Nonlinear problems in analysis of Krylov subspace methods

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Nonlinear problems in optimization

- Nonlinear problems are solved
  as a sequence of its local linear approximations.

- Order of convergence (p, linear, quadratic, ...) is determined as a limit of a locally evaluated decrease of the error. Convergence is viewed asymptotically. The approach is relevant for evaluation of approximation error in practical computations.

- Computational kernels use efficient solvers for linear algebraic systems $A\,x = b$. Sometimes they aim at highly accurate approximate solution x_n , which is very rare in solving linear algebraic systems arising from discretized integral or differential equations.

Classical linear iterative solvers

Linear stationary iterative methods (Jacobi, Gauss-Seidel, SOR, SSOR), semiterative methods (Chebyshev) and also the steepest descent method for minimizing of quadratic functionals fit within the locally-based asymptotic description frame.

- Construction of the k-th iteration is based on local information (in the Chebyshev method on an estimate of the edges of the spectrum).
- Rate of convergence is described via the asymptotic convergence factors (which means linearization at infinity). The description is independent of the right hand side and initial approximation.
- Apart from a possible transient phase, their behaviour is essentially linear. An example - steepest descent:

$$\|x - x_k\|_A \leq \left(\frac{\kappa - 1}{\kappa + 1}\right)^k \|x - x_0\|_A .$$

Krylov subspace methods

Construction of iterations is in Krylov subspace methods based from the first step on a very complex information about the operator A and its relationship with the right hand side b and the initial approximation x_0. The finite termination property i.e. global information is present in construction of *each iteration.* As a consequence, no meaningful asymptotic, no meaningful linearized description can be used (apart from uninteresting cases).

Identification of the conjugate gradients rate of convergence with the linear bound of Meinardus (1963)

$$\|x - x_k\|_A \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \|x - x_0\|_A ,$$

which is still frequent in the literature, illustrates the persisting locally linearized view which does not consider the fundamental difference between the Krylov subspace and classical iterative methods.

Historical remark

1950 - Iterative methods for elliptic PDE
- Ph.D. Thesis by D. Young at Harvard (published in 1954)

1951, 1952 - Lanczos algorithm, conjugate gradient method
by C. Lanczos, M. Hestenes and E. Stiefel

1962 - Book Matrix Iterative Analysis by R. Varga

1971 - Book Iterative methods by D. Young

1971 - Lecture of J. Reid in Dundee (published in 1971)

1971 - Ph.D. Thesis of C.C. Paige at the University of London
(published in 1972, 1976 and 1980)

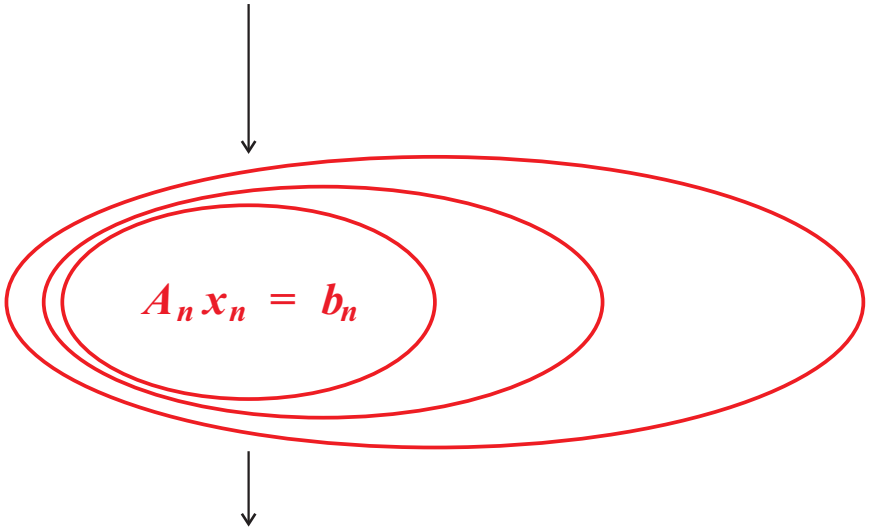
Historical remark (cont.)

- Classical iterative methods naturally responded to finite difference schemes used in discretization of PDE problems which produced banded matrices with nice structure and, in the SPD case, close to homogeneous spectra.

- The mathematical beauty and success of the analysis by Young and Varga may have paradoxically decreased an interest in later analysis of Krylov subspace methods, which is based on different principles and techniques. Though the analysis of classical iterative methods is a part of the common knowledge in computational mathematics, the modern analysis of Krylov subspace methods developed in the last decades is much less known (which is true even within the matrix computation community).

Projections on Krylov subspaces

$$A\,x \;=\; b, \quad A \in \mathbb{R}^{N\times N}, \quad r_0 = b - Ax_0$$



Here x_n approximates the solution x using the projection onto low dimensional subspaces

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

.

Nonlinearity

The projection process using Krylov subspaces is highly nonlinear in A and r_0 .

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

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.

The story goes back to Gauss (1814).

Outline

1. Krylov subspace methods as the problems of moments
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. CG in finite precision arithmetic
5. Spectral information and convergence of GMRES
6. MGS GMRES is normwise backward stable

1. Krylov subspace methods as the problems of moments

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, *Über 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 (1883-4), 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 : Matrix computation: Lanczos $\equiv$ Stieltjes

In matrix computations, T_n results from the Lanczos process (1951) applied to T_n starting with e_1. Therefore $p_1(\lambda) \equiv 1, p_2(\lambda), \ldots, p_n(\lambda)$ are orthonormal with respect to the inner product

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

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 : Model reduction via matching moments I

Polynomial formulation:

$$\int_0^\infty f(\lambda)\, d\omega(\lambda) \;\approx\; \sum_{i=1}^{n} \omega_i^{(n)} f(\lambda_i^{(n)})\,,$$

where the reduced model given by the distribution function with n points of increase $\omega^{(n)}$ matches the first $2n$ moments

