Moments, Krylov subspace methods, model reduction and RCWA in elipsometry

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Historical remark on iterative methods

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

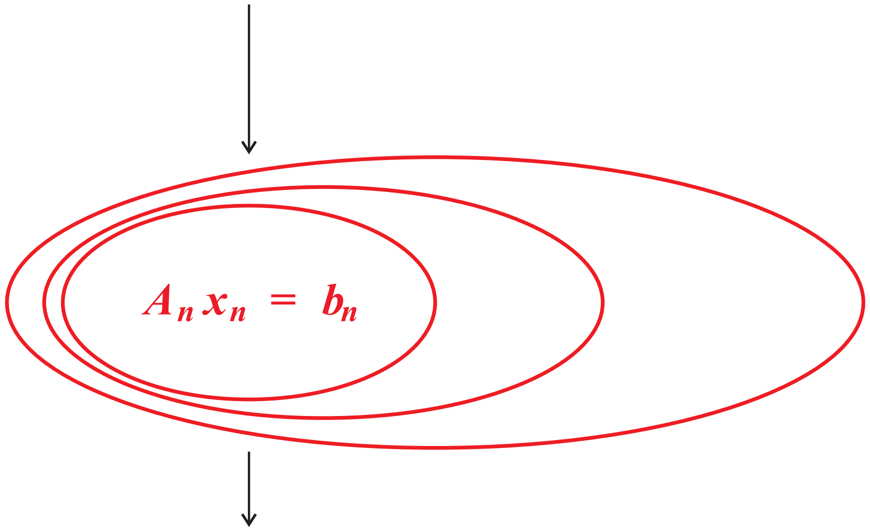
1971 - Book Iterative methods by D. Young

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)

Projections onto Krylov subspaces

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



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 and moments

The projection process using Krylov subspaces is highly nonlinear in A and it depends on r_0 ,

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

$\mathcal{K}_n(A, r_0)$ 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 matching moments model reduction

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. Application to scattering amplitude estimation in elipsometry

1 : Matching moments

Consider a non-decreasing distribution function $\omega(\lambda)$, $\lambda \geq 0$ with the moments given by the Riemann-Stieltjes integral

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

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,

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

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),

and the description given in H. H. J. Goldstine, *A History of Numerical Analysis from the 16th through the 19th Century,* (1977).

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

1 : Model reduction via matching moments I

Gauss-Christoffel quadrature 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 : 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 $p_1(\lambda) \equiv 1, \, p_2(\lambda), \, \dots, \, p_n(\lambda)$ 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 $\theta_i^{(n)}, \, i = 1, \dots, n$.

Consequently,

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

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

1 : Linear algebraic equation

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

Consider the spectral decomposition

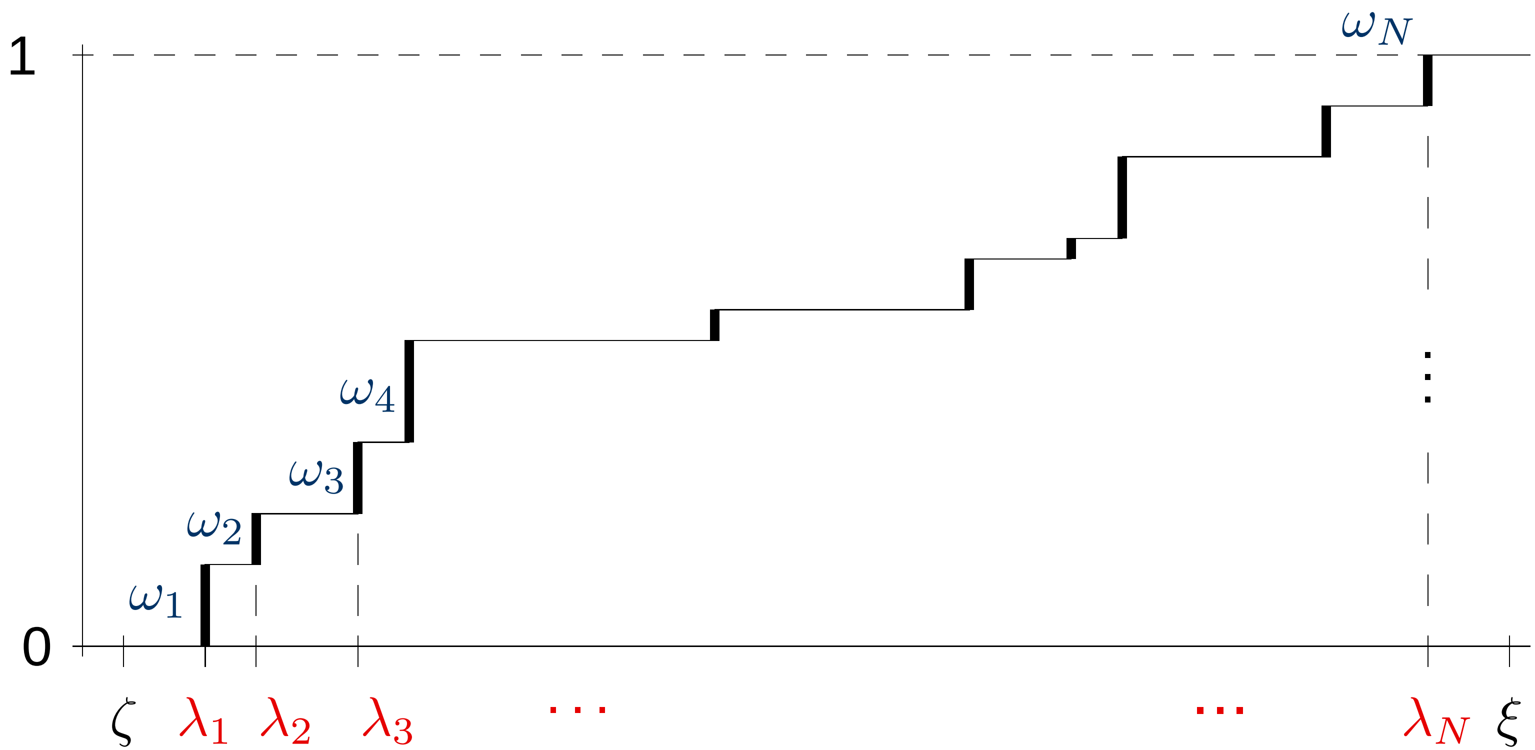
$$A = S \,\text{diag}(\lambda_i)\, S^* \,,$$

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 $\omega(\lambda)$



Matrix formulation:

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

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

matching the first $2n$ moments therefore means

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

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

The A-norm of the error is minimal! See Elman, Silvester and Wathen (2005), p. 71.

