments do not help



Condition numbers of the matrix of the modified moments (GM) and the matrix of the mixed moments (MM). Left - enlarged supports, right - shifted supports.

3 : Summary

1. Gauss-Christoffel quadrature for a small number of quadrature nodes can be highly sensitive to small changes in the distribution function. 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 and with no singularity close to the interval of integration.

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4 : Sensitivity of the Lanczos recurrences

$A \in \mathbb{R}^{N \times N}$ diagonal SPD,

$$A,\, w_1 \quad \longrightarrow \quad T_n \quad \longrightarrow \quad T_N = W_N^T\, A\, W_N$$

$$A + E,\, w_1 + e \quad \longrightarrow \quad \tilde{T}_n \quad \longrightarrow \quad \tilde{T}_N = \tilde{W}_N^T\, (A + E)\, \tilde{W}_N$$

$\tilde{T}_N$ has all its eigenvalues close to that of A.

Is $\tilde{T}_n$ for sufficiently small perturbations of A, w_1 close to T_n?

4 : Literature on the subject

Gelfand and Levitan (1951), Burridge (1980),
Natterer (1989),
Xu (1993), Druskin, Borcea and Knizhnermann (2005),

Carpraux, Godunov and Kuznetsov (1996), Kuznetsov (1997),
Paige and van Dooren (1999);

Here, however, sensitivity of Krylov subspaces has to be investigated as a part of the problem!

4 : Different view

Computation of the inverse eigenvalue problem - reconstruction of T_N from the nodes and weights:

Stieltjes (1884),

de Boor and Golub (1978), Gautschi (1982, 1983, 2004, 2005),
Gragg and Harrod (1984),
Boley and Golub (1987), Reichel (1991), H. J. Fischer (1998),

Rutishauser (1957, 1963, 1990), Fernando and Parlett (1994), Parlett (1995), Parlett and Dhillon (97),

Laurie (99, 01);

4 : Accurate recovery of recursion coefficients

Laurie (99): A constructive proof of the following statement:

Given the weights and the $N-1$ positive differences between the consecutive nodes, the main diagonal entries of the corresponding Jacobi matrix (shifted by the smallest node) and the off-diagonal entries can be computed in $\frac{9}{2}N^2+O(N)$ arithmetic operations, all of which can involve only addition, multiplication and division of positive numbers.

Consequently, in finite precision arithmetic they can be computed to a relative accuracy no worse than $\frac{9}{2}N^2\varepsilon+O(N\varepsilon)$, where ε denotes machine precision.

4 : Sensitivity result

Laurie (99, 01): This result also bounds the conditioning of the problem:

If the weights and the $N-1$ positive differences between the consecutive nodes are perturbed, with the size of the relative perturbations of the individual entries bounded by some small ϵ , then such a perturbation cannot cause a relative change of larger than $\frac{9}{2}N^2\epsilon + O(N\epsilon)$ in the individual entries of the shifted main diagonal or off-diagonal of the Jacobi matrix.

The resulting algorithm combines ideas from earlier works from approximation theory, orthogonal polynomials, and numerical linear algebra.

