The perfidious condition number

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The class of elliptic PDEs, an example

\[- \nabla \cdot (k(x) \nabla u) = 0,\]

Morin, Nocheto, Siebert, SIREV (2002),
linear FE, standard uniform triangulation, \(N = 3969\) DOF.

**ICHOL PCG** (drop-off tolerance 1e-02), \(\kappa \approx 16;\)
Laplace operator PCG, \(\kappa \approx 160.\)
Predicting the computational cost?

\[ \| x - x_k \|_A / \| x - x_0 \|_A \]

PCG iteration

- \text{Laplace}
- \text{ICHOL}
Consider a linear bounded invertible operator $G : S \to S$ and the equation on Hilbert space

$$Gu = f, \quad f \in S.$$  

(Infinite dimensional) Krylov subspace methods at step $n$ implicitly construct a finite dimensional approximation $G_n$ of $G$ with the desired approximate solution $u_n$ defined by ($u_0 = 0$)

$$u_n := p_{n-1}(G_n)f \approx u = G^{-1}f,$$

where $p_{n-1}(\lambda)$ is the associated polynomial of degree at most $n - 1$ and $G_n$ is obtained by restricting and projecting $G$ onto the $n$th Krylov subspace

$$\mathcal{K}_n(G, f) := \text{span}\{f, Gf, \ldots, G^{n-1}f\}.$$  

Finite dimensional self-adjoint operators (finite Hermitian matrices)

\[ G = \frac{1}{2\pi i} \int_{\Gamma} \lambda (\lambda I_N - G)^{-1} d\lambda = \frac{1}{2\pi i} \sum_{\ell=1}^{N} \int_{\Gamma_{\ell}} \lambda (\lambda I_N - G)^{-1} d\lambda \]

\[ = \sum_{\ell=1}^{N} Y \text{diag} \left( \frac{1}{2\pi i} \int_{\Gamma_{\ell}} \frac{\lambda}{\lambda - \lambda_{\ell}} \, d\lambda \right) Y^* = \sum_{\ell=1}^{N} \lambda_{\ell} y_{\ell} y_{\ell}^* \]

\[ = \int \lambda \, dE(\lambda). \]

Compact infinite dimensional self-adjoint operators

Bounded infinite dimensional self-adjoint operators

Generalization to bounded normal and non-normal operators
Using the spectral decomposition \( G = \sum_{\ell=1}^{N} \lambda_\ell \, y_\ell y_\ell^* \)

Symbolically

\[
    w_1^* G \, w_1 = w_1^* \left( \sum_{\ell=1}^{N} \lambda_\ell \, y_\ell y_\ell^* \right) w_1 \equiv w_1^* \left( \int \lambda \, dE(\lambda) \right) w_1
\]

\[
    = \sum_{\ell=1}^{N} \lambda_\ell \, |(y_\ell, w_1)|^2 = \sum_{\ell=1}^{N} \lambda_\ell \, \omega_\ell = \int \lambda \, d\omega(\lambda) ,
\]

where the spectral function \( E(\lambda) \) of \( G \) is understood to be a nondecreasing family of projections with increasing \( \lambda \), symbolically \( dE(\lambda_\ell) \equiv y_\ell y_\ell^* \) and

\[
    I = \sum_{\ell=1}^{N} y_\ell y_\ell^* = \int dE(\lambda) .
\]

CG and Gauss quadrature relationship - the size of errors are equal!

At any iteration step \( n \), CG represents the matrix formulation of the \( n \)-point Gauss quadrature of the Riemann-Stieltjes integral determined by \( A \) and \( r_0 \),

\[
\int_0^\infty \phi(\lambda) \, d\omega(\lambda) = \sum_{i=1}^{n} \omega_i^{(n)} \phi(\theta_i^{(n)}) + R_n(\phi).
\]

For the function \( \phi(\lambda) \equiv \lambda^{-1} \),

\[
\frac{\|x - x_0\|^2_A}{\|r_0\|^2} = n\text{-th Gauss quadrature} + \frac{\|x - x_n\|^2_A}{\|r_0\|^2}.
\]

