Numerical Linear Algebra

Basic iterative methods

Gerard Sleijpen and Martin van Gijzen

October 1, 2008

Program October 1

- Basic methods for eigenproblems.
  - Standard Power method
  - Shift-and-invert Power method
  - QR algorithm
- Basic iterative methods for linear systems
  - Richardson's method
  - Jacobi, Gauss-Seidel and SOR
  - Iterative refinement
- Steepest decent and the Minimal residual method

Basic methods for eigenproblems

The eigenvalue problem

$$Ax = \lambda x$$

can not be solved in a direct way for problems of order > 4, since the eigenvalues are the roots of the characteristic equation

$$det(A - \lambda I) = 0 \; .$$

Today we will discuss two *iterative* methods for solving the eigen-problem.

The Power method

The Power method is the classical method to compute largest eigenvalue and eigenvector of a matrix.

Multiplying with a matrix amplifies strongest the eigendirection corresponding to the (in modulus) largest eigenvalues most.

Successively multiplying and scaling (to avoid overflow or underflow) yields a vector in which the direction of the largest eigenvector becomes more and more dominant.

Algorithm

The Power method

$q_0 \in \mathbb{C}^n$ is given

for $k = 1, 2, ...$

$$z_k = Aq_{k-1}$$
$$q_k = z_k / \|z_k\|_2$$
$$\lambda^{(k)} = q_{k-1}^H z_k$$

endfor

It can easily be seen that if q_{k-1} is an eigenvector corresponding to λ_j then

$$\lambda^{(k)} = q_{k-1}^H A q_{k-1} = \lambda_j q_{k-1}^H q_{k-1} = \lambda_j \|q_{k-1}\|_2^2 = \lambda_j .$$

Convergence (1)

Assume that the n eigenvalues are ordered such that $|\lambda_1| > |\lambda_2| \geq ... \geq |\lambda_n|$ and the eigenvectors by $x_1, ..., x_n$ so $Ax_i = \lambda_i x_i$. Each arbitrary starting vector q_0 can be written as:

$$q_0 = a_1 x_1 + a_2 x_2 + ... + a_n x_n$$

and if $a_1 \neq 0$ it follows that

$$A^k q_0 = a_1 \lambda_1^k (x_1 + \sum_{j=2}^{n} \frac{a_j}{a_1} \left(\frac{\lambda_j}{\lambda_1} \right)^k x_j) \ .$$

Convergence (2)

Using this equality we conclude that

$$|\lambda_1 - \lambda^{(k)}| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right) \quad , \quad \text{and also}$$

the angle between q_k and x_1 is of order $|\frac{\lambda_2}{\lambda_1}|^k$.

Convergence (3)

Note that there is a problem if $|\lambda_1| = |\lambda_2|$, which is the case for instance if $\lambda_1 = \bar{\lambda}_2$. A vector q_0 which has a nonzero component in x_1 and x_2 can be written as

$$q_0 = a_1 x_1 + a_2 x_2 + \sum_{j=3}^{n} a_j x_j \ .$$

The component in the direction of $x_3, ..., x_n$ will vanish in the Power method, but q_k will not tend to a limit.

Shifting

Clearly, the (asymptotic) convergence depends on $|\frac{\lambda_2}{\lambda_1}|$. To speed-up convergence the Power method can also be applied to the shifted problem

$$(A - sI)x = (\lambda - s)x$$

The asymptotic rate of convergence now becomes

$$|\frac{\lambda_2 - s}{\lambda_1 - s}|$$

Moreover, by choosing a suitable shift (*how?*) convergence can be forced towards the smallest eigenvalue of A.

Shift-and-invert

Another way to speed-up convergence is to apply the Power method to the *shifted and inverted* problem

$$(A - sI)^{-1}x = \mu x \quad \lambda = \frac{1}{\mu} + s$$

This technique allows us to compute eigenvalues near the shift. However, for this the solution of a system is required in every iteration!

Assignment: Show that the shifted and inverted problem and the original problem share the same eigenvectors.

The QR method (1)

A popular techniqu,e in particular to solve small or dense eigenvalue problems, is the QR method.
The method starts with the matrix A_0, factors it by Gram-Schmidt into $Q_0 R_0$ and then reverses the factors: $A_1 = R_0 Q_0$.

Assignment: Show that A_0 and A_1 are similar (share the same eigenvectors).

The QR method (1)

A popular techniqu,e in particular to solve small or dense eigenvalue problems, is the QR method.
The method starts with the matrix A_0, factors it by Gram-Schmidt into $Q_0 R_0$ and then reverses the factors: $A_1 = R_0 Q_0$.

Assignment: Show that A_0 and A_1 are similar (share the same eigenvectors).

$$Q_0^{-1} A_0 Q_0 = Q_0^{-1} Q_0 R_0 Q_0 = A_1$$

The QR method (2)

Repeating this process yields

$$A_k = Q_k R_k \qquad A_{k+1} = R_k Q_k$$

The matrix A_k becomes more and more upper triangular and finally the eigenvalues will be on the main diagonal.