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

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

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

and the CG approximation given by

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

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 Hestenes and Stiefel (1952), . . .
nice Ph.D. Thesis by Kent (1989, Stanford), book by B. Fischer (1996), paper by Fischer and Freund (1992).

$$Ax = b\,,\; x_0 \qquad \longleftrightarrow \qquad \int_\zeta^\xi \lambda^{-1}\, d\omega(\lambda)$$

$$\uparrow \qquad\qquad\qquad\qquad \uparrow$$

$$T_n\, y_n \;=\; \|r_0\|\, e_1 \qquad \longleftrightarrow \qquad \sum_{i=1}^{n} \omega_i^{(n)} \left(\theta_i^{(n)}\right)^{-1}$$

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

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

1 : Matching moments model reduction

CG (Lanczos) reduces for A HPD at the step n the original model

$$A\,x \;=\; b\,,\; r_0 = b - Ax_0$$

to

$$T_n\, y_n \;=\; \|r_0\|\, e_1\,,$$

such that the the $2n$ moments are matched,

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

1 : Comments on literature

Proofs of results related to moments or model reduction are in the literature typically based on factorizations of the matrix of moments, Golub and Welsh (1969), Dahlquist, Golub and Nash (1978), . . . , Kent(1989), . . . , which is also true for Antoulas (2005).

Moment matching techniques has been used for decades in computational physics and in computational chemistry, see Gordon (1968).

Gauss quadrature formulation related to the nonsymmetric Lanczos process and to the Arnoldi process was given by Freund and Hochbruck (1993), motivated by Fischer and Freund (1992). Gauss quadrature was formally extended to the complex plane by Saylor and Smolarski (2001), with motivation from inverse scattering problems in electromagnetics by Warnick (1997), . . . , Golub, Stoll and Wathen (2008).

Here we avoid using matrix of moments, and do not need any formal generalization of the Gauss quadrature formulas to the complex plane.

1 : Vorobyev moment problem - 1958, 1965

Find a linear HPD operator $\mathcal{A}_n$ on $\mathcal{K}_n(A, r_0)$ such that

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

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

By construction,

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

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

$$Q_n \left(A^n w_1\right) \; - \; A_n^n w_1 \; = \; Q_n \left(A^n w_1 - A_n^n w_1\right) \; = \; 0$$

gives (note that A is Hermitian)

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

1 : Matching moments model reduction

Using the unitary basis W_n with $Q_n = W_n W_n^*$,

$$A_n \quad = \quad Q_n\, A\, Q_n \;=\; W_n W_n^*\, A\, W_n W_n^* \;=\; W_n\, T_n\, W_n^*\,,$$

$$A_n^k \quad = \quad W_n\, T_n^k\, W_n^*\,,$$

which gives the result

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

1 : Non-Hermitian Lanczos

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

The non-Hermitian Lanczos algorithm can be written in the form

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

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

We assume that the algorithm does not break down in steps 1 through n (it can break down later).

1 : Non-Hermitian Lanczos

Here

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

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

$$Q_n = W_n V_n^* \,.$$

1 : Vorobyev moment problem for N. L.

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

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

Using ortogonality to the basis vectors $v_1, A^* v_1, \ldots, (A^*)^{n-1} v_1$,

$$
v_1^*\, A^{k+n}\, w_1 \;=\; v_1^*\, A^k\, A_n^n\, w_1\,, \quad k = 0, 1, \ldots, n-1\,.
$$

1 : Matching moments in nonsymmetric L.

$$\begin{aligned} A_n &= Q_n\, A\, Q_n \;=\; W_n V_n^*\, A\, W_n V_n^* \;=\; W_n\, T_n\, V_n^*\,, \\ A_n^n &= W_n\, T_n^n\, V_n^*\,, \end{aligned}$$

$$v_1^*\, A^k \;=\; e_1^T\, T_n^k\, V_n^*\,, \qquad k = 0, 1, \ldots, n-1\,,$$

we finally get (using a simple multiplication argument for the first n moments)

$$v_1^*\, A^k\, w_1 \;\equiv\; e_1^T\, T_n^k\, e_1\,, \qquad k = 0, 1, \ldots, 2n-1\,,$$

i.e., n steps of the nonsymmetric Lanczos (or BiCG) represent the model reduction which matches $2n$ moments.