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

1 : Linear algebraic equation

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

Consider the spectral decomposition

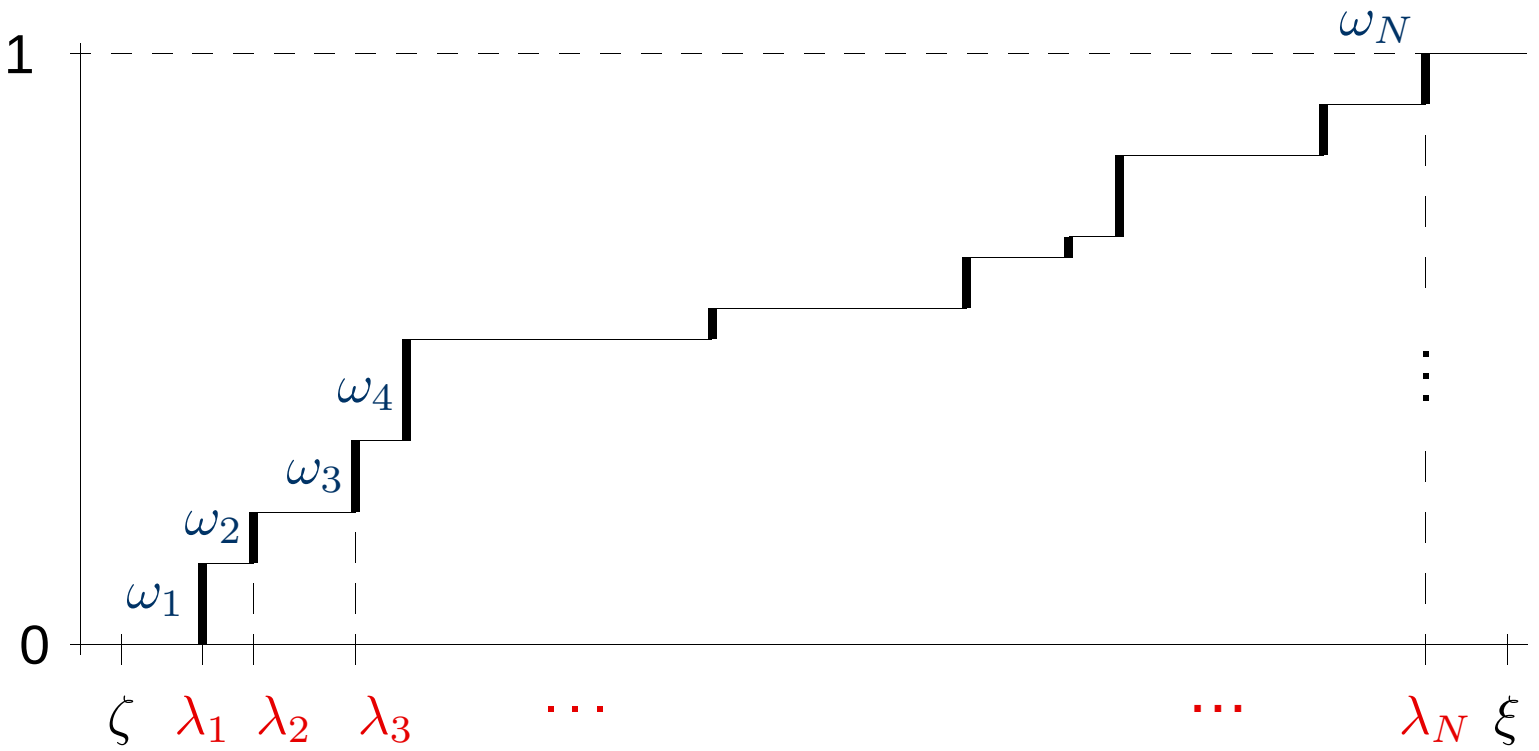
$$A = S\,\mathrm{diag}(\lambda_i)\,S^T ,$$

where for clarity of exposition we assume that the eigenvalues are distinct,

$$0 < \lambda_1 < \ldots < \lambda_N , \quad S = [s_1, \ldots , s_N] .$$

A and $w_1(b, x_0)$ determine the distribution function $\omega(\lambda)$ with
N points of increase λ_i and weights $\omega_i = |(s_i, w_1)|^2$, $i = 1, \ldots , N$.

1 : Distribution function $\omega(\lambda)$



1 : Conjugate gradients (CG) for $Ax = b$

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

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 projections

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

1 : Alternative descriptions

- Stay with A, b, r_0, w_1 and work with the matrix formulation using the Lanczos process (CG) applied to A with w_1 .

- Using the basis of eigenvectors S , the matrix formulation reduces to the mathematically equivalent polynomial formulation, Lanczos (CG) reduces to the Stieltjes process applied to the distribution function $\omega(\lambda)$.

In both descriptions the n-th step gives the Jacobi matrix T_n and the distribution function $\omega_n(\lambda)$.

The relationship was pointed out by Hesteness and Stiefel (1952), . . . nice Ph.D. Thesis by Kent (1989, Stanford), book by B. Fischer (1996), paper by Fischer and Freund (1992).

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

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

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

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

1 : Model reduction via matching moments II

Matrix formulation:

$$\int_0^\infty \lambda^k \, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_j \, (\lambda_j)^k \;=\; w_1^T \, A^k \, w_1 \,,$$

$$\sum_{i=1}^{n} \omega_i^{(n)} \, (\lambda_i^{(n)})^k \;=\; \sum_{i=1}^{n} \omega_i^{(n)} \, (\theta_i^{(n)})^k \;=\; e_1^T \, T_n^k \, e_1 \,.$$

matching the first $2n$ moments therefore means

$$w_1^T \, A^k \, w_1 \;\equiv\; e_1^T \, T_n^k \, e_1 \,, \quad k = 0, 1, \ldots, 2n-1 \,.$$

1 : Equivalent Vector moment problem

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 $\mathcal{K}_n$.

1 : Literature

Vorobyev (1958 R.), Chapter III, (1965 E.)

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*). It has been used and popularized by Brezinski (1997), see also Kent (1989).

Connections to continued fractions and Padé approximation, *qd and LR algoritms* were developed by Stiefel (1958), Rutishauser (1954, 1959), Henrici (1967), Sack and Donovan (1972), . . .

Development towards the applications in dynamical systems and control (partial realization problem) in Gragg (1972), Grag (1974), Gragg and Lindquist (1983), Gallivan, Grimme and Van Dooren (1994), Feldman and Freund (1995), Grimme (1997, Ph.D. Thesis, UIUC), . . .

A nice survey given at the Lanczos Centenary Conference by M. Gutknecht (1993), published (1994).

1 : Literature (cont.)

Proofs of results related to moments are in the literature typically based on factorizations of the matrix of moments, see Golub and Nash (1969), Dahlquist, Golub and Nash (1978), . . . , Kent(1989), . . . , which is also true for the recent comprehensive description of matching moment techniques in dynamical systems and control by Antoulas (2005).

Moment matching techniques has been used (with relationship to orthogonal polynomials, Pade and continued fractions) for decades in computational physics and in computational chemistry, for a remarkable early work see Gordon (1968).

Gauss quadrature interpretation related to the nonsymmetric Lanczos process and to the Arnoldi process was given by Freund and Hochbruck (1993), motivated by the very insightful work on the Hermitian Lanczos process by Fischer and Freund (1992). Interpretation of the nonsymmetric moment matching as a Gauss quadrature in the complex plane was given by Saylor and Smolarski (2001), with references to application in inverse scattering problems in electromagnetics by Warnick (1997), . . .

