Stopping criteria in iterative methods – a miscellaneous issue?

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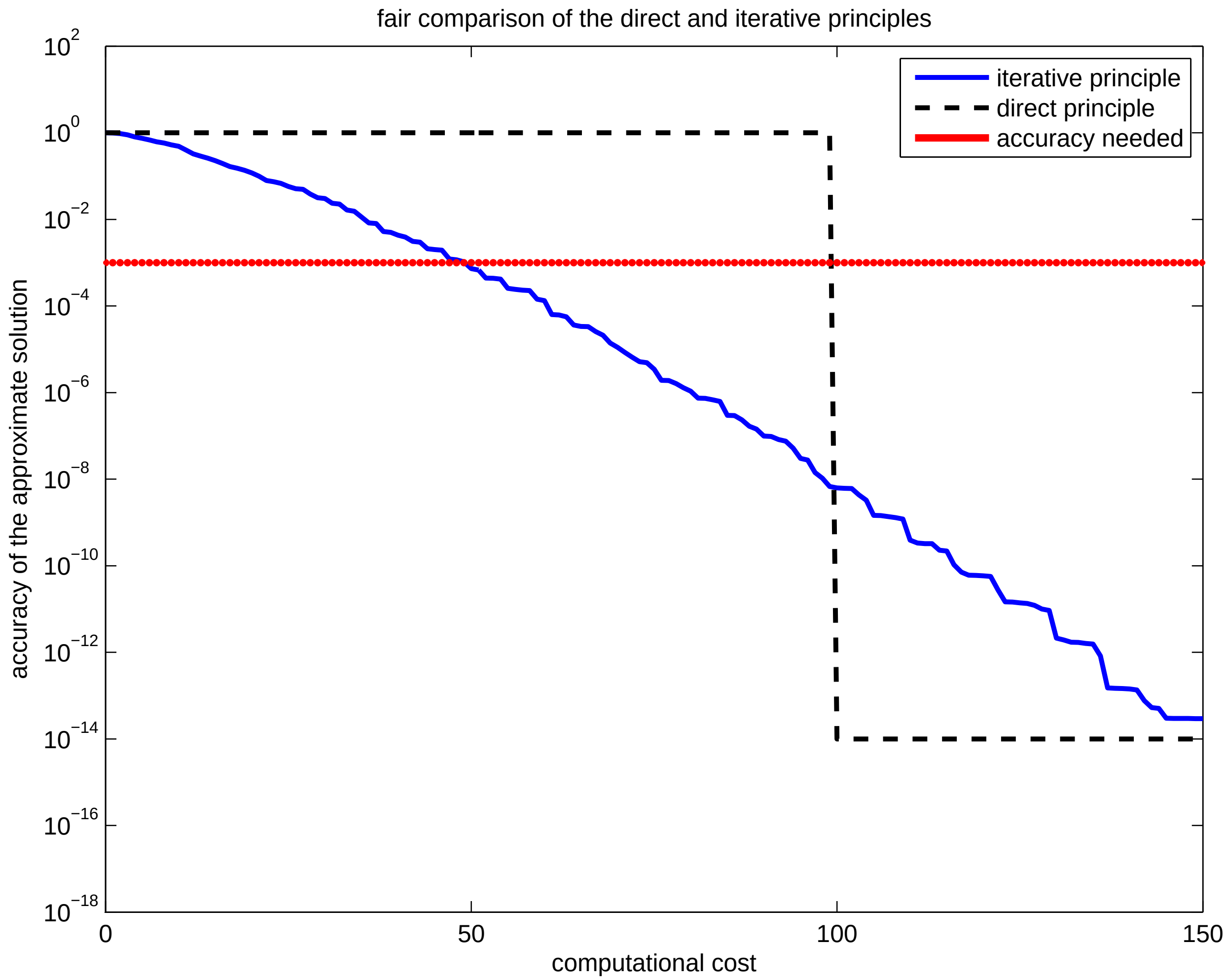
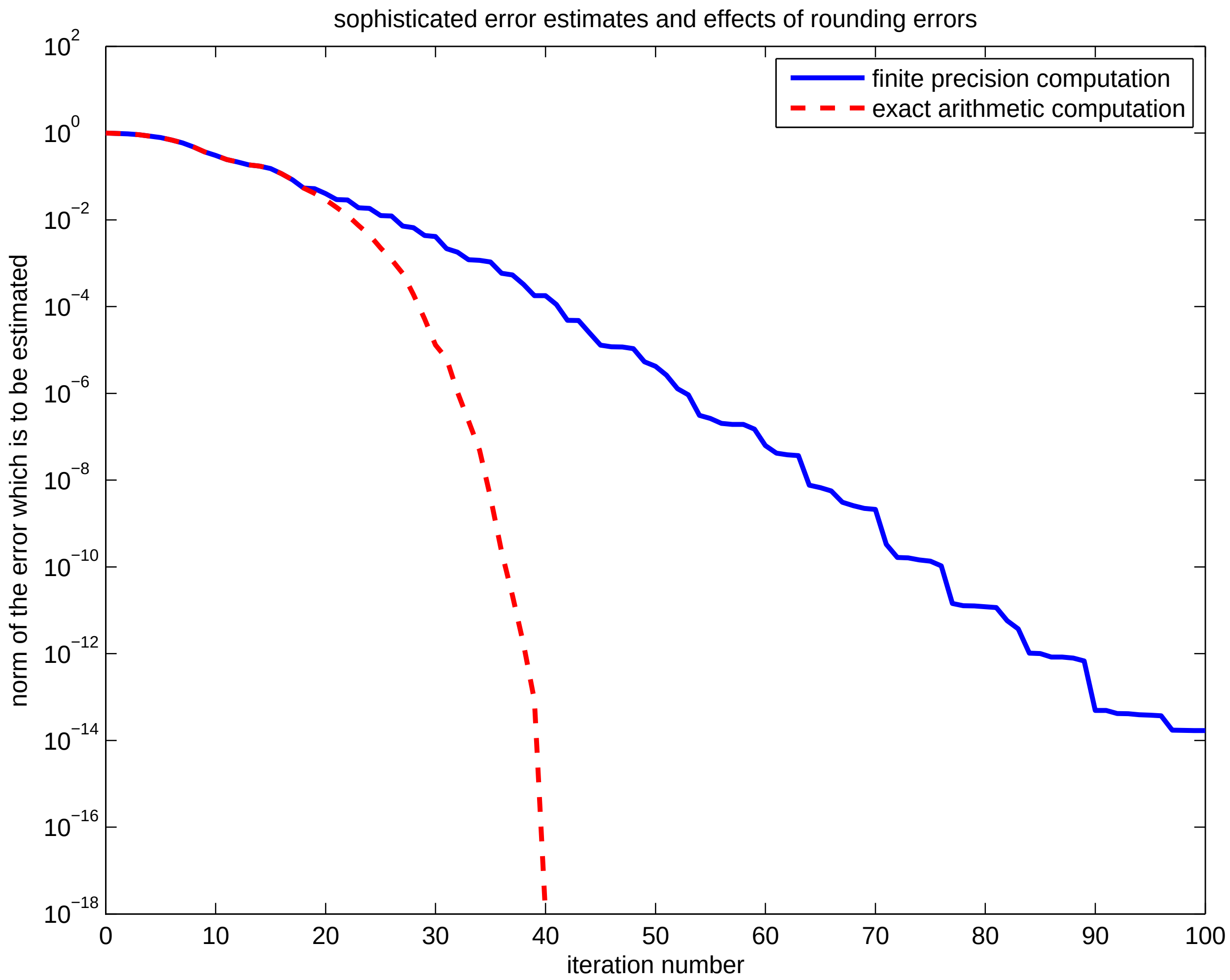
Fair comparison of the direct and iterative principle



