Contribution

We present numerical experiments which illustrate that the idea of the so-called composite bounds may get to significant troubles when applied to computations in FP arithmetic.

Idea of composite bounds

The theoretical convergence rate of the Conjugate Gradient Method for solving linear systems $Ax = b$ with SPD matrix $A$ is often estimated by the minimax problem

$$
\min_{p \in \mathbb{P}_k} \max_{i=1, \ldots, N} |p(\lambda_i)|,
$$

where $\mathbb{P}_k$ is the set of polynomials of degree $k$.

Consequences of theoretical analysis

Backward-like analysis. The results of Greenbaum and Strakoš (see e.g. [3, 4]) explain that the numerical behaviour of FP CG computations applied to the original problem $Ax = b$ can be (up to small inaccuracy) described via the convergence behaviour of exact CG computations applied to larger perturbed system $\hat{A}x = b$ where the eigenvalues of the matrix $\hat{A}$ are clustered in tiny intervals located around each eigenvalue of $A$. Matrix $\hat{A}$ of the perturbed system depends in mathematically precise formulation on the number of computed iterations $k$. These results are based on strong relationship between CG and Lanczos algorithms; it is known that delay of convergence in FP CG computations goes together with generating multiple approximations of the eigenvalues of $A$.

Failure of the composite bound. Since the perturbed problem has more eigenvalues, it can not be guaranteed that (4) works also for the perturbed problem in exact arithmetic and, consequently, for the original problem in FP arithmetic. In the upper part of the figure, bounds are plotted for different number of eigenvalues considered as outliers ($m = 0, \ldots, 20$). We observe failure of the composite bound (red dashed lines) for FP CG (solid line). If we take into consideration all eigenvalues of $\hat{A}$ the corresponding upper bound with the use of $R^m_\sigma(\lambda)$ gives the quantity

$$
\max_{\lambda \in \sigma(\hat{A})} \left| R^m_\sigma(\lambda) \right| \text{ instead of } \max_{i=1, \ldots, N} \left| R^m_i(\lambda_i) \right|,
$$

where $\sigma(\hat{A})$ is the spectrum of $\hat{A}$. However, as illustrated in the bottom part of the figure, this corrected upper bound (black dashed line) turns out to be totally useless. Observed blow up is an unavoidable consequence of evaluating of $R^m_\sigma(\lambda)$ in the neighborhoods of outliers. We observe that the behaviour of exact CG applied to the perturbed problem (dotted line) is very similar to FP CG of the original problem.

Further numerical experiments

Numerical experiments were performed on simple linear systems with a diagonal matrix $A \in \mathbb{R}^{N \times N}$ and with the right hand side of ones. The spectrum of diagonal matrices is of two types. Both are based on spectrum introduced in [8] which, for given $n$, $\lambda_1, \lambda_2$, and for parameter $\rho \in (0, 1]$ determining the non-uniformity of the spectrum, is distributed as

$$
\lambda_i = \lambda_1 + \frac{(\lambda_2 - \lambda_1)\rho^{i-1}}{\rho^{i-1} - 1},
$$

for $i = 2, \ldots, n$. The polynomial $R^m_\sigma(\lambda)$ has roots at the outlying eigenvalues. Application of the polynomial $C^m_{\lambda_1, \lambda_2 - m}(\lambda)$ to the rest of the spectrum gives the bound

$$
\|x - x_k\|_A \leq 2 \left( \sqrt{\kappa_{N-m}} - 1 \right) k \frac{\kappa_{N-m}}{\kappa_{N-m} + 1},
$$

where $\kappa_{N-m} = \lambda_{N-m}/\lambda_1$ may be substantially smaller than $\kappa$. On the other hand, there is a delay of $m$ iterations which are necessary to zero out eigenvalues, i.e., the bound is applicable at the steps $m, m+1, \ldots$.

We illustrate several other shortcomings of the composite upper bound. The difficulty is fundamental. The backward-like analysis implies that bounds valid in FP computations must be based on polynomials which are small on the union of tiny intervals located around original eigenvalues, for detail theoretical analysis see e.g. [7] or [5, Chapter 5].

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References