1 : Proof using Vorobyev moment problem

The elegant formulation of the Vorobyev moment problem gives proofs without using moment matrices or quadrature formulations. This allows straightforward generalizations to nonsymmetric cases (presented later). By construction,

$$w_1^T\, A^k\, w_1 \;=\; w_1^T\, A_n^k\, w_1\,, \quad k = 1, \ldots, n-1\,.$$

Since $\mathcal{K}_n(A, w_1) = \text{span}\{w_1, \ldots, A^{n-1} w_1\}\,,$

$$Q_n\,(A^k\, w_1) \;-\; A_n^k\, w_1 \;=\; Q_n\,(A^k\, w_1 - A_n^k\, w_1) \;=\; 0$$

gives

$$w_1^T\, A^k\, w_1 \;=\; w_1^T\, A_n^k\, w_1\,, \quad k = 0, 1, \ldots, 2n-1\,.$$

1 : Proof using Vorobyev m. p. (cont.)

With the restriction onto $\mathcal{K}_n(A, w_1)$, A_n is uniquely determined by its action on n basis vectors (Q_n leaves the vectors from $\mathcal{K}_n(A, w_1)$ unchanged)

$$A_n\,(A^{j-1}w_1) \;=\; (Q_n\,A)\,(A^{j-1}w_1)\;, \quad j = 1,\,\ldots\,n\,.$$

Consequently, using the ON basis W_n with $Q_n = W_n W_n^T$,

$$\begin{aligned} A_n &= Q_n\,A \;=\; W_n W_n^T\,A\,, \\ A_n^k &= W_n\,(W_n^T\,A\,W_n)^{k-1}\,W_n^T\,A \;=\; W_n\,T_n^{k-1}\,W_n^T\,A \end{aligned}$$

which finally gives

$$w_1^T\,A^k\,w_1 \;=\; w_1^T\,A_n^k\,w_1 = \; e_1^T\,T_n^k\,e_1\;, \quad k = 0, 1,\,\ldots\,, 2n-1\,.$$

1 : Nonsymmetric Lanczos

Given a nonsingular $A \in \mathbb{R}^{N\times N}$, $v \in \mathbb{R}^N$, $w \in \mathbb{R}^N$, $v^T w = 1$.

The nonsymmetric Lanczos algorithm can be written in the form

$$
\begin{aligned}
A\,W_n &= W_n\,T_n + \delta_{n+1}\,w_{n+1}\,e_n^T, \\
A^T\,V_n &= V_n\,T_n^T + \beta_{n+1}\,v_{n+1}\,e_n^T,
\end{aligned}
$$

$$
V_n^T\,W_n = I_n, \quad T_n = V_n^T(A, v_1, w_1)\,A\,W_n(A, v_1, w_1).
$$

We assume that the algorithm does not break down
in steps 1 through n.

1 : Nonsymmetric Lanczos (cont.)

Here

$$T_n \equiv \begin{pmatrix} \gamma_1 & \beta_2 & & \\ \delta_2 & \gamma_2 & \ddots & \\ & \ddots & \ddots & \beta_n \\ & & \delta_n & \gamma_n \end{pmatrix}, \quad \beta_l > 0,\, \delta_l \neq 0\,,$$

The columns of W_n form a basis of $\mathcal{K}_n(A, w_1)$, while the columns of V_n a basis of $\mathcal{K}_n(A_T, v_1)$. Since $V_n^T W_n = I_n$ the oblique projector onto $\mathcal{K}_n(A, w_1)$ orthogonal to $\mathcal{K}_n(A^T, v_1)$ can be written as

$$Q_n = W_n V_n^T .$$

1 : Matching moments in nonsymmetric L.

We will prove that under the given assumption the nonsymmetric Lanczos represents the model reduction which matches the first $2n$ moments

$$v_1^T A^k w_1 \equiv e_1^T T_n^k e_1 , \quad k = 0, 1, \ldots, 2n-1 .$$

1 : Vorobyev moment problem for N. L.

Find a linear operator A_n on $\mathcal{K}_n(A, w_1)$ such that

$$\begin{aligned} A_n\, w_1 &= A\, w_1\,, \\ A_n\, (A\, w_1) &= A^2\, w_1\,, \\ &\vdots \\ A_n\, (A^{n-2}\, w_1) &= A^{n-1}\, w_1\,, \\ \\ A_n\, (A^{n-1} w_1) &= (W_n\, V_n^T)\, (A^n w_1)\,. \end{aligned}$$

Analogously to the symmetric Lanczos

$$v_1^T\, A^k\, w_1 \;\equiv\; v_1^T\, A_n^k\, w_1\,, \quad k = 0, 1, \ldots, 2n-1\,.$$

1 : Final step

Since

$$
\begin{aligned}
A_n &= Q_n A = W_n V_n^T A\,, \\
A_n^k &= W_n (V_n^T A W_n)^{k-1} V_n^T A = W_n T_n^{k-1} V_n^T A\,,
\end{aligned}
$$

$$
V_n^T A_n^k W_n = T_n^k\,,
$$

we finally get

$$
v_1^T A^k w_1 = v_1^T A_n^k w_1 = e_1^T T_n^k e_1\,, \quad k = 0, 1, \ldots, 2n-1\,.
$$

1 : 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, $w_1 \;=\; r_0/\|r_0\|\,,$

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

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 projections

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

1 : Arnoldi moment matching

We will not give the Vorobyev moment problem description of GMRES (which would require a slight generalization), but of the Arnoldi process:

Find a linear operator A_n on $\mathcal{K}_n(A, w_1)$ such that

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

Consider $v_1 \in \mathbb{R}^N$, $\|v_1\| = 1$.

1 : Final step

Due to the nonsymmetry of A , the last line of the Vorobyev moment problem can not be used for extension of the moment matching beyond n moments:

$$v_1^T A^k w_1 \equiv v_1^T A_n^k w_1 , \quad k = 0, 1, \ldots, n-1 .$$

Since

$$\begin{aligned} A_n &= Q_n A = W_n W_n^T A , \\ A_n^k &= W_n (W_n^T A W_n)^{k-1} W_n^T A = W_n T_n^{k-1} W_n^T A , \\ & W_n^T A_n^k W_n = T_n^k , \end{aligned}$$

we finally get

$$w_1^T A^k w_1 = w_1^T A_n^k w_1 = e_1^T T_n^k e_1 , \quad k = 0, 1, \ldots, n-1 .$$

Outline

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Exact arithmetic !