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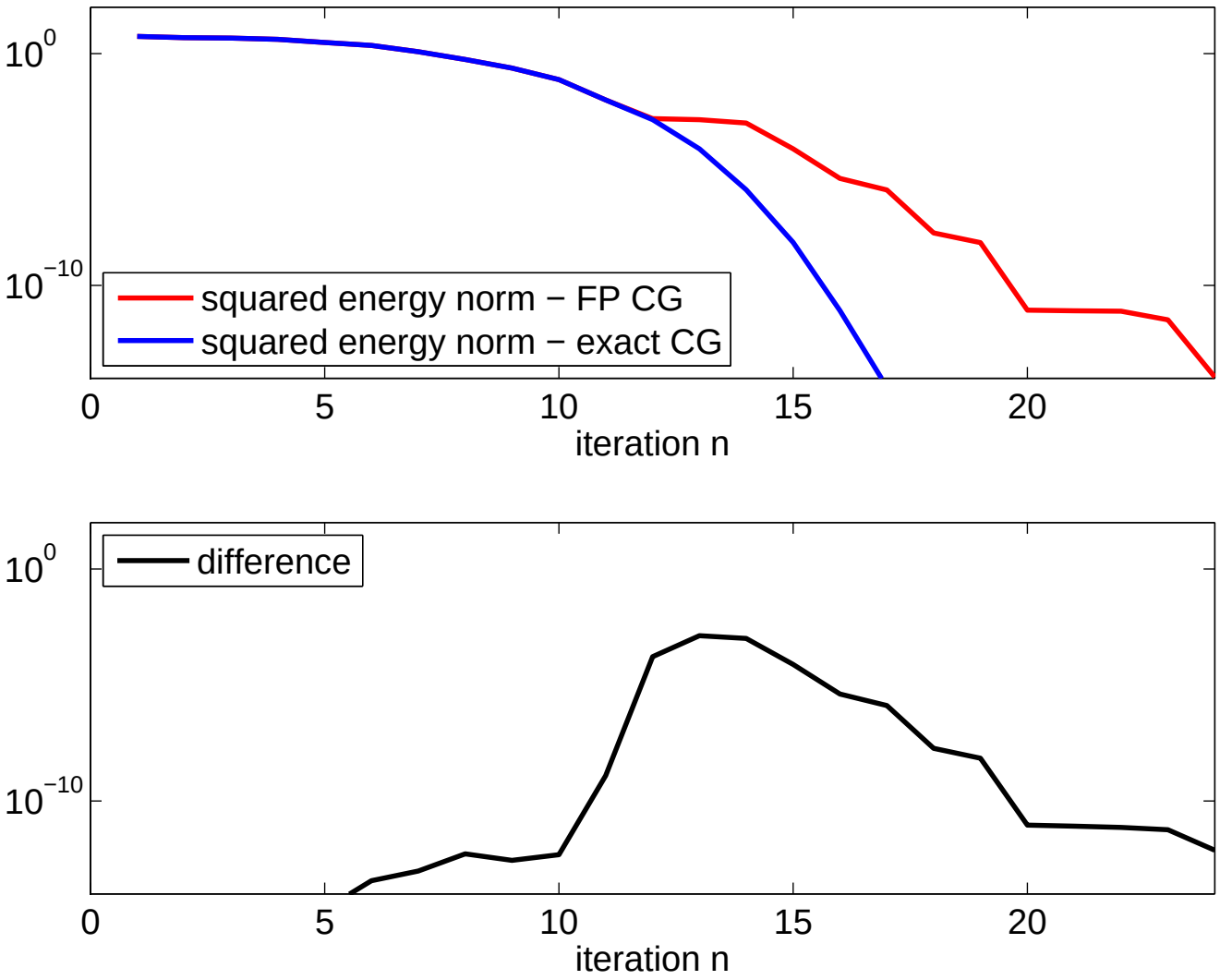
5 : CG in finite precision arithmetic



5 : Back to finite precision CG

Mathematical model of finite precision Lanczos and CG computations, see

Paige (1971–80), Greenbaum (1989),
S (1991), Greenbaum and S (1992),
(also Parlett (1990)),

Recent review and update in Meurant and S (2006).

Numerical stability of MGS GMRES

and core problems

in errors-in-variables modeling

Outline

1. Gauss-Christoffel quadrature, moments and CG
2. Convergence of CG in the presence of close eigenvalues
3. Gauss-Christoffel quadrature can be sensitive to small perturbations of the distribution function
4. Sensitivity of Jacobi matrices to spectral data
5. Back to CG in finite precision arithmetic
6. From MGS GMRES to updating of singular values
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6 : Generalized minimal residuals (GMRES)

$$\|b - A\,x_n\| = \min_{u \in x_0 + \mathcal{K}_n(A,r_0)} \|b - A\,u\|$$

$$= \min_y \; \|\,\|r_0\|\,w_1 - A\,W_n\,y\|\,.$$

Observation (exact arithmetic): $\|b - A\,x_n\|$ small $\longrightarrow$

w_1 must be well approximated by the columns of $A\,W_n$.