Outline

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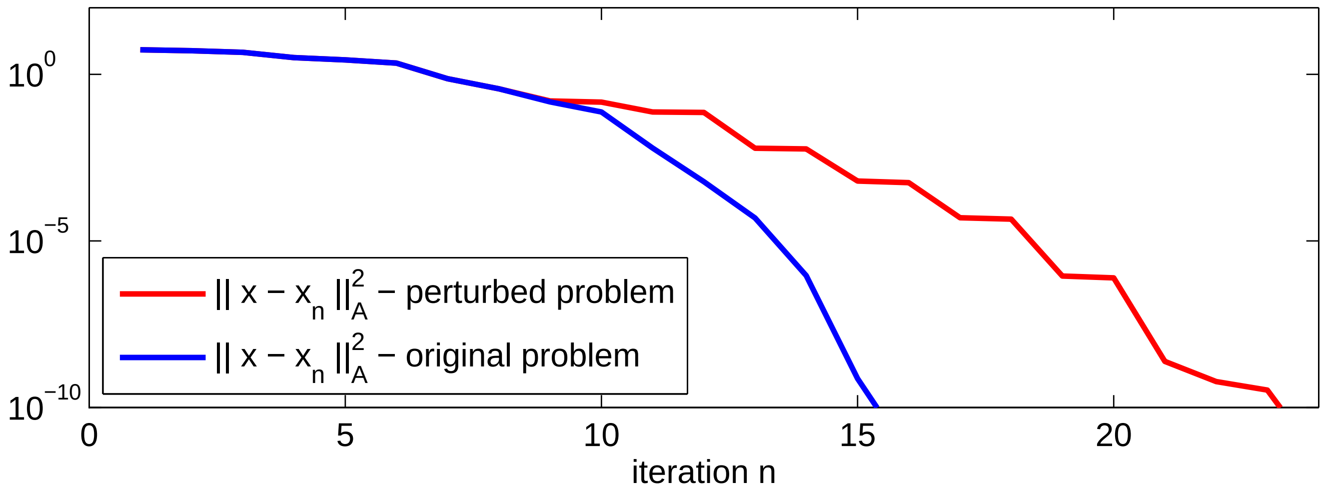
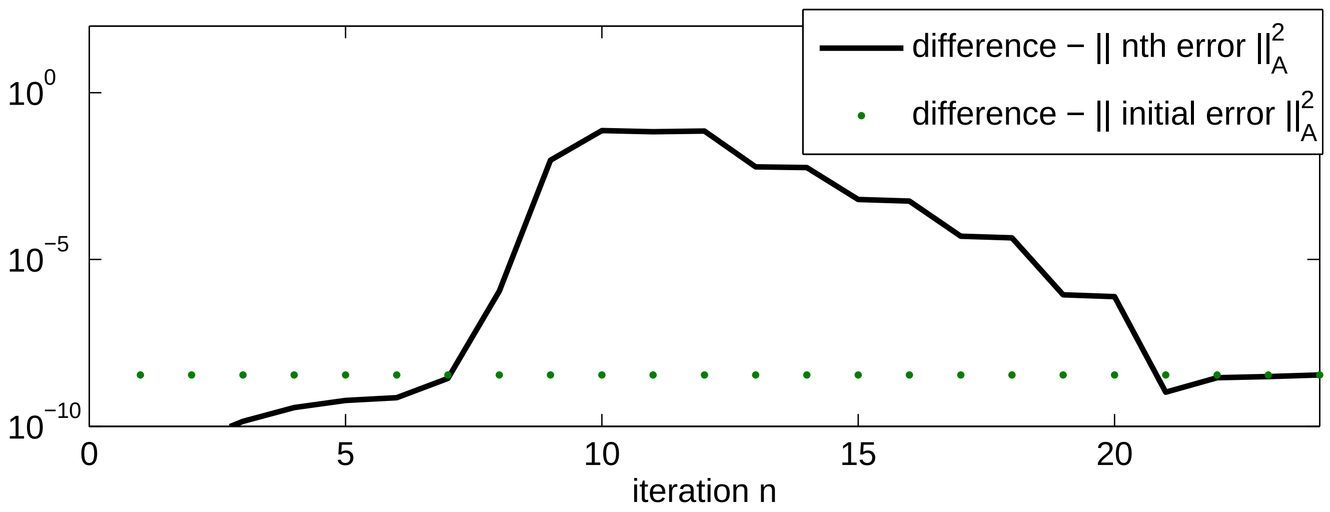
Exact arithmetic !

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





2 : Observations

- Replacing single eigenvalues by two close ones causes large delays. Clusters can not be replaced by single representatives! Matching moment property is responsible for the possibly large difference.
- 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).

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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,

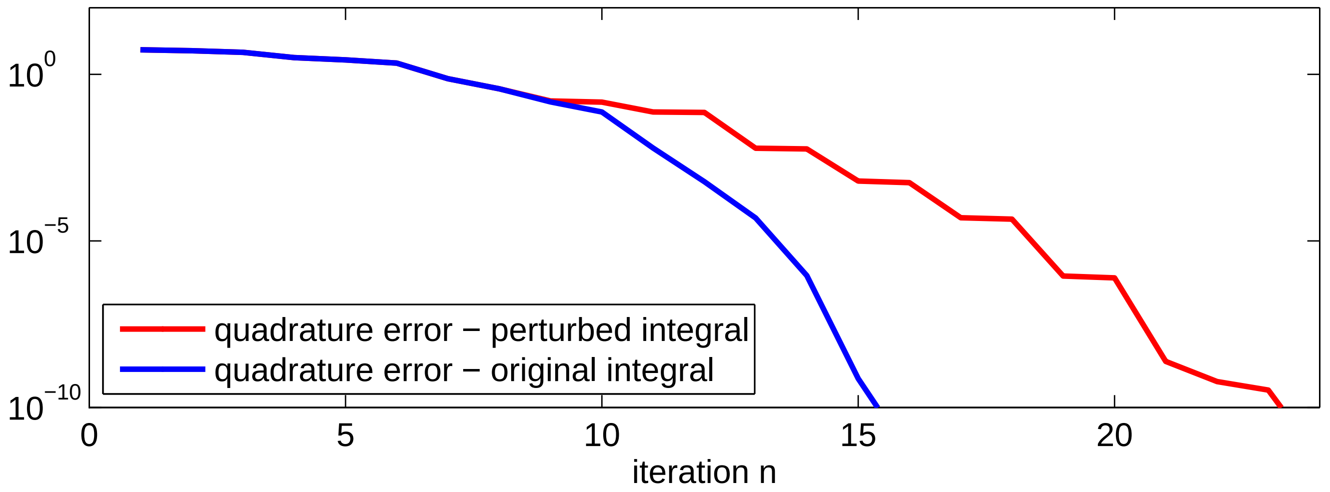
$$\int_{\zeta}^{\xi} f(\lambda)\, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} f(\theta_i^{(n)}) \;+\; R_n(f)\,.$$