2 : Basic problem

$A \in \mathbb{R}^{N\times N}$ is diagonal positive definite (SPD),
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 (starting vector $w_1 \in \mathbb{R}^N$) has been generated randomly.
Lanczos process:

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

2 : A particular larger problem

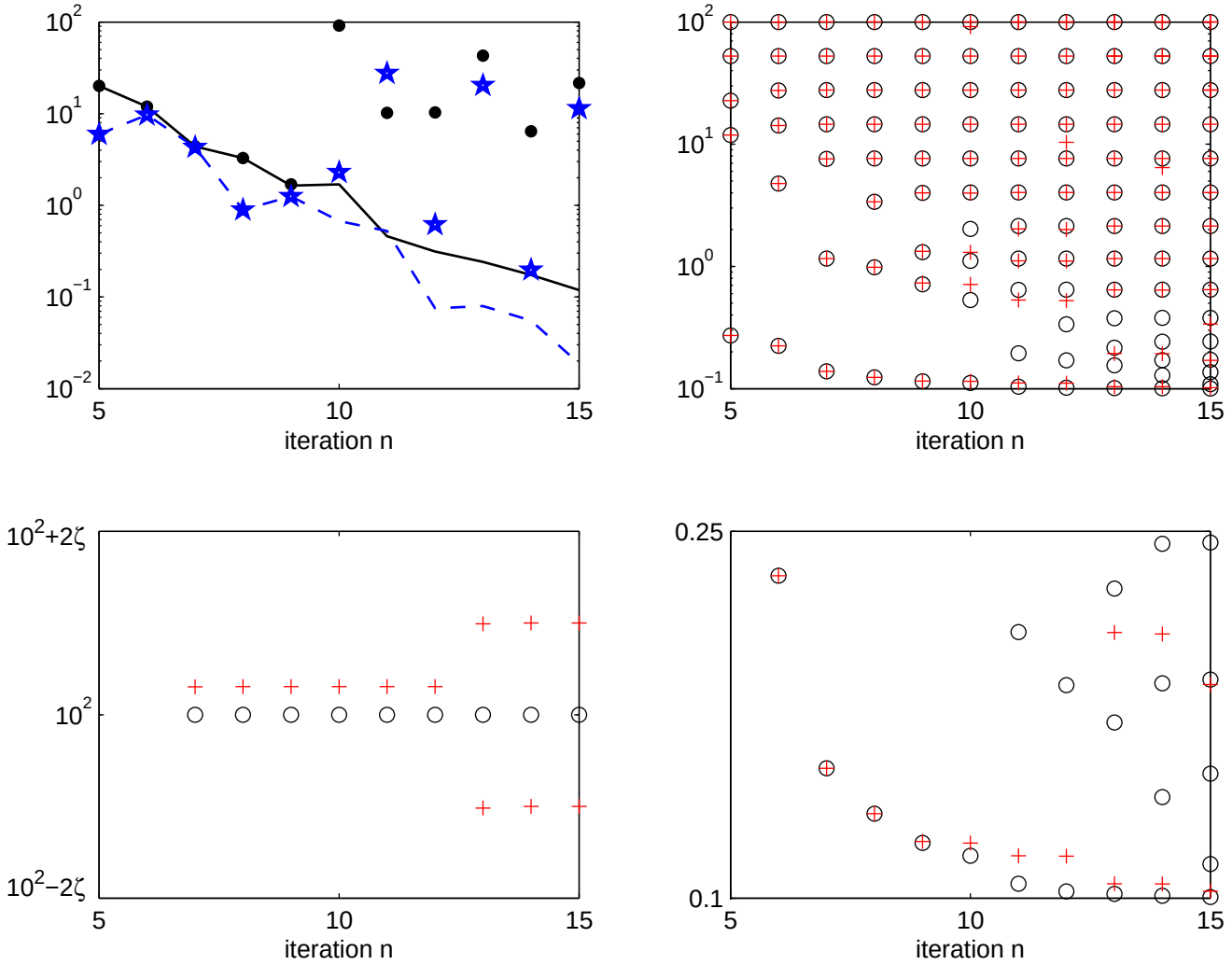
$\hat{A} \in \mathbb{R}^{2N \times 2N}$ diagonal SPD, $\hat{w}_1 \in \mathbb{R}^{2N}$, obtained by replacing each eigenvalue of A by a pair of very close eigenvalues of $\hat{A}$ sharing the weight of the original eigenvalue. In terms of the distribution functions, $\hat{\omega}(\lambda)$ has doubled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

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

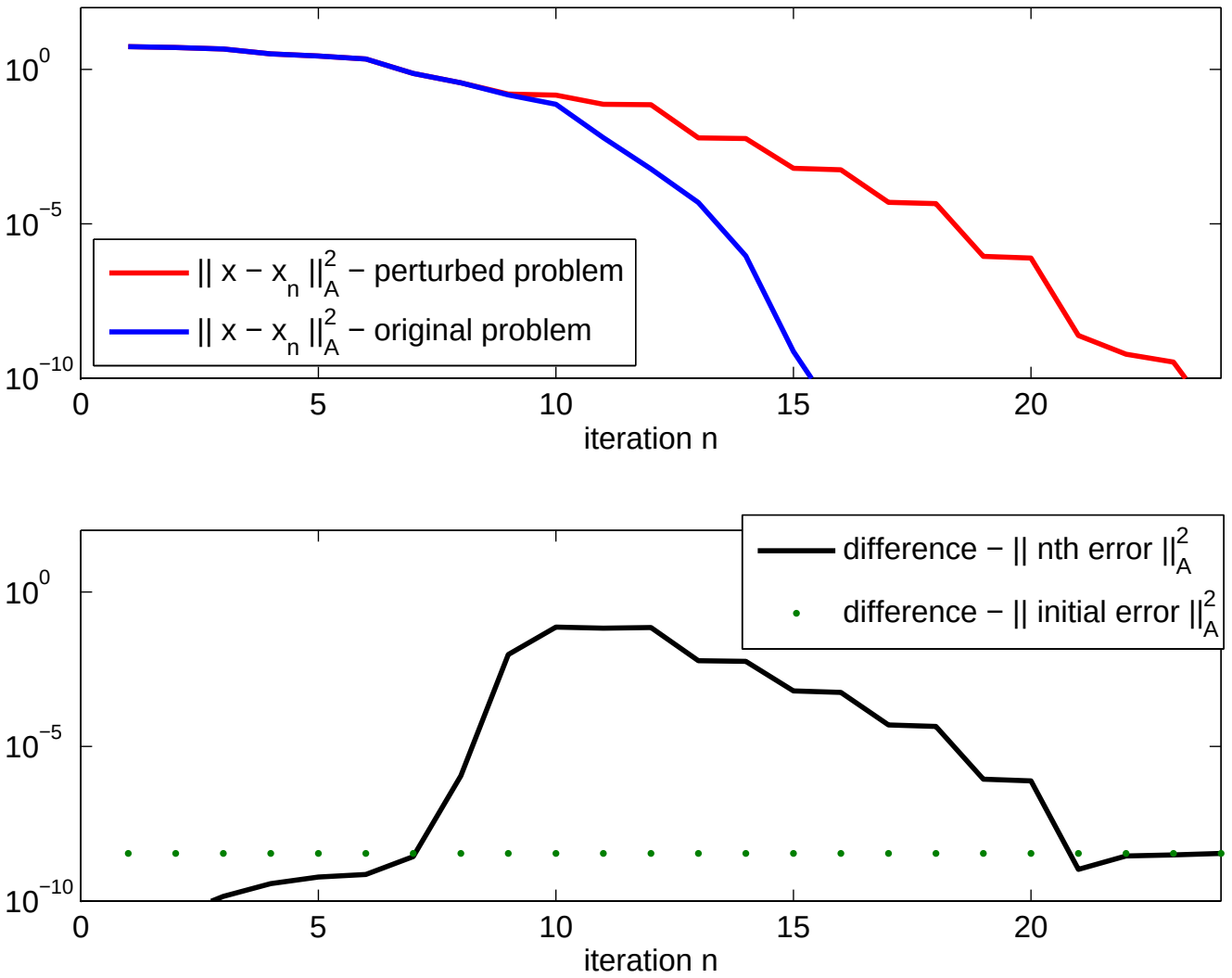
$\hat{T}_{2N}$ has all its eigenvalues close to those of A.

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 : Observations

- Replacing single eigenvalues by two close ones causes 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 global information.

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 : 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).

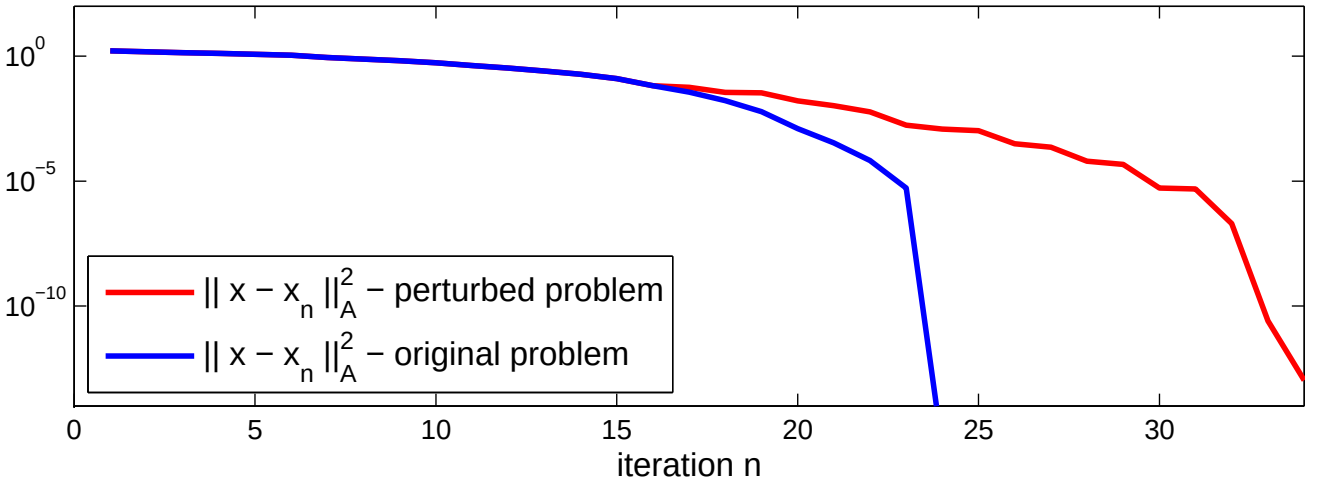
2 : Caution

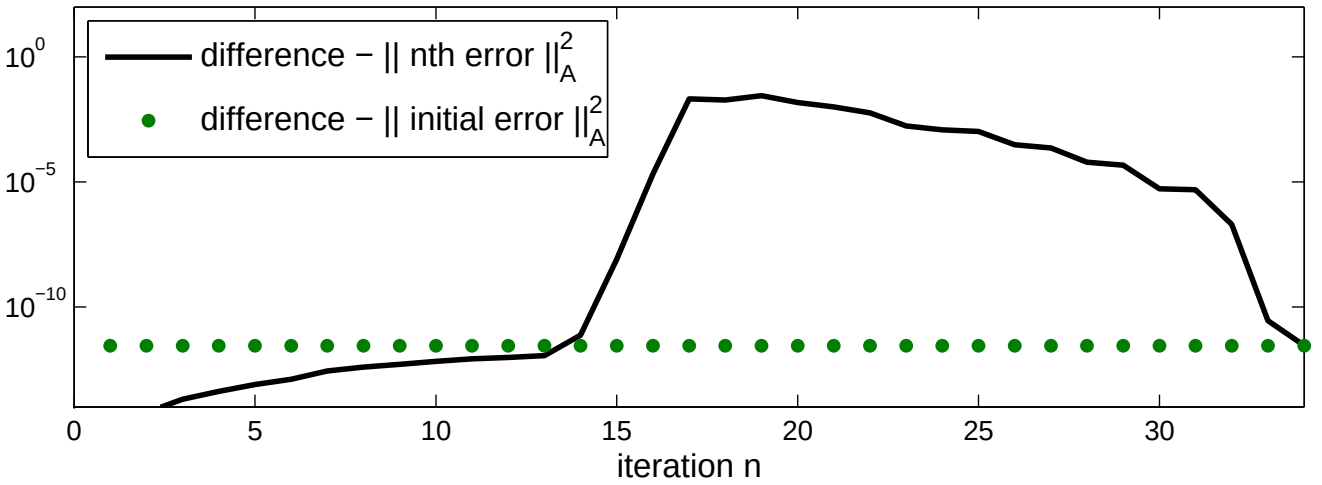
Kratzer, Parter and Steuerwalt, *Block splittings for the conjugate gradient method*, Computers and Fluids 11, (1983), pp. 255-279. The statement on p. 261, second paragraph, in our notation says:

> 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 $\hat{A}$).

2 : CG results for A, w_1 and $\hat{A}, \hat{w}_1$, $\gamma = 0.8$:





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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,