In order to describe the relationship quantitatively while suppressing the influence of $\|b\|,\ \|A\|$ and $\|x_n\|$, it seems convenient to relate

$$\frac{\|b - A\,x_n\|}{\|b\| + \|A\|\|x_n\|} \quad \text{with} \quad \kappa\left(\left[w_1, \frac{1}{\|A\|}\,A\,W_n\right]\right)\,.$$

6 : Updating the smallest singular value

Paige, S (2002, SISC)

$$\frac{1}{\sqrt{2}} \;\le\; \frac{\|b - A\,x_n\|}{\|b\| + \|A\|\|x_n\|}\;\kappa\left(\left[w_1, \frac{1}{\|A\|}\,A\,W_n\right]\right) \;\le\; \frac{\sqrt{2}}{1-\delta_n^2}\,,$$

where

$$\delta_n \;=\; \frac{\sigma_{\min}\left(\left[w_1, \frac{1}{\|A\|}\,A\,W_n\right]\right)}{\sigma_{\min}\left(\left[\frac{1}{\|A\|}\,A\,W_n\right]\right)}\,.$$

When does the smallest singular value not change (or change a little) while updating a column?

6 : Solution - TLS fundamentals

Paige, S (2002, Numerische Math. I) gave the solution within the context of the orthogonally invariant linear approximation problem:

$\tilde{A}$ nonzero N by M matrix, $\tilde{b}$ nonzero N-vector,

$$\tilde{A}\,\tilde{x} \;\approx\; \tilde{b}, \qquad (\tilde{A}^T\,\tilde{b} \neq 0 \quad \text{for simplicity}),$$

where $\approx$ means using data corrections of the prescribed type in order to get the nearest compatible system. When errors are contained in both $\tilde{A}$ and $\tilde{b}$,

$$(\tilde{A} + \tilde{E})\,\tilde{x} \;=\; \tilde{b} + \tilde{r}, \quad \min \|[\tilde{r},\, \tilde{E}]\|_F,$$

which represents the total least squares problem (TLS).

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7 : Sufficient condition for TLS solution

Theorem

If $\sigma_{\min}(\tilde{A}) > \sigma_{\min}([\tilde{b}, \tilde{A}])$, then the unique TLS solution is given by

$$[\tilde{b}, \tilde{A}] = \tilde{U}\,\tilde{\Sigma}\,\tilde{V}^T = \sum_{i=1}^{k+1} \tilde{u}_i\,\tilde{\sigma}_i\,\tilde{v}_i^T, \quad \tilde{v}_{k+1} = \begin{bmatrix} \nu \\ w \end{bmatrix},$$

$$\tilde{x} = -\frac{1}{\nu}\,w, \quad [\tilde{r}, \tilde{E}] = -\,\tilde{u}_{k+1}\,\tilde{\sigma}_{k+1}\,\tilde{v}_{k+1}^T.$$

Golub and Reinsch (1970), Golub (1973), van der Sluis (1975), Golub and Van Loan (1980), Golub, Hoffman and Stewart (1987).

7 : Remaining difficulty

The condition $\sigma_{\min}(\tilde{A}) > \sigma_{\min}([\tilde{b}, \tilde{A}])$ is sufficient, but not necessary. If

$$\sigma_{\min}(\tilde{A}) = \sigma_{\min}([\tilde{b}, \tilde{A}]),$$

then there might be a solution, or it can happen that the TLS formulation does not have a solution.

Van Huffel, Vandewalle (1991) completed the TLS theory in an ingenious but complicated way by introducing the concept of a nongeneric solution, which eliminates some (not all!) unwanted directions in the columnspace of $\tilde{A}$ (nonpredictive colinearities) uncorrelated with the vector $\tilde{b}$.