The QR method (3)

Normally the algorithm is used with shifts

$$A_k - \alpha_k I = Q_k R_k \qquad A_{k+1} = R_k Q_k + \alpha_k I$$

This is justified by the fact that A_{k+1} is similar to A_k (**Check this!**).

Normally the shifted algorithm converges quadratically.

Iterative methods for linear systems

Iterative methods construct successive approximations x_k to the solution of the linear systems $Ax = b$. Here k is the iteration number, and the approximation x_k is also called the *iterate*. The vector $r_k = b - Ax_k$ is the *residual*.

The iterative methods are composed of only a few different basic operations:

- Products with the matrix A
- Vector operations (updates and inner product operations)
- *Preconditioning operations*

Preconditioning

Usually iterative methods are applied not to the original system

$$Ax = b$$

but to the preconditioned system

$$M^{-1}Ax = M^{-1}b$$

where the preconditioner is chosen such that:

- Preconditioning operations (operations with M^{-1}) are cheap;
- The iterative method converges much faster for the preconditioned system.

Basic iterative methods

The first iterative methods we will discuss are the *basic iterative methods*. Basic iterative methods only use information of the previous iteration.

Until the 70's they were quite popular. Some are still used but as preconditioners in combination with an acceleration technique. They also still play a role in multigrid techniques where they are used as smoothers.

Basic iterative methods (2)

Basic iterative methods are usually constructed using a splitting of A:

$$A = M - R.$$

Successive approximations are then computed using the iterative process

$$Mx_{k+1} = Rx_k + b$$

which is equivalent too

$$x_{k+1} = x_k + M^{-1}(b - Ax_k)$$

The vector $r_k = b - Ax_k$ is called the *residual*, and the matrix M is a *preconditioner*. The next few slides we look at $M = I$.

Richardson's method

The choice $M = I$, $R = I - A$ gives Richardson's method, which is the most simple iterative method possible.

The iterative process becomes

$$x_{k+1} = x_k + (b - Ax_k) = b + (I - A)x_k$$

Richardson's method (2)

This process yields the following iterates:

Initial guess $x_0 = 0$

$$x_1 = b$$

$$x_2 = b + (I - A)x^{(1)} = b + (I - A)b$$

$$x_3 = b + (I - A)x^{(2)} = b + (I - A)b + (I - A)^2 b$$

Repeating this gives

$$x_{k+1} = \sum_{i=0}^{k} (I - A)^i b$$

Richardson's method (3)

So Richardson's method generates the series expansion for $\frac{1}{1-z}$ with $z = I - A$. If this series converges we have

$$\sum_{i=0}^{\infty} (I - A)^i = A^{-1}$$

The series expansion for $\frac{1}{1-z}$ converges if $|z| < 1$. If A is diagonalizable then the series $\sum_{i=0}^{\infty} (I - A)^i$ converges if

$$|1 - \lambda| < 1$$

with λ any eigenvalue of A. For λ real this means that

$$0 < \lambda < 2$$

Richardson's method (4)

In order to increase the radius of convergence and to speed up the convergence, one can introduce a parameter α:

$$x_{k+1} = x_k + \alpha(b - Ax_k) = \alpha b + (I - \alpha A)x_k$$

It is easy to verify that if all eigenvalues are real and positive the optimal α is given by

$$\alpha_{opt} = \frac{2}{\lambda_{max} + \lambda_{min}}.$$

Richardson's method (5)

Before, we assumed for the initial guess $x_0 = 0$.
Starting with another initial guess x_0 only
means that we have to solve a shifted system

$$A(y + x_0) = b \Leftrightarrow Ay = b - Ax_0 = r_0$$

So the results obtained before remain valid, irrespective of the initial guess.

Richardson's method (6)

We want to stop once the error $\|x_k - x\| < \epsilon$, with ϵ some prescribed tolerance e. Unfortunately we do not know x, so this criterion does not work in practice.

Alternatives are:

- $\|r_k\| = \|b - Ax_k\| = \|Ax - Ax_k\| < \epsilon$
  Disadvantage: criterion not scaling invariant
- $\frac{\|r_k\|}{\|r_0\|} < \epsilon$
  Disadvantage: good initial guess does not reduce the number of iterations
- $\frac{\|r_k\|}{\|b\|} < \epsilon$
  Seems best

Convergence of Basic Iterative Methods

To investigate the convergence of Basic Iterative Methods in general, we look again at the formula

$$Mx_{k+1} = Rx_k + b.$$

Remember that $A = M - R$. If we subtract $Mx = Rx + b$ from this equation we get a recursion for the error $e = x_k - x$:

$$Me_{k+1} = Re_k$$

Convergence of Basic Iterative Methods

We can also write this as

$$e_{k+1} = M^{-1}Re_k$$

This is a power iteration and hence the error will ultimately point in the direction of the largest eigenvector of $M^{-1}R$. The rate of convergence is determined by the *spectral radius* $\rho(M^{-1}R)$ of $M^{-1}R$:

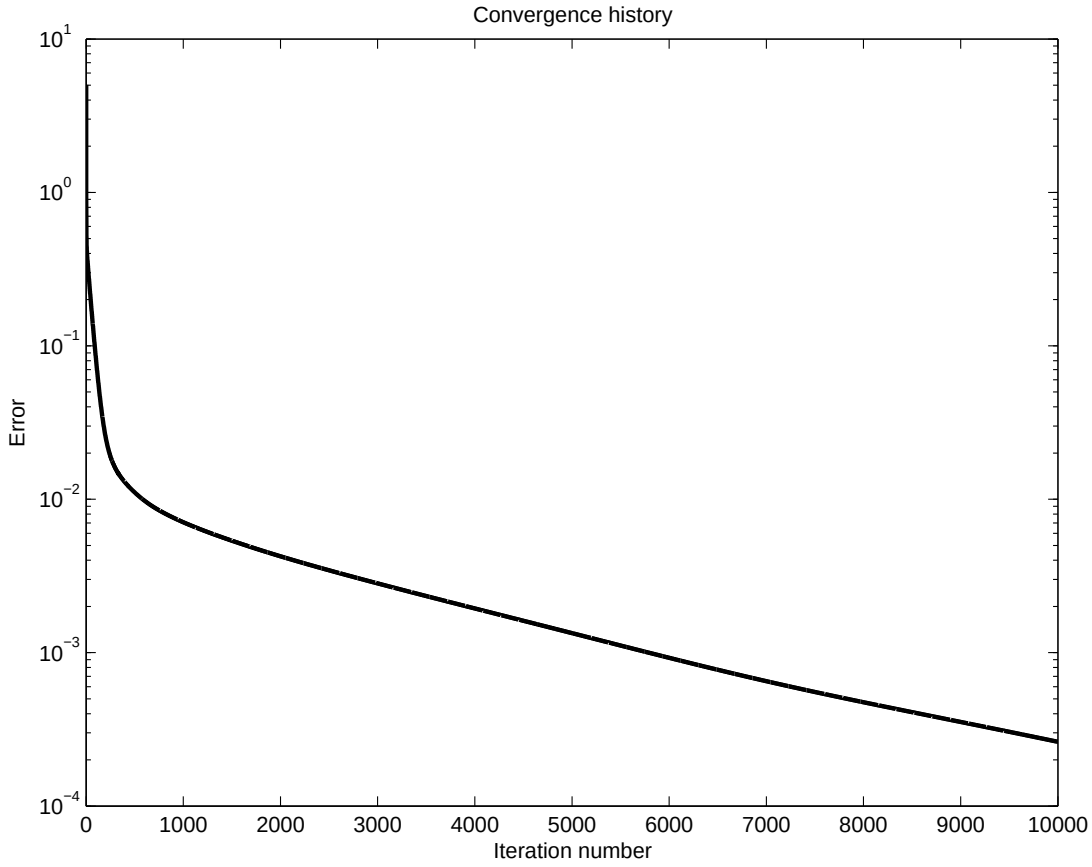
$$\rho(M^{-1}R) = |\lambda_{max}(M^{-1}R)| \ .$$

For convergence we must have that

$$\rho(M^{-1}R) < 1 \ .$$

Linear convergence

Ultimately, we have $\|e_{k+1}\| \approx \rho(M^{-1}R)\|e_k\|$, which means that we have linear convergence



Classical Basic Iterative Methods

We will now briefly discuss the three best known basic iterative methods

- Jacobi's method
- The method of Gauss-Seidel
- Successive overrelaxation

These methods can be seen as Richardson's method applied to the preconditioned system

$$M^{-1}Ax = M^{-1}b \; .$$

Jacobi's method

We first write $A = L + D + U$, with L the strictly lower triangular part of A, D the main diagonal and U the strictly upper triangular part. Jacobi's method is now defined by the choice $M = D$, $R = -L - U$. The process is given by

$$Dx_{k+1} = (-L - U)x_k + b$$

or equivalently by

$$x_{k+1} = x_k + D^{-1}(b - Ax_k)$$

The Gauss-Seidel method

We write again $A = L + D + U$. The Gauss-Seidel method is now defined by the choice $M = L + D$, $R = -U$. The process is given by

$$(L + D)x_{k+1} = -Ux_k + b$$

or equivalently by

$$x_{k+1} = x_k + (L + D)^{-1}(b - Ax_k)$$

Successive overrelaxation (SOR)

We write again $A = L + D + U$. The SOR method is now defined by the choice $M = D + \omega L$, $R = (1 - \omega)D - \omega U$. The parameter ω is called the relaxation parameter. The process is given by

$$(D + \omega L)x_{k+1} = ((1 - \omega)D - \omