The conjugate gradient method in finite precision computations

Krystyna Ziętak

Wrocław University of Technology
Institute of Mathematics and Computer Science

Warsaw, October 7, 2006

Lanczos method

C. Lanczos,
An iteration method for the solution of the eigenvalue problem of linear differential and integral equation,
J. Res. Nat. Bur. Standards 45 (1950), 255–282.

Conjugate gradient method

M.R. Hestenes, E. Stiefel,
Methods of conjugate gradients for solving linear systems,
J. Nat. Bur. Standards 49 (1952), 409–436.

Pioneering papers of Woźniakowski

1. H. Woźniakowski, Numerical stability of the Chebyshev method for the solution of large linear systems, **Numer. Math. 28 (1977), 191–209**.
2. H. Woźniakowski, Roundoff error analysis iterations for large linear systems, **Numer. Math. 30 (1978), 301–314**.
3. H. Woźniakowski, Roundoff-error analysis of a new class of conjugate-gradient algorithms, **Linear Alg. Appl. 29 (1980), 507–529**.

Pioneering papers of Woźniakowski

1. H. Woźniakowski, Numerical stability of the Chebyshev method for the solution of large linear systems,
   Numer. Math. 28 (1977), 191–209.
2. H. Woźniakowski, Roundoff error analysis iterations for large linear systems,
   Numer. Math. 30 (1978), 301–314.
3. H. Woźniakowski, Roundoff-error analysis of a new class of conjugate-gradient algorithms,
   Linear Alg. Appl. 29 (1980), 507–529.

Pioneering papers of Woźniakowski

1. H. Woźniakowski, Numerical stability of the Chebyshev method for the solution of large linear systems,
   Numer. Math. 28 (1977), 191–209.
2. H. Woźniakowski, Roundoff error analysis iterations for large linear systems,
   Numer. Math. 30 (1978), 301–314.
3. H. Woźniakowski, Roundoff-error analysis of a new class of conjugate-gradient algorithms,
   Linear Alg. Appl. 29 (1980), 507–529.

Pioneering PhD thesis

1. **C.C. Paige**, The computation of eigenvalues and eigenvectors of very large sparse matrices, *University of London 1971*.
2. **A. Greenbaum**, Convergence properties of the conjugate gradient algorithm in exact and finite precision arithmetic, *University of California, Berkeley 1981*.

Review paper

- **G. Meurant, Z. Strakoš**, The Lanczos and conjugate gradient algorithms in finite precision arithmetic, **Acta Numerica 2006, 471–542**.

Pioneering PhD thesis

1. **C.C. Paige**, The computation of eigenvalues and eigenvectors of very large sparse matrices, *University of London 1971*.
2. **A. Greenbaum**, Convergence properties of the conjugate gradient algorithm in exact and finite precision arithmetic, *University of California, Berkeley 1981*.

Review paper

- **G. Meurant, Z. Strakoš**, The Lanczos and conjugate gradient algorithms in finite precision arithmetic, **Acta Numerica 2006, 471–542**.

Pioneering PhD thesis

1. **C.C. Paige**, The computation of eigenvalues and eigenvectors of very large sparse matrices, *University of London 1971*.
2. **A. Greenbaum**, Convergence properties of the conjugate gradient algorithm in exact and finite precision arithmetic, *University of California, Berkeley 1981*.

Review paper

- **G. Meurant, Z. Strakoš**, The Lanczos and conjugate gradient algorithms in finite precision arithmetic, **Acta Numerica 2006, 471–542**.

Roundoff error analysis of iterations for linear systems

$$Ax = b, \quad A \text{ Hermitian positive definite}$$

$$\alpha \quad \text{exact solution}, \quad y \text{ computed solution in } fl$$

Numerical stability of method

$$||y - \alpha|| \quad \text{is of order } 2^{-t}||A||\;||A^{-1}||\;||\alpha||$$

Well behaviour

$$(A + \Delta A)y = b, \quad ||\Delta A|| \text{ is of order } 2^{-t}||A||$$

Numerical stability of iterative method

$$x_k \quad \text{computed} \quad \text{sequence in } fl$$

$$\overline{\lim_k} ||x_k - \alpha|| \quad \text{is of order } 2^{-t} ||A|| \; ||A^{-1}|| \; ||\alpha||$$

Woźniakowski 1977

- Chebyshev method is numerically stable,
- but not well-behaved
- residuals

$$||Ax_k - b|| \quad \text{are of order } 2^{-t} ||A||^2 ||A-1|| \; ||\alpha||$$

Numerical stability of iterative method

$$x_k \quad \text{computed} \quad \text{sequence in } fl$$

$$\overline{\lim_k} ||x_k - \alpha|| \quad \text{is of order } 2^{-t}||A|| \; ||A^{-1}|| \; ||\alpha||$$