The TLS theory has been revisited in
Paige and S (2002, NM I + II), Paige and S (2006).

7 : Core problem theorem

Let B be a nonzero N by M real matrix and b a nonzero real $N-$vector, $B^T b \neq 0$. Then there exists a decomposition

$$P^T \left[\begin{array}{c|c} b & BQ \end{array} \right] = \left[\begin{array}{c|c|c} b_1 & B_{11} & 0 \\ \hline 0 & 0 & B_{22} \end{array} \right] ,$$

where $P^{-1} = P^T$, $Q^{-1} = Q^T$, $b_1 = \beta_1 e_1$ and B_{11} is a lower bidiagonal matrix with nonzero bidiagonal elements.

Such a decomposition is given by the Golub-Kahan bidiagonalization of the matrix $[b, B]$. Its properties are:

7 : Core problem theorem - continuation

S1. The matrix B_{11} has full column rank and its singular values are simple. Consequently, any zero singular values or repeats that B has must appear in B_{22}.

S2. The matrix B_{11} has minimal dimensions, and B_{22} has maximal dimensions, over all orthogonal transformations giving the block structure above, without any additional assumptions on the structure of B_{11} and b_1.

S3. All components of $b_1 = \beta_1 e_1$ in the left singular vector subspaces of B_{11}, i.e., the first elements of all left singular vectors of B_{11}, are nonzero.

$B_{11}\, x_1 \approx b_1$ represents the core approximation problem. The core problem contains all necessary and sufficient information for solving the approximation problem with the original data, its TLS solution always exists and it is unique, $x = Q\,[x_1, 0]^T$.

7 : A surprising path

Numerical stability analysis of MGS GMRES led to questions on

nonexistence of the Total Least Squares solution and the LS - TLS relationship, which resulted in the core problem formulation, Paige and S (2006), with an alternative proof based on the properties of Jacobi matrices and the relationship between the Lanczos tridiagonalization and the Golub - Kahan bidiagonalization in Hnětynková and S (2007).

Further developments: Björck (2005a, 2005b), Van Huffel and Sima (2005), Sima (2006), Van Huffel, Hnětynková, Plešinger, Sima and S (200?), Chang, Paige and Titley-Peloquin (2006), ...

Hnětynková, Plešinger, and S (2008) : Noise revealing in discrete ill-posed problems.

7 : A comment on history

Golub and Kahan would clearly have presented the core problem decomposition, together with its properties, SVD-based and {Jacobi matrices, the Lanczos tridiagonalization and the Golub and Kahan bidiagonalization}-based proof, had the use for it been put to them in 1965. The same is undoubtedly true for Paige and Saunders in 1982.

It is worth reading the founding papers.

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8 : Numerical stability of GMRES

Björck (1967), Karlson (1991), Björck and Paige (1992),

Drkošová, Greenbaum, Rozložník and S (1995), Arioli and Fassino (1996), Rozložník (1997), Greenbaum, Rozložník and S (1997),

Paige and S (2002, NM I + II, SISC), Giraud and Langou (2002), Langou (2003), Giraud, Graton and Langou (2007),

Paige, Rozložník, and S (2006):

MGS GMRES is normwise backward stable

Conclusions

- It is good to look for interdisciplinary links and for different lines of thought. Such as linking the Krylov subspace methods with model reduction and matching moments, Gauss-Christoffel quadrature, the inverse eigenvalue problem for Jacobi matrices etc.

- Rounding error analysis of Krylov subspace methods has had unexpected side effects in understanding of general mathematical phenomena independent of any numerical stability issues such as the sensitivity of the Gauss-Christoffel quadrature.

- Analysis of Krylov subspace methods for solving linear problems has to deal with highly nonlinear finite dimensional phenomena.

- The pieces of the mosaic coming from numerical linear algebra, approximation theory, numerical quadrature, matrix theory etc. fit together.

Thank you!