Combination of the direct and iterative principle

- In order to reduce the disadvantages and profit from the advantages.
- Principal advantage of the iterative part is in stopping the computation at the desired accuracy level.
- It requires a meaningful stopping criterion. The errors of the model, discretization error and the computational error should be of the same order.
- Due to difficulties with the previous point this (potential) principal advantage is often presented as a disadvantage (a need for a stopping criteria . . .).

Stopping criteria and rounding error analysis



Backward error approach

How good is an approximate solution?

Consider a linear algebraic system $Ax = b$, and a computed approximation x_n . Then

$$Ax_n = b - r_n \, , \quad r_n = b - Ax_n \, .$$

Thus, $-r_n$ represents the (unique) perturbation Δb of the right hand side b such that x_n is the exact solution of the perturbed system.

A simple one-sided example of the perturbation theory – backward error approach.

How good is an approximate solution?

[Goldstine, Von Neumann - 47], [Turing], [Wilkinson - 63, 65]

Perturbation theory: $(A + \Delta A)\,\hat{x} \;=\; b + \Delta b\;.$

Normwise relative backward error:

Given $\hat{x}$, construct ΔA , Δb such that both
$\|\Delta A\|_2 / \|A\|_2$ and $\|\Delta b\|_2 / \|b\|_2$ are minimal;

$$\hat{x} \;\longrightarrow\; \frac{\|\Delta A\|_2}{\|A\|_2} \;=\; \frac{\|\Delta b\|_2}{\|b\|_2} \;=\; \frac{\|b - A\hat{x}\|_2}{\|b\|_2 + \|A\|_2 \|\hat{x}\|_2}\;.$$

NRBE stopping criterion

We ask and answer the question

"How close is the problem $(A + \Delta A)\, x_n \; = \; b + \Delta b$, which is solved by x_n accurately, to the original problem $A\, x \; = \; b$?"

Perhaps this is what we need – the matrix A and the right hand side b are inaccurate anyway.

Is the computed convergence curve close to the exact one?