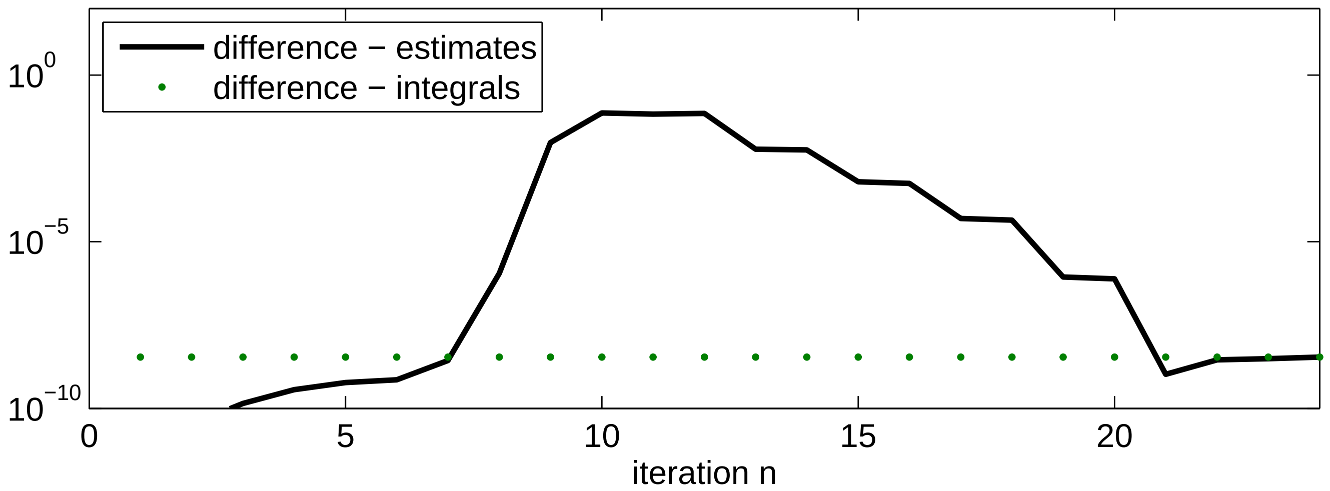
For $f(\lambda) \equiv \lambda^{-1}$ the formula takes the form

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

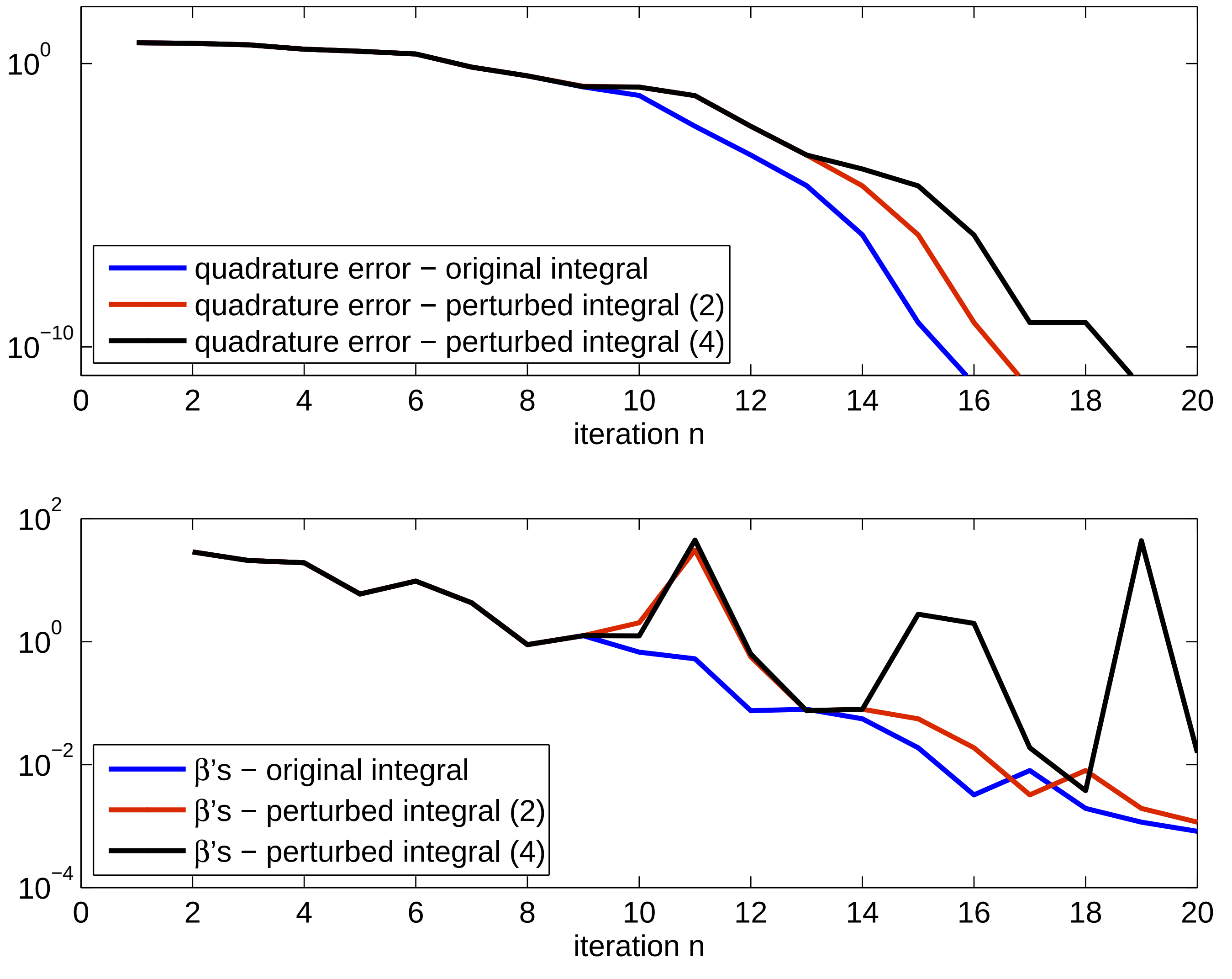
This was a base for the CG error estimation in
[DaGoNa-78, GoFi-93, GoMe-94, GoSt-94, GoMe-97, ...]