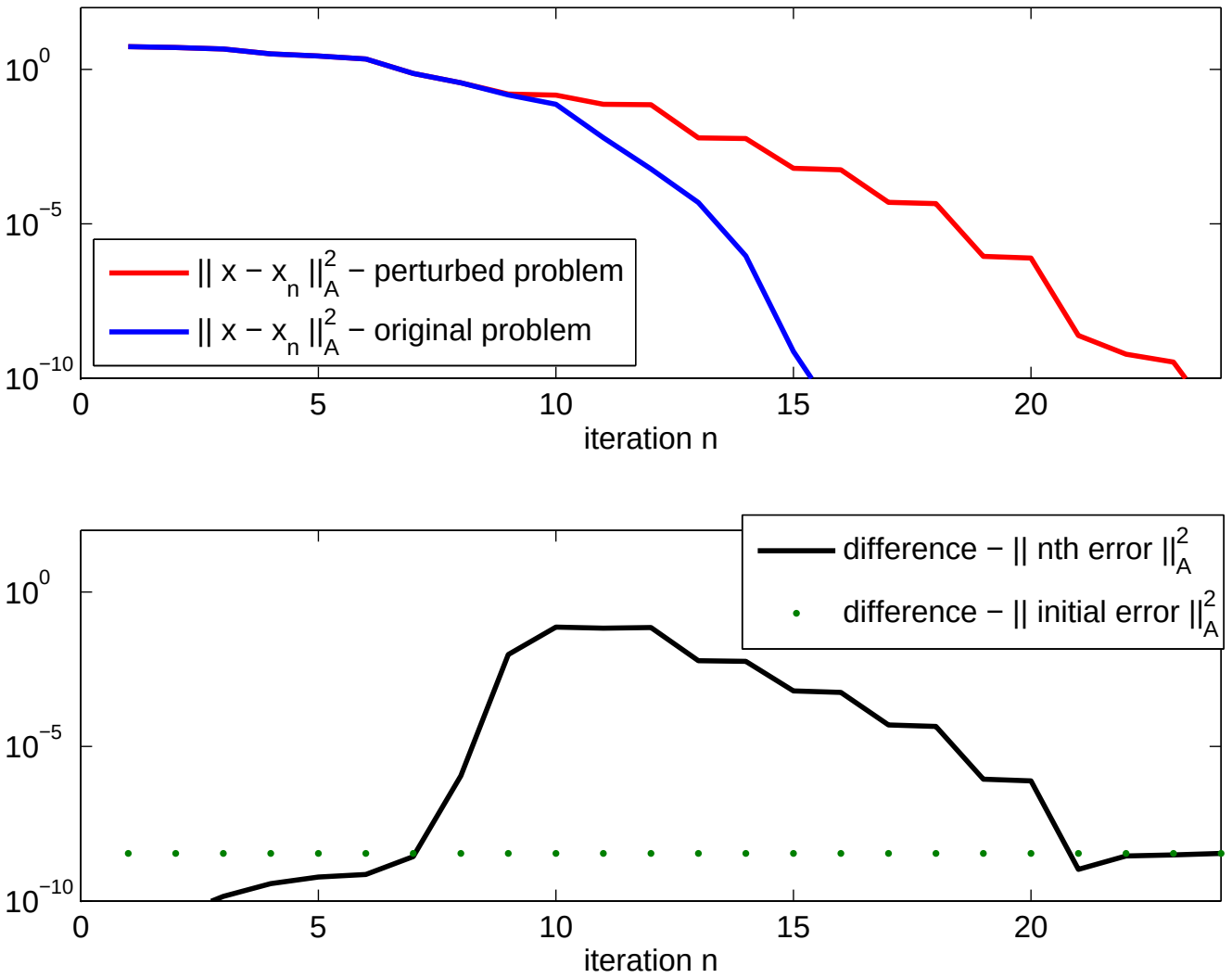
$$\int_{\zeta}^{\xi} f(\lambda)\, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} f(\theta_i^{(n)}) \;+\; R_n(f)\,.$$

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

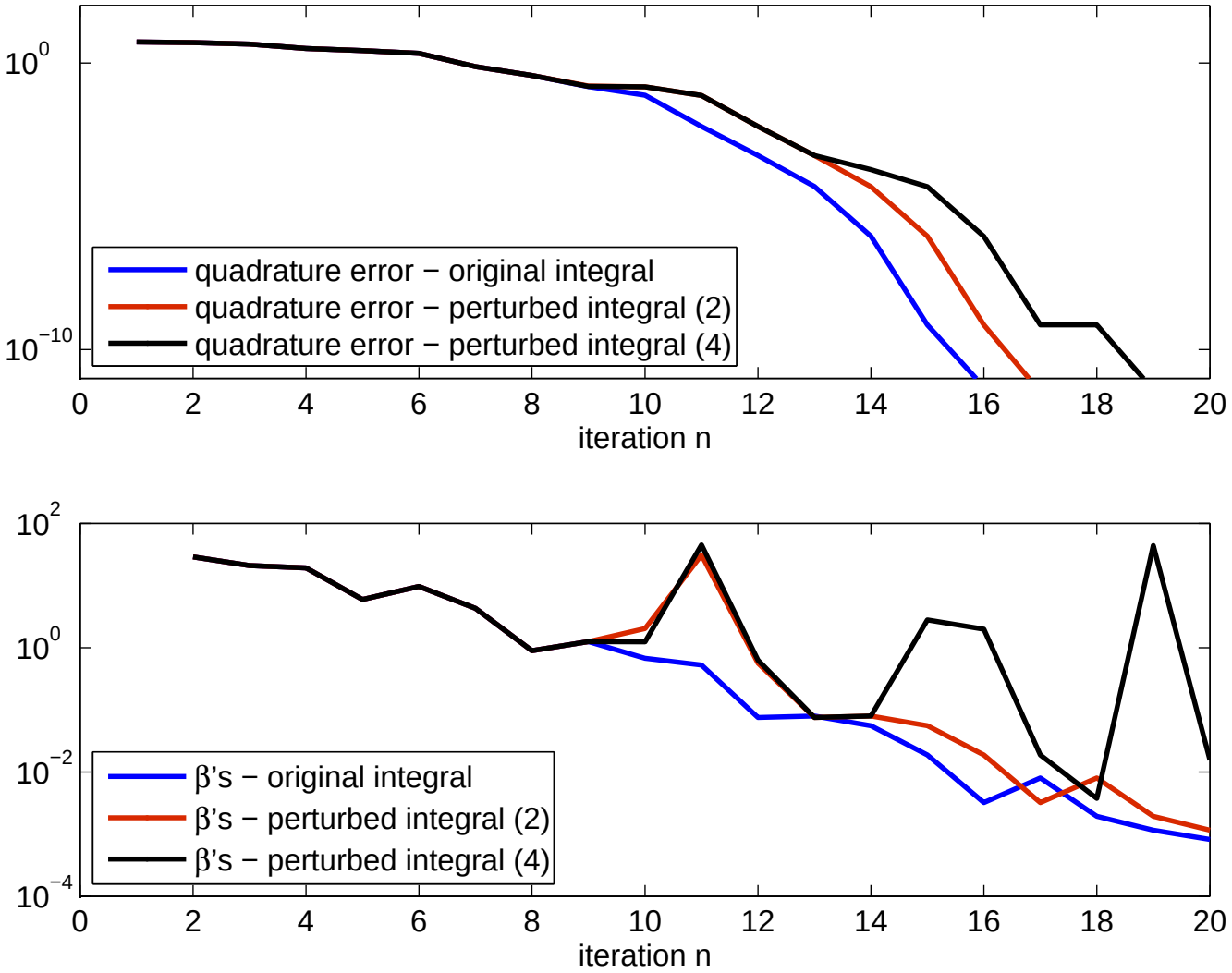
$$\frac{\|x - x_0\|_{\mathbf{A}}^2}{\|r_0\|^2} \;=\; n\text{-th Gauss quadrature} \;+\; \frac{\|x - x_n\|_{\mathbf{A}}^2}{\|r_0\|^2}\,.$$

This was a base for the CG error estimation in
[DaGoNa-78, GoFi-93, GoMe-94, GoSt-94, GoMe-97, . . .]