Woźniakowski 1977

- Chebyshev method is numerically stable,
- but not well-behaved
- residuals

$$||Ax_k - b|| \quad \text{are of order } 2^{-t}||A||^2||A{-}1|| \; ||\alpha||$$

Numerical stability of iterative method

$$x_k \quad \text{computed} \quad \text{sequence in } fl$$

$$\overline{\lim_k} ||x_k - \alpha|| \quad \text{is of order } 2^{-t}||A|| \; ||A^{-1}|| \; ||\alpha||$$

Woźniakowski 1977

- Chebyshev method is numerically stable,
- but not well-behaved
- residuals

$$||Ax_k - b|| \quad \text{are of order } 2^{-t}||A||^2||A{-}1|| \; ||\alpha||$$

Chebyshev method

$$x_k - \alpha = W_k(A)(x_0 - \alpha)$$

$$W_k(z) = \frac{T_k(f(z))}{T_k(f(0))}, \qquad f(z) = \frac{b+a}{b-a} - 2\frac{z}{b-a}$$

$T_k(z)$ Chebyshev polynomial

$$r_k := Ax_k - b, \quad x_{k+1} := x_k + [p_{k-1}(x_k - x_{k-1}) - r_k]/q_k,$$

new algorithm for computing p_k and q_k

Jacobi, Gauss-Seidel, SOR

$$A = A^H > 0 \quad \text{has property A}$$

consistently ordered, $\quad A = D - L - U, \quad \gamma D^{-1}U + \gamma^{-1}D^{-1}U$

$$A = \begin{bmatrix} D_1 & A_{12} \\ A_{21} & D_2 \end{bmatrix}$$

Woźniakowski 1978

- Jacobi, Richardson, SOR methods are numerically stable, but not well-behaved
- Gauss-Seidel is well-behaved

Jacobi, Gauss-Seidel, SOR

$$A = A^H > 0 \quad \text{has property A}$$

consistently ordered, $\quad A = D - L - U, \quad \gamma D^{-1} U + \gamma^{-1} D^{-1} U$

$$A = \begin{bmatrix} D_1 & A_{12} \\ A_{21} & D_2 \end{bmatrix}$$

Woźniakowski 1978

- Jacobi, Richardson, SOR methods are numerically stable, but not well-behaved
- Gauss-Seidel is well-behaved

Conjugate gradient method *cg*

$$Ax = b$$

$$A = A^H > 0, \quad \text{order } n$$

- In exact arithmetic *cg* generates orthogonal residual vectors $r_k = b - Ax_k$

$$< r_i, r_j >= 0$$

- in exact arithmetic $\alpha = A^{-1}b$ is obtained after at most n steps.

Conjugate gradient method *cg*

$$Ax = b$$

$$A = A^H > 0, \quad \text{order } n$$

- In exact arithmetic *cg* generates orthogonal residual vectors $r_k = b - Ax_k$

$$< r_i, r_j >= 0$$

- in exact arithmetic $\alpha = A^{-1}b$ is obtained after at most n steps.

Hestenes-Stiefel formulation of *cg*

- given x_0, $\quad r_0 = b - Ax_0$, $\quad p_0 = r_0$
- for $j = 1, 2, \ldots$

$$x_j = x_{j-1} + \gamma_{j-1} p_{j-1}$$

$$\gamma_{j-1} = \frac{< r_{j-1}, r_{j-1}}{< p_j, Ap_{j-1} >}, \qquad \delta_j = \frac{< r_j, r_j >}{< r_{j-1}, r_{j-1} >}$$

$$p_j = r_j + \delta_j p_{j-1}, \qquad r_j = r_{j-1} - \gamma_{j-1} A p_{j-1},$$

Woźniakowski 1980

- new class of conjugate gradient algorithms
- numerical stability of these algorithms with iterative refinement
- numerical well behaviour if $2^{-t}[\mathrm{cond}_2(A)]^2$ is at most of order unity

Gatlinburg VII at Asilomar 1977

Woźniakowski 1980

- new class of conjugate gradient algorithms
- numerical stability of these algorithms with iterative refinement
- numerical well behaviour if $2^{-t}[\text{cond}_2(A)]^2$ is at most of order unity

Gatlinburg VII at Asilomar 1977

Woźniakowski 1980

- new class of conjugate gradient algorithms
- numerical stability of these algorithms with iterative refinement
- numerical well behaviour if $2^{-t}[\mathrm{cond}_2(A)]^2$ is at most of order unity

Gatlinburg VII at Asilomar 1977

Woźniakowski algorithm

Woźniakowski *cg*

$$r_k = Ax_k - b, \qquad z_k = x_k - c_k r_k$$

$$y_k = x_{k-1} - z_k, \qquad c_k = \frac{< r_k, r_k >}{< r_k, Ar_k >}$$

$$\mathbf{x_{k+1} = z_k - u_k y_k}$$

algorithm for computation of u_k is not given explicitly

Classical version of *cg*: $x_{k+1} = x_k + \gamma_k p_k$

In: *Accuracy and Stability of Numerical Algorithms* Higham writes:

1. Woźniakowski (1980) analyses a class of conjugate gradient algorithms (which does not include the usual conjugate gradient method).
2. Woźniakowski obtains a forward error bound proportional to $[\mathrm{cond}(A)]^{3/2}$ and a residual bound proportional to $\mathrm{cond}(A)$.

In: *Accuracy and Stability of Numerical Algorithms* Higham writes:

1. Woźniakowski (1980) analyses a class of conjugate gradient algorithms (which does not include the usual conjugate gradient method).
2. Woźniakowski obtains a forward error bound proportional to $[\mathrm{cond}(A)]^{3/2}$ and a residual bound proportional to $\mathrm{cond}(A)$.

In: *Accuracy and Stability of Numerical Algorithms* Higham writes:

1. Greenbaum (1989) presents a detailed error analysis of the conjugate gradient method, but her concern is with the rate of convergence rather than the attainable accuracy.
2. Notay (1993) analyses how rounding errors influence the convergence rate of the conjugate gradient method for matrices with isolated eigenvalues at the ends of the spectrum.

In: *Accuracy and Stability of Numerical Algorithms* Higham writes:

1. Greenbaum (1989) presents a detailed error analysis of the conjugate gradient method, but her concern is with the rate of convergence rather than the attainable accuracy.
2. Notay (1993) analyses how rounding errors influence the convergence rate of the conjugate gradient method for matrices with isolated eigenvalues at the ends of the spectrum.

Woźniakowski class of *cg* algorithms

For these algorithms there exists computed vector x_k such that

$||A^{1/2}(x_k - \alpha)|| \leq c_n 2^{-t} ||A^{1/2}|| \, ||x_k||$

If $||A^{1/2}|| \, ||x_k||$ is of order $||A^{1/2} x_k||$

then these *cg* algorithms

are numerically stable in A-norm:

$$||A^{1/2}(x_k - \alpha)|| = 0(2^{-t}\mathrm{cond}(A)||A^{1/2}x_k||),$$

but not well behaved

Relationship between *cg* and Lanczos

Krylov subspace

$$A \; n \times n, \quad \text{nonsingular sym. posit. def.,} \; ||v||_2 = 1$$

$$\mathcal{K}_k(v, A) = \text{span}\{v, Av, \ldots, A^{k-1}v\},$$

$$Ax = b, \qquad r_0 = b - Ax_0$$

$$x_k = x_0 + V_k y_k$$

V_k is the matrix of orthonormal basis of $\mathcal{K}_k(v_1, A)$, where Krylov subspace is generated by Lanczos algorithm with $v_1 = r_0/||r_0||$

Conjugate gradient method *cg* and Lanczos

Matrix notation Lanczos algorithm

$$AV_k = V_k T_k + \eta_{k+1} v_{k+1} e_k^T, \qquad T_k \text{ sym. tridiag.}$$

$$(*) \quad T_k y_k = ||r_0|| e_1, \qquad x_k = x_0 + V_k y_k$$

(*) is equivalent to *cg* method of Hestenes and Stiefel

Properties of cg

If $r_k = b - Ax_k = r_0 - AV_k y_k$ is orthogonal to V_k then $r_{n+1} = 0$

- $r_0 = b - Ax_0, \quad v_1 = r_0/||r_0||$
- $\mathcal{K}_k(v_1, A) = \mathrm{span}\{r_0, \ldots, r_{k-1}\}$
- $< r_i, r_j >= 0, \quad r_k \perp \mathcal{K}_k(v_1, A)$
- $$v_{k+1} = (-1)^k \frac{r_k}{||r_k||}$$

Properties of cg

If $r_k = b - Ax_k = r_0 - AV_k y_k$ is orthogonal to V_k then $r_{n+1} = 0$

- $r_0 = b - Ax_0, \quad v_1 = r_0/||r_0||$
- $\mathcal{K}_k(v_1, A) = \mathrm{span}\{r_0, \ldots, r_{k-1}\}$
- $< r_i, r_j >= 0, \quad r_k \perp \mathcal{K}_k(v_1, A)$
- $$v_{k+1} = (-1)^k \frac{r_k}{||r_k||}$$

Properties of cg

If $r_k = b - Ax_k = r_0 - AV_k y_k$ is orthogonal to V_k then $r_{n+1} = 0$

- $r_0 = b - Ax_0, \quad v_1 = r_0/||r_0||$
- $\mathcal{K}_k(v_1, A) = \mathrm{span}\{r_0, \ldots, r_{k-1}\}$
- $< r_i, r_j >= 0, \quad r_k \perp \mathcal{K}_k(v_1, A)$
- $$v_{k+1} = (-1)^k \frac{r_k}{||r_k||}$$

Properties of *cg*

If $r_k = b - Ax_k = r_0 - AV_k y_k$ is orthogonal to V_k then $r_{n+1} = 0$

- $r_0 = b - Ax_0, \quad v_1 = r_0/||r_0||$
- $\mathcal{K}_k(v_1, A) = \mathrm{span}\{r_0, \dots, r_{k-1}\}$
- $< r_i, r_j >= 0, \quad r_k \perp \mathcal{K}_k(v_1, A)$
- $$v_{k+1} = (-1)^k \frac{r_k}{||r_k||}$$

Error norms in *cg*

1. Lanczos and *cg* can be formulated in terms of orthogonal polynomials and Gauss quadrature of some integral determined by A, v_1
2. Lanczos and *cg* can be viewed as matrix representations of Gauss quadrature
3. $A-$norm of the error $x_k - \alpha$ and Euclidean norm of the error in *cg* can be computed using Gauss quadrature.

Error norms in *cg*

1. Lanczos and *cg* can be formulated in terms of orthogonal polynomials and Gauss quadrature of some integral determined by A, v_1
2. Lanczos and *cg* can be viewed as matrix representations of Gauss quadrature
3. $A-$norm of the error $x_k - \alpha$ and Euclidean norm of the error in *cg* can be computed using Gauss quadrature.

Error norms in *cg*

1. Lanczos and *cg* can be formulated in terms of orthogonal polynomials and Gauss quadrature of some integral determined by A, v_1
2. Lanczos and *cg* can be viewed as matrix representations of Gauss quadrature
3. $A-$norm of the error $x_k - \alpha$ and Euclidean norm of the error in *cg* can be computed using Gauss quadrature.

Error norms in *cg*

1. Computing $A-$norm of the error $x_k - \alpha$ is closely related to approximating quadratic forms.
2. This has been studied extensively by **Gene Golub with many collaborators during the last thirty-five years** (see the review paper of Meurant and Strakoš)

Error norms in *cg*

1. Computing $A-$norm of the error $x_k - \alpha$ is closely related to approximating quadratic forms.
2. This has been studied extensively by **Gene Golub with many collaborators during the last thirty-five years** (see the review paper of Meurant and Strakoš)

Lanczos and *cg* in finite precision

1. What happens numerically to the equivalence of Lanczos and *cg* as well as to the equivalence with orthogonal polynomials and Gauss quadrature?
2. How do we evaluate convergence of *cg* in finite precision arithmetic?
3. see **Z. Strakoš and P. Tichy**, On error estim. in *cg* and why it works in finite precision computation, *Electr. Trans. Numer. Anal.* 13 (2002).

Lanczos and *cg* in finite precision

1. What happens numerically to the equivalence of Lanczos and *cg* as well as to the equivalence with orthogonal polynomials and Gauss quadrature?
2. How do we evaluate convergence of *cg* in finite precision arithmetic?
3. see **Z. Strakoš and P. Tichy**, On error estim. in *cg* and why it works in finite precision computation, *Electr. Trans. Numer. Anal.* 13 (2002).

Lanczos and *cg* in finite precision

1. What happens numerically to the equivalence of Lanczos and *cg* as well as to the equivalence with orthogonal polynomials and Gauss quadrature?
2. How do we evaluate convergence of *cg* in finite precision arithmetic?
3. see **Z. Strakoš and P. Tichy**, On error estim. in *cg* and why it works in finite precision computation, *Electr. Trans. Numer. Anal.* 13 (2002).

Conclusion
from Strakoš and Tichy talk:

Hestenes and Stiefel cg (1952)

should be celebrated,

but also studied,
even after 50 years!

Most important of all

My congratulations to
Henryk
who was the pioneer
in this field!!!

Many happy and fruitful years!!!