3 : Sensitivity of the Gauss-Ch. Quadrature





3 : Simplified problem



3 : Sensitivity statement

1. Gauss-Christoffel quadrature can be highly sensitive to small changes in the distribution function of the approximated integral.
   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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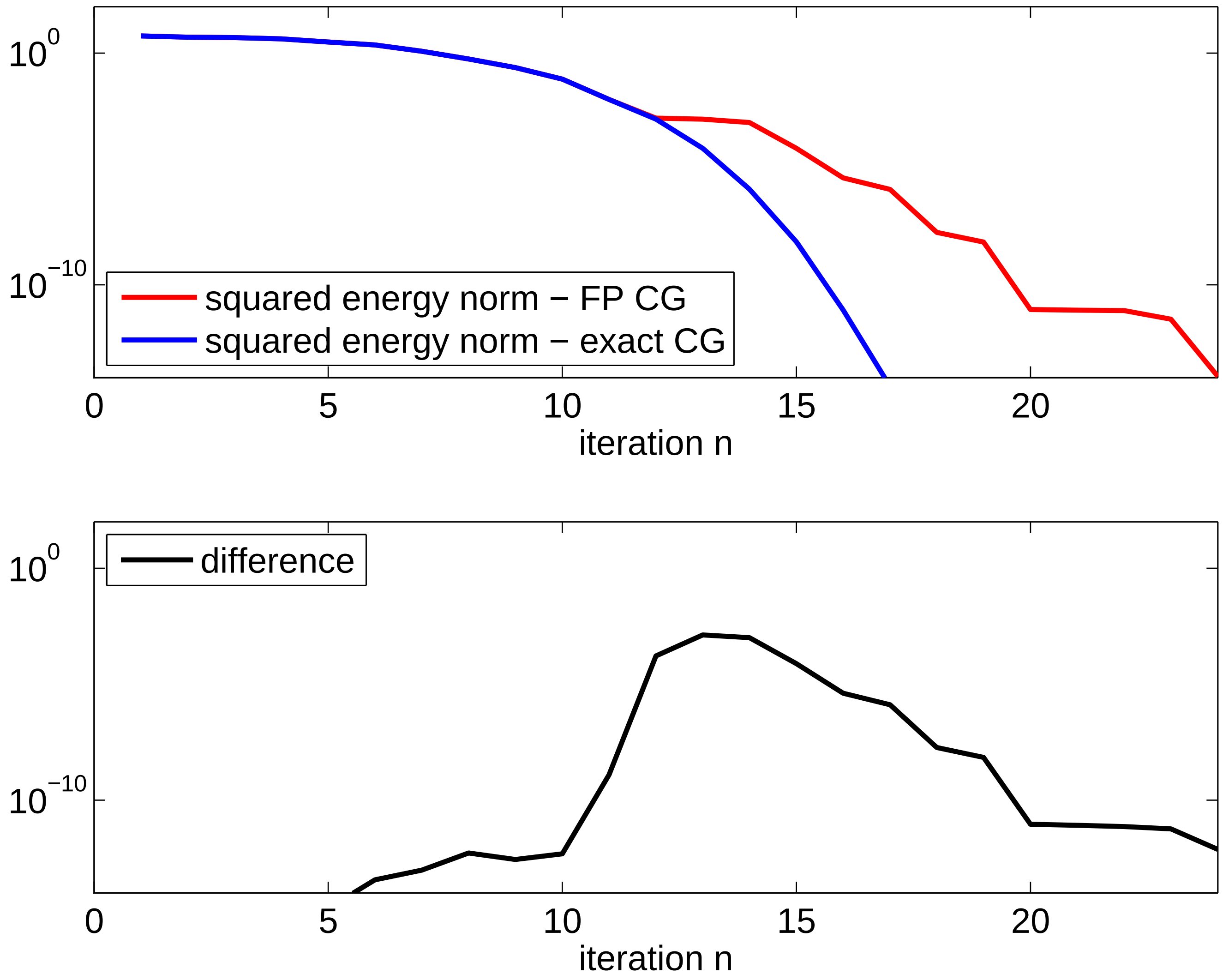
4 : Exact and FP CG applied to A, w_1



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 Meurant and S, Acta Numerica, (2006).

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5 : Diffraction of light

Consider Maxwell equations of electrodynamics for space with no sources

$$\operatorname{div} \widehat{\mathbf{E}} = 0 \,, \qquad \operatorname{div} \widehat{\mathbf{H}} = 0 \,,$$

$$\operatorname{curl} \widehat{\mathbf{E}} = -\mu \frac{\partial \widehat{\mathbf{H}}}{\partial t} \,, \qquad \operatorname{curl} \widehat{\mathbf{H}} = \varepsilon \frac{\partial \widehat{\mathbf{E}}}{\partial t} \,,$$

which gives the wave equations corresponding to the space invariant ε, μ,

$$\Delta \widehat{\mathbf{E}} = \varepsilon \, \mu \frac{\partial^2 \widehat{\mathbf{E}}}{\partial t^2} \,, \qquad \Delta \widehat{\mathbf{H}} = \varepsilon \, \mu \frac{\partial^2 \widehat{\mathbf{H}}}{\partial t^2} \,.$$

Maxwell equations for the conductive material

$$\operatorname{div} \widehat{\mathbf{E}} = 0\,, \qquad \operatorname{div} \widehat{\mathbf{H}} = 0\,,$$

$$\operatorname{curl} \widehat{\mathbf{E}} = -\,\mu\,\frac{\partial \widehat{\mathbf{H}}}{\partial t}\,, \qquad \operatorname{curl} \widehat{\mathbf{H}} = \varepsilon\,\frac{\partial \widehat{\mathbf{E}}}{\partial t} + \gamma\,\widehat{\mathbf{E}}\,,$$

If ε and μ are space invariant, then we get, similarly as above, the generalized wave equations

$$\Delta\,\widehat{\mathbf{E}} = \varepsilon\,\mu\,\frac{\partial^2 \widehat{\mathbf{E}}}{\partial t^2} + \gamma\,\mu\,\frac{\partial \widehat{\mathbf{E}}}{\partial t}\,, \qquad \Delta\,\widehat{\mathbf{H}} = \varepsilon\,\mu\,\frac{\partial^2 \widehat{\mathbf{H}}}{\partial t^2} + \gamma\,\mu\,\frac{\partial \widehat{\mathbf{H}}}{\partial t}\,.$$