3 : Sensitivity of the Gauss-Ch. Quadrature



3 : Simplified problem



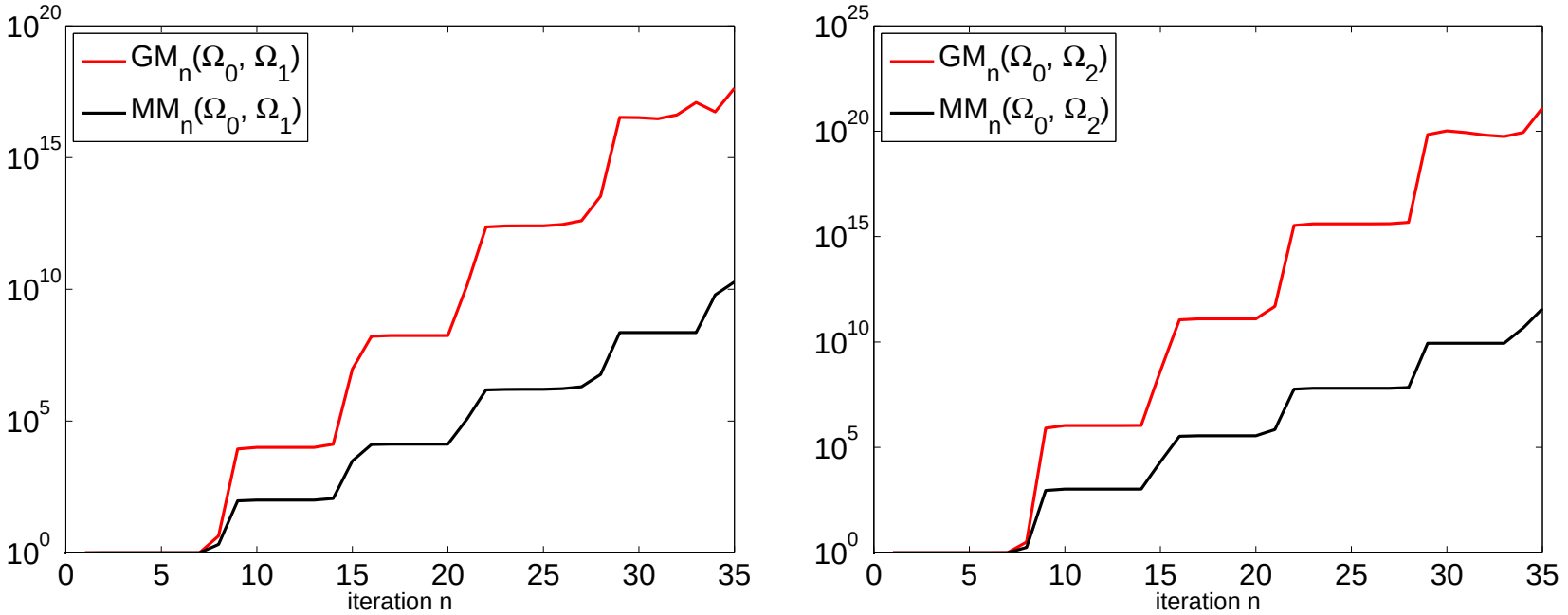
3 : Theorem - O'Leary, S, Tichý (2007)

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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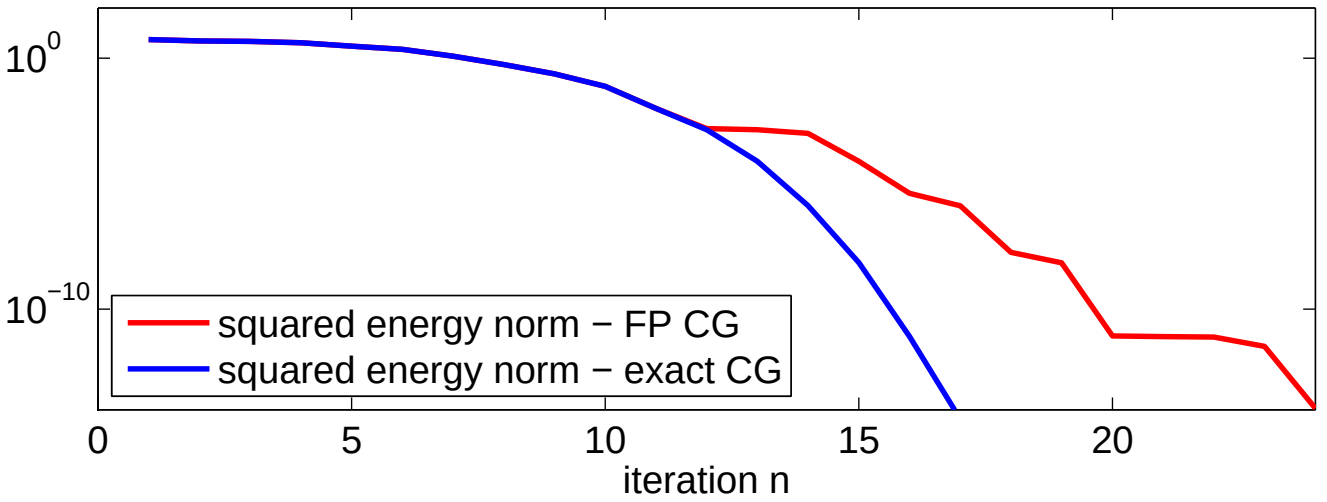
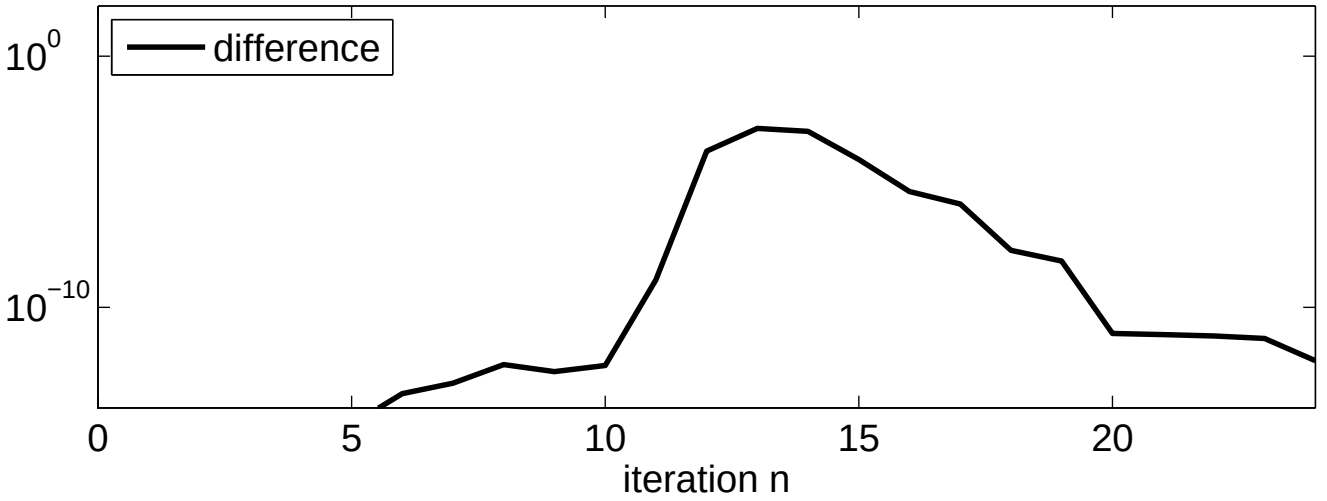
4 : CG applied to the basic problem





4 : Observations - FP CG

- 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),

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

4 : Close to the exact CG for $\hat{A}\,\hat{x} = \hat{b}$???