This has become the basis for CG error estimation; see Golub, 1994; and, e.g., the surveys in S and Tichý, 2002; Meurant and S, 2006; Golub and Meurant, 2010; Liesen and S, 2013.
Condition number and contraction bound(s)??

\[ \frac{\|x - x_n\|_A}{\|x - x_0\|_A} \leq 2 \left( \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^n \]
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- Daniel (1967) did not identify CG convergence with the Chebyshev polynomials-based bound. He carefully writes (modifying slightly his notation)

  “...assuming only that the spectrum of the matrix \( A \) lies inside the interval \([\lambda_1, \lambda_N]\), we can do no better than Theorem 1.2.2.” [see the bound above]
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That means that the Chebyshev polynomials-based bound holds for any distribution of eigenvalues between $\lambda_1$ and $\lambda_N$ and for any distribution of the components of the initial residuals in the individual invariant subspaces.
Back to the elliptic PDE problem example
Various parts of the spectra and convergence behavior
Information on the whole spectrum is available a priori!

**Theorem**: (Pairing the eigenvalues and the FE discretization nodal values \( k_j, \ j = 1, \ldots, N \))

Let \( 0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N \) be the eigenvalues of \( L^{-1} A \). Let \( k(x) \) be bounded and piecewise continuous. Then there exists a (possibly non-unique) permutation \( \pi \) such that the eigenvalues above satisfy

\[
\lambda_{\pi(j)} \approx k_j, \quad j = 1, \ldots, N.
\]


Here we assume for simplicity a Lagrange FE discretization. The results of the paper are more general.
Clusters of eigenvalues?
It is not true that CG (or other Krylov subspace methods used for solving systems of linear algebraic equations with symmetric matrices) applied to a matrix with $t$ distinct well separated tight clusters of eigenvalues produces in general a large error reduction after $t$ steps; see Sections 5.6.5 and 5.9.1 in Liesen, S (2013). The associated myth has been proved false more than 25 years ago; see Greenbaum (1989); S (1991); Greenbaum, S (1992). Still it is persistently repeated in the literature as an obvious fact.
It is not true that CG (or other Krylov subspace methods used for solving systems of linear algebraic equations with symmetric matrices) applied to a matrix with \( t \) distinct well separated tight clusters of eigenvalues produces in general a large error reduction after \( t \) steps; see Sections 5.6.5 and 5.9.1 in Liesen, S (2013). The associated myth has been proved false more than 25 years ago; see Greenbaum (1989); S (1991); Greenbaum, S (1992). Still it is persistently repeated in the literature as an obvious fact.

As for systems with nonsymmetric matrices, without specific (strong) assumptions on the structure of invariant subspaces it can not be claimed that distribution of eigenvalues provides insight into the asymptotic behavior of Krylov subspace methods (such as GMRES); see Sections 5.7.4, 5.7.6 and 5.11 of Liesen, S (2013). As above, the relevant results Greenbaum, S (1994); Greenbaum, Pták, S (1996) and Arioli, Pták, S (1998) are more than 20 years old.
Krylov subspace methods adapt to the problem. Exploiting this adaptation is the key to their efficient use.

Unlike nonlinear problems and/or multilevel methods, the analysis of Krylov subspace methods cannot be based, in general, on contraction arguments.

Individual steps modeling-analysis-discretization-computation should not be considered separately within isolated disciplines. They form a single problem. Operator preconditioning follows this philosophy.

HPC computations require handling all involved issues. A posteriori error analysis and stopping criteria are essential ...

Assumptions must be honored.
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Málek, S, Preconditioning and the Conjugate Gradient Method in the Context of Solving PDEs, SIAM Spotlights, SIAM (2015), Chapter 13:

“Here we do not argue against using condition numbers ... where appropriate. We argue against using them as general unquestioned tools which are considered fully descriptive ... as arguments closing the door for further investigation.”
“We will go on pondering and meditating, the great mysteries still ahead of us, we will err and stumble on the way, and if we win a little victory, we will be jubilant and thankful, without claiming, however, that we have done something that can eliminate the contribution of all the millenia before us.”
“There remains this: we beech the skilled in these things, that we thought worth showing, they will think openly receiving, and whatever it hides, worth imparting more properly by themselves to the wider mathematical community.”
Thank you very much for your kind patience!