Relative residual stopping criteria

Difference between the normwise relative backward error and the relative residual norm:

Backward error restricted to the right hand side only is given by

$$\|r_n\|_2 / \|b\|_2 \, .$$

Moreover, for an unwise choice of x_0 this may differ greatly from the frequently used relative residual norm

$$\|r_n\|_2 / \|r_0\|_2 \, .$$

Literature

On the backward error

The theory and history is given elegantly by Higham, 2nd Edn., 2002:
§1.10; pp. 29–30; Chapter 7, in particular §7.1, 7.2 and 7.7;

and also by Stewart & Sun, 1990, Section III/2.3;
Meurant, 1999, Section 2.7; among others —

but this is not easily accessible to non-experts.

The original BE references are:

Rigal & Gaches, J. Assoc. Comput. Mach. 1967,
for normwise analysis (used here);

Oettli & Prager, Num. Math. 1964,
for componentwise analysis.

Relation to stopping criteria

Explained and thoroughly discussed in

Higham, 2nd Edn., 2002, §17.5; and in
"Templates", Barrett *et al.*, 1995, Section 4.2.

These ideas have been used for constructing stopping criteria for years.

For example, in Paige & Saunders, ACM Trans. Math. Software 1982, the backward error idea is used to derive a family of stopping criteria which quantify the levels of confidence in A and b, and which are implemented in the generally available software realization of the LSQR method.

Stopping criteria

General considerations, methodology and applications:

Arioli, Duff & Ruiz, SIAM J. Mat. An. Appl. 1992;
Arioli, Demmel & Duff,
SIAM J. Matrix Anal. Appl. 1989;
Chatelin & Frayssé, 1996;
Kasenally & Simoncini, SIAM J. Numer. An. 1997.

Arioli, Noulard & Russo, Calcolo, 2001;
Arioli, Loghin & Wathen, Numer. Math. 2005;
Paige & Strakoš, SIAM J. Sci. Comput. 2002;
Strakoš & Liesen, ZAMM, 2005.

Stopping criteria

These ideas are not widely used by the applications community, apparently because very little attention has been paid to stopping criteria in some major numerical linear algebra or iterative methods text books, or reference books.

It would be healthy for users and also for our community if stopping criteria were considered to be fundamental parts of iterative computations, and not treated among the miscellaneous issues (or not treated at all).

Stopping criteria based on error estimates

An example when some more sophisticated stopping criteria may be preferable:

(Preconditioned) Conjugate gradient method
for solving discretized elliptic self-adjoint PDEs,

see:

Arioli, Numer. Math. 2004;
Hestenes & Stiefel, J. Res. Nat. Bur. St. 1952;
Meurant, Numerical Algorithms 1999;
Strakoš & Tichý, ETNA 2002;
Strakoš & Tichý, BIT 2005.
Meurant & Strakoš, Acta Numerica 2006;

Inaccurate data:

Normwise Backward Error Summary

Inaccurate data – stop early!

Usually $A \approx \tilde{A}$, $b \approx \tilde{b}$ where $\tilde{A}$ & $\tilde{b}$ are ideal unknowns. Suppose we know α, β where

$$\left.\begin{array}{ll} \tilde{A} = A + \delta A, & \tilde{b} = b + \delta b, \\ \|\delta A\|_2 \leq \alpha \|A\|_2, & \|\delta b\|_2 \leq \beta \|b\|_2. \end{array}\right\} \quad (*)$$

Justification for stopping criterion: If

$$\frac{\|b - Ax_k\|_2}{\beta \|b\|_2 + \alpha \|A\|_2 \|x_k\|_2} \leq 1,$$

$\exists$ δA_k, δb_k satisfying $(*)$, and

$$(A + \delta A_k)\, x_k = b + \delta b_k.$$

x_k the exact answer to a possible problem $\tilde{A} x_k = \tilde{b}$.

Proof

Rigal & Gaches, J. Assoc. Comp. Mach. 1967, showed: given $E, \; f$,

$$\eta_{E,f}(x_k) \quad = \quad \frac{\|b - Ax_k\|_2}{\|f\|_2 + \|E\|_2 \|x_k\|_2}$$

$$= \min_{\eta, \delta A, \delta b} \{ \eta : (A + \delta A)\, x_k = b + \delta b, \quad \|\delta A\|_2 \le \eta \|E\|_2, \; \|\delta b\|_2 \le \eta \|f\|_2 \}.$$

Take $E = \alpha A, \quad f = \beta b,$ and the result follows.

Important refinement

$$\eta'_{E,f}(x_k) = \frac{\|b - Ax_k\|_2}{\|f\|_2 + \|E\|_F \|x_k\|_2}$$

$$= \min_{\eta', \delta A, \delta b} \{ \eta' : (A + \delta A)\, x_k = b + \delta b,$$

$$\|\delta A\|_F \leq \eta' \|E\|_F, \; \|\delta b\|_2 \leq \eta' \|f\|_2 \}$$

gives the directly applicable NRBE' criterion
based on the Frobenius matrix norm.

One more reference

More details can be found in

"Modified Gram-Schmidt (MGS), Least Squares,
and backward stability of MGS-GMRES"
C. C. Paige, M. Rozložník, and Z. Strakoš,

to appear in SIAM J. Matrix Anal Appl.

Thank you for your kind attention!