5 : Problem setting

We will consider only time-harmonic fields, where any field vector $\widehat{\mathbf{V}}(x, y, z, t)$ will be represented by its associated space dependent complex vector $\mathbf{V}(x, y, z)$ such that

$$\widehat{\mathbf{V}}(x, y, z, t) \;=\; \mathrm{Re}[\mathbf{V}(x, y, z) \exp(-\mathbf{i}\,\omega\, t)]\,,$$

Maxwell’s equations take the form

$$\begin{aligned} \operatorname{div} \mathbf{E} \;&=\; 0\,, \qquad & \operatorname{div} \mathbf{H} \;&=\; 0\,, \\ \operatorname{curl} \mathbf{E} \;&=\; \mathbf{i}\,\mu\,\omega\,\mathbf{H}\,, \qquad & \operatorname{curl} \mathbf{H} \;&=\; -\,\mathbf{i}\,\varepsilon\,\omega\,\mathbf{E}\,. \end{aligned}$$

5 : Problem setting

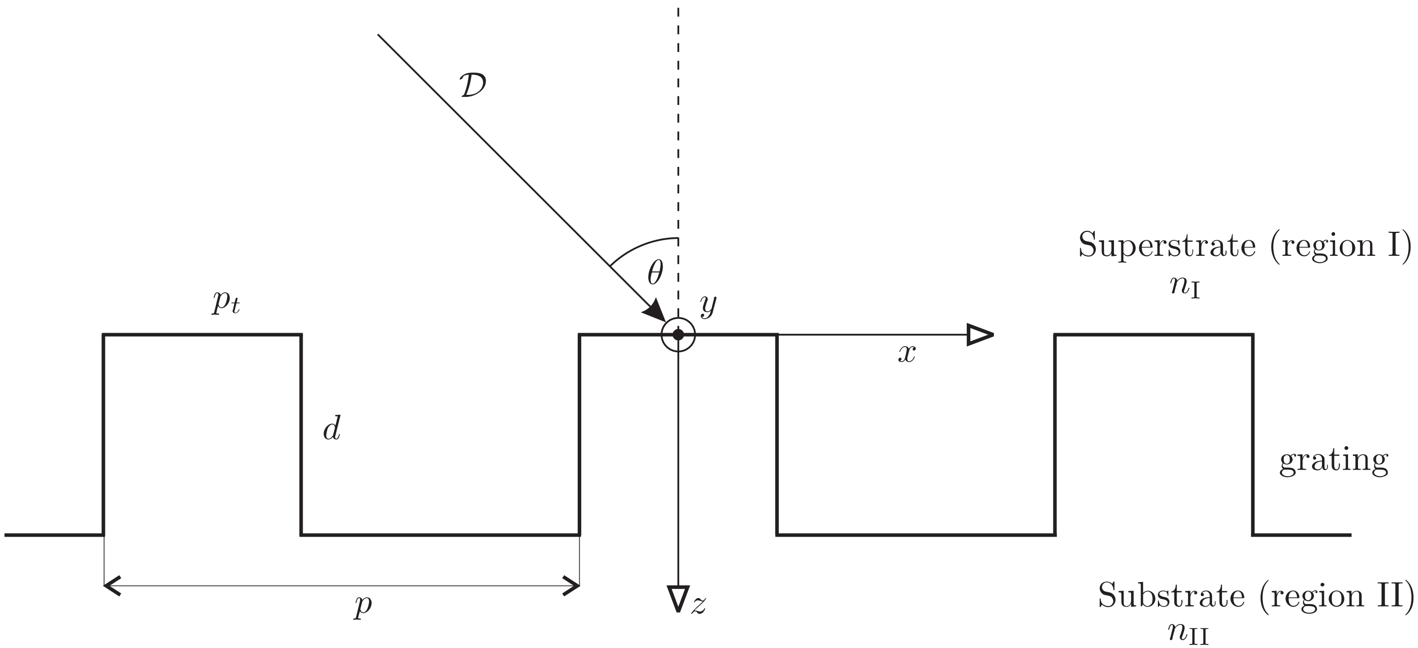
If the electric permittivity ε and the magnetic permeability μ are space invariant,

$$\Delta\,\mathbf{E} \;=\; -\,\varepsilon\,\mu\,\omega^2\,\mathbf{E}\,, \qquad \Delta\,\mathbf{H} \;=\; -\,\varepsilon\,\mu\,\omega^2\,\mathbf{H}\,.$$

In our application, the permeability, μ, is space invariant, but the permittivity, ε, may be space dependent, $\varepsilon = \varepsilon(x, y, z)$,

$$\Delta\,\mathbf{H} \;=\; -\,\varepsilon\,\mu\,\omega^2\,\mathbf{H} - \frac{1}{\varepsilon}\,\mathrm{grad}\,\varepsilon \otimes \mathrm{curl}\,\mathbf{H}\,.$$

5 : Simple 2D x-periodic grating



Rectangular grating.

5 : TE polarization

The electric field in the TE polarization is then described by the equation

$$\Delta E_y \;=\; -\,k_0^2\,\varepsilon_r(x)\,E_y\,, \qquad\quad E_x \;=\; E_z \;=\; 0\,,$$

with the magnetic field

$$(H_x, 0, H_z) \;=\; \frac{\mathbf{i}}{\mu_0\,\omega}\left(\frac{\partial E_y}{\partial z}\,,\,0\,,-\frac{\partial E_y}{\partial x}\right)\,.$$