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).

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5 : Eigenvalues and convergence of GMRES ?

Consider any nonzero eigenvalues and a nonincreasing sequence (desired convergence curve sampled at the steps 0 to N)

$$f(0) \geq f(1) \geq \ldots \geq f(N-1) > f(N) = 0\,.$$

Then the size of the component of the initial residual eliminated in the jth GMRES step is $\phi_j = (f(j-1)^2 - f(j)^2)^{\frac{1}{2}}$. Let R_{N-1} be a nonsingular upper triangular matrix, $h = (\phi_1, \ldots, \phi_N)^T$, be the first column of

$$\Phi = \left(\begin{array}{c|c} h & \\ & R_{N-1} \end{array} \right),$$

5 : Theorem

The following two assertions are equivalent:

1° The spectrum of A is $\{\lambda_1, \ldots, \lambda_N\}$ and GMRES applied to A with r_0 yields residuals such that $\|r_k\| = f(k)\,, \quad k = 0, 1, \ldots, N\,.$

2° $A = U\,(\,\Phi\,C\,\Phi^{-1})\,U^*$ and $r_0 = U\,h$,
where C is the companion matrix corresponding to the spectrum of A and U is unitary.

Theorem gives a complete parametrization of the set of **all pairs** $\{A, r_0\}$ for which GMRES gives the prescribed convergence curve while the matrix A has the prescribed eigenvalues.

Greenbaum and S (1994), Greenbaum, Pták and S (1996),
Arioli, Pták and S (1998).

5 : Spectrum not sufficient. Spectral bounds?

Interpretation of the term $C(A, r_0)$ in the bounds of the type

$$\|r_n\| \leq C(A, r_0)\ F(sp(A), N)$$

needs a proper care. Since, by Theorem, the spectrum is in general not sufficient for description of convergence, the dependence of $C(A, r_0)$ on the data can not be ignored. A bound

$$\|r_n\| \leq \text{const}\ F(sp(A), N)$$

is either not valid for all data A, r_0, or it is completely irrelevant.

5 : Pathological initial residuals?

Our conclusion seems to be in conflict with common practice.

Convergence is often related to eigenvalue distributions without any assumption on the existence or conditioning of the eigenvector basis and/or restriction on applicability of the bounds. Then, however, the derived conclusions lack a proper justification.

In many cases there are indeed good reasons for linking convergence to eigenvalues. The point is that the reasons should be given and examined (contrary to common practice).

The cases in which poor convergence can be observed with nice spectra and vice versa do exist in practice. Convection dominated diffusion problems can lead to such linear algebraic systems, as described by Reddy and Trefethen (1994), Trefethen (1997), see also Ernst (2000), Liesen and S (2005).

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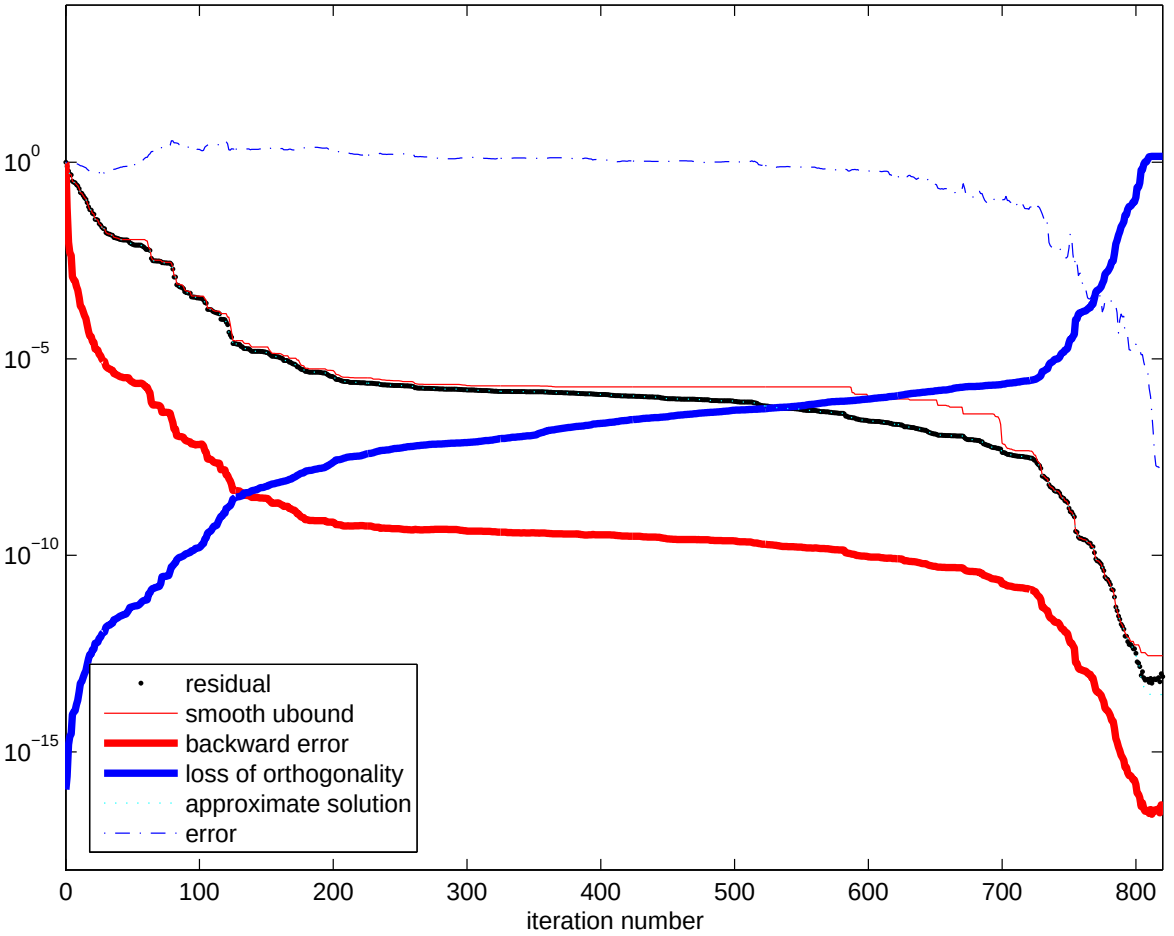
6 : MGS GMRES in finite precision



Sherman2 from Matrix market, problem rhs.

6 : Observations - MGS GMRES

- 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.

6 : 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), Core problem theory in Errors-in-Variables Modelling, (2002, NM I, 2006, SIMAX)

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.

- Rounding error analysis of Krylov subspace methods has had unexpected side effects such as understanding of general mathematical phenomena in matrix theory, quadrature approximations and Errors-in Variables Modeling, which are independent of any numerical stability issues.

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

Thank you!