Matrices, moments and quadrature with applications

Gérard MEURANT

January-February, 2012
1 Motivations
2 Applications
Motivations

Assume we are solving a linear system $Ax = b$ where $A$ is a square symmetric positive definite matrix of order $n$

The method of choice is the Conjugate Gradient (CG) algorithm

Problem: when to stop the iterations?

Most people use $\|r^k\| \leq \epsilon \|r^0\|$ or $\|r^k\| \leq \epsilon \|b\|

But this can be misleading as we will see in the next slide

Consider the matrix BCSSTK01, $n = 48$, $\|A\| = 3.0152 \times 10^9$, $\|A^{-1}\| = 2.9263 \times 10^{-4}$ (origin: Matrix Market)
Conjugate Gradient for BCSSTK01, $n = 48$

In this example, we will stop too late, the error norm is smaller than the norm of the residual
Error norms in solving linear systems

Let \( \tilde{x} \) an approximate solution of

\[
Ax = b
\]

The residual \( r \) is defined as

\[
r = b - A\tilde{x}
\]

Note that \( r \) can be computed

The error \( \epsilon \) is defined as \( \epsilon = x - \tilde{x} \) and

\[
\epsilon = A^{-1}r
\]

Of course, \( \epsilon \) is generally unknown (except for test problems)
For $A$ symmetric positive definite (SPD), the $A$–norm of the error is
\[ \|\epsilon\|_A^2 = \epsilon^T A \epsilon = r^T A^{-1} A A^{-1} r = r^T A^{-1} r \]

The $l_2$ norm is $\|\epsilon\|^2 = r^T A^{-2} r$

Can we compute estimates of $r^T A^{-1} r$ or $r^T A^{-2} r$?

These are quadratic forms $I[f] = u^T f(A) u$

One idea is to write $I[f]$ as an integral and to use quadrature rules to compute approximations
Ingredients

To achieve our goal we will use

- Orthogonal polynomials
- Tridiagonal matrices
- The Lanczos and conjugate gradient methods
- Quadrature rules
Here are some applications in which quadratic forms are involved:

- Computation of elements of functions of matrices
- Estimates of the norm of the error in iterative methods
- Least squares problems
- Total least squares
- Regularization of discrete ill-posed problems
- ...