5 : TM polarization

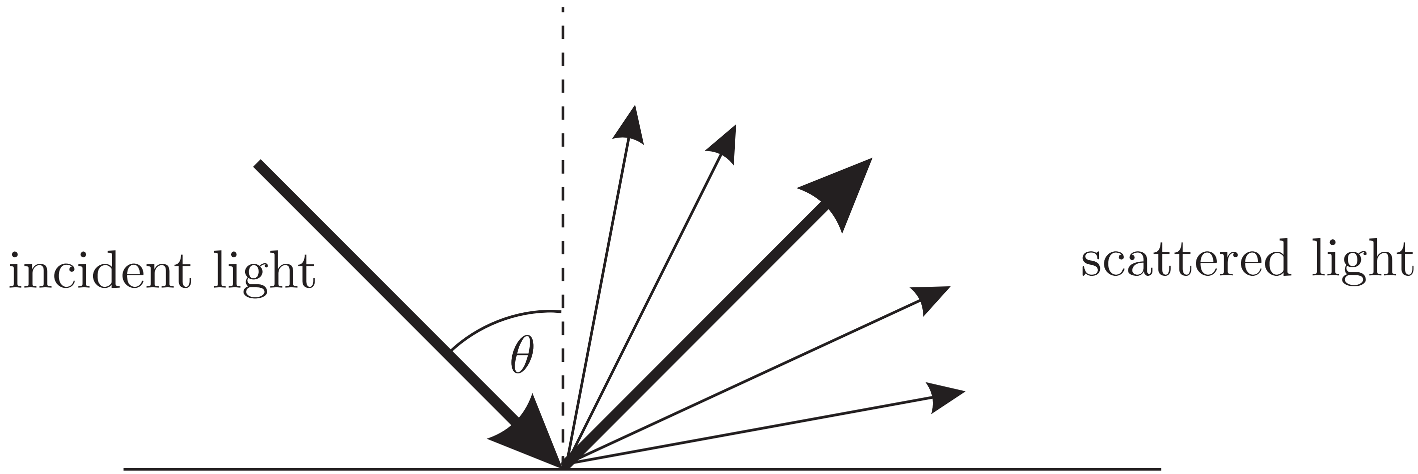
The magnetic field in the TM polarization is described by the equation

$$\Delta\, H_y \;-\; \frac{1}{\varepsilon_r(x)}\,\frac{d\varepsilon_r(x)}{dx}\,\frac{\partial H_y}{\partial x} \;=\; -\,k_0^2\,\varepsilon_r(x)\,H_y\,, \qquad H_x \;=\; H_z \;=\; 0\,,$$

with the electric field

$$(E_x, 0, E_z) \;=\; \frac{\mathbf{i}}{\varepsilon_0\varepsilon_r(x)\,\omega}\left(-\frac{\partial H_y}{\partial z}\,,\,0\,,\,\frac{\partial H_y}{\partial x}\right)\,.$$

5 : Diffraction on a periodic media



Discrete diffraction orders

Floquet conditions, separation of variables

$$F(x,z) \equiv e^{-\mathbf{i}\; k_{\mathrm{I}}\; x\; \sin\theta} E_y(x,z)$$

is strictly periodic in x with a period p. Using the Fourier expansion,

$$E_y\,(x,z) \;=\; \sum_{s=-\infty}^{+\infty} f_s\,(z)\, e^{\mathbf{i}\, k_{xs}\; x}\;,$$

where

$$k_{xs} \;\equiv\; k_{\mathrm{I}}\;\sin\theta \;+\; s\,\frac{2\pi}{p} \;=\; k_0\left(n_{\mathrm{I}}\sin\theta \;+\; s\,\frac{\lambda}{p}\right)\;,\quad s = 0, 1, -1, \ldots\;,$$

5 : RCWA (TE polarization)

In the homogenous superstrate and substrate ε_r is constant,
and E_y solves the Helmholtz equation

$$\Delta E_y = -k_\ell^2 \, E_y, \quad E_x = E_z = 0, \quad \ell = \mathrm{I}, \mathrm{II} \, ,$$

$$\left[\frac{d^2}{dz^2} + k_{\ell,zs}^2 \right] f_s^{(\ell)}(z) = 0, \quad \ell = \mathrm{I}, \mathrm{II}, \quad s = 0, 1, -1, \ldots \, ,$$

where

$$k_{\ell,zs}^2 = k_\ell^2 - k_{xs}^2 \, .$$

A general solution can be written as

$$f_s^{(\ell)}(z) = A_s^{(\ell)} \, e^{-\mathbf{i} k_{\ell,zs} \, z} + B_s^{(\ell)} \, e^{\mathbf{i} k_{\ell,zs} \, z} \, .$$

5 : RCWA

In the grating region, $\varepsilon_r(x)$ represents a periodic function with respect to x with period p . It can therefore be expressed by its Fourier series

$$\varepsilon_r\,(x) = \sum_{h=-\infty}^{+\infty} \epsilon_h \, e^{\mathbf{i}\, h \, \frac{2\pi}{p} \, x} \, .$$

For the TM polarization it is convenient to consider also the subsequent Fourier expansions (not used here)

$$\frac{1}{\varepsilon_r(x)} = \sum_{h=-\infty}^{+\infty} a_h \, e^{\mathbf{i}\, h \, \frac{2\pi}{p} x} \, .$$

5 : RCWA (TE polarization)

Fourier amplitudes in the grating region are coupled,

$$\sum_{j=-\infty}^{+\infty} \left\{ \left[\frac{d^2}{dz^2} - k_{xj}^2 \right] f_j(z) \right\} e^{\mathbf{i}\, j\, \frac{2\pi}{p}\, x} = -k_0^2 \sum_{j=-\infty}^{+\infty} \left\{ \sum_{s=-\infty}^{+\infty} \epsilon_{j-s}\, f_s(z) \right\} e^{\mathbf{i}\, j\, \frac{2\pi}{p}\, x} .$$

Equating for the index j leaves the result

$$\frac{d^2 f_j(z)}{dz^2} = k_{xj}^2\, f_j(z) - k_0^2 \sum_{s=-\infty}^{+\infty} \epsilon_{j-s}\, f_s(z) .$$

5 : RCWA (TE polarization)

Product of two Fourier expansions:

$$
\begin{aligned}
e^{-\mathbf{i}\, k_{\mathrm{I}}\, x \sin\theta}\, \varepsilon_r\, E_y &= \sum_{h=-\infty}^{+\infty} \epsilon_h\, e^{\mathbf{i}\, h\, \frac{2\pi}{p}\, x} \sum_{s=-\infty}^{+\infty} f_s(z)\, e^{\mathbf{i}\, s\, \frac{2\pi}{p}\, x} \\
&= \sum_{j=-\infty}^{+\infty} \left\{ \sum_{s=-\infty}^{+\infty} \epsilon_{j-s}\, f_s(z) \right\} e^{\mathbf{i}\, j\, \frac{2\pi}{p}\, x} \\
&= \lim_{N\to\infty} \sum_{j=-N}^{N} \left(\lim_{M\to\infty} \sum_{s=-M}^{M} \epsilon_{j-s}\, f_s(z) \right) e^{\mathbf{i}\, j\, \frac{2\pi}{p}\, x} \,.
\end{aligned}
$$

RCWA (TE polarization)

Simultaneous truncation - how fast does it converge?

$$e^{-\mathbf{i}\,k_{\mathrm{I}}\,x\sin\theta}\,\varepsilon_r(x)\,E_y(x,z) \;=\; \lim_{N\to\infty}\sum_{j=-N}^{N}\psi_{1,j}^{(N)}(z)\,e^{\mathbf{i}\,j\,\frac{2\pi}{p}\,x}\,,$$

where

$$\psi_{1,j}^{(N)}(x) \;=\; \sum_{s=-N}^{N}\epsilon_{j-s}\,f_s(z)\,.$$

5 : RCWA - linear algebraic system (TE)

After discretisation and expressing the approximate solutions in terms of matrix functions, the matching of the boundary conditions gives

$$\begin{bmatrix} -I & I & e^{\mathbf{i}\sqrt{C}dk_0} & 0 \\ Y_I & \sqrt{C} & -\sqrt{C}e^{\mathbf{i}\sqrt{C}dk_0} & 0 \\ 0 & e^{\mathbf{i}\sqrt{C}dk_0} & I & -I \\ 0 & \sqrt{C}e^{\mathbf{i}\sqrt{C}dk_0} & -\sqrt{C} & -Y_{\mathrm{II}} \end{bmatrix} \begin{bmatrix} r_{\mathrm{TE}} \\ g_{\mathrm{TE}}^{+} \\ g_{\mathrm{TE}}^{-} \\ t_{\mathrm{TE}} \end{bmatrix} = \begin{bmatrix} e_0 \\ n_{\mathrm{I}} \cos\theta \, e_0 \\ 0 \\ 0 \end{bmatrix}$$

Here only $e_{n+1}^T g_{\mathrm{TE}}^{+}$ is needed.

5 : RCWA - scattering amplitude - moments

Estimating the scattering amplitude is based on

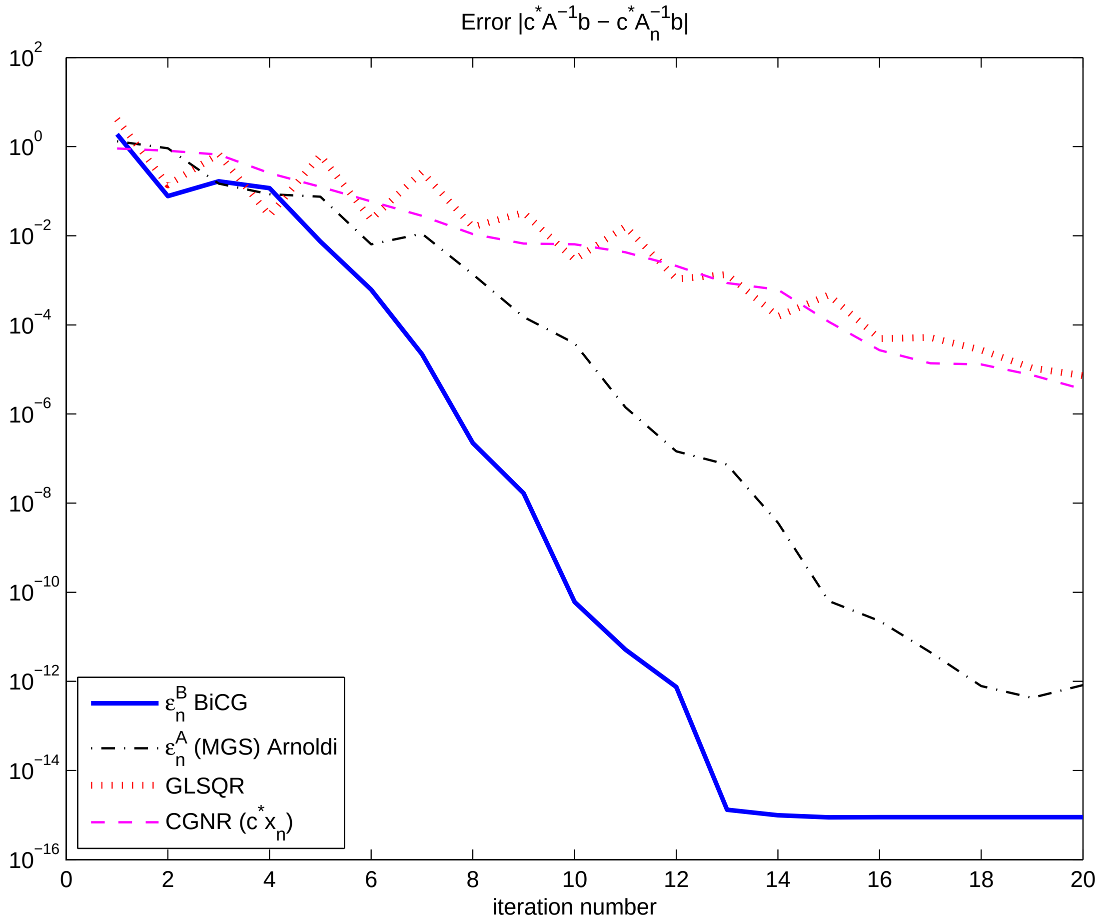
$$c^* A^{-1} b \approx c^* A_n^{\dagger} b ,$$

where $A_n^{\dagger}$ is the matrix representation of the inverse of the restricted operator A_n ,

$$A_n^{\dagger} = W_n T_n^{-1} V_n^* ,$$

and T_n matches the $2n$ moments

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



Results with simple block preconditioning.

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 independent of any numerical stability issues.

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

- The pieces of the mosaic fit together.

Recent references

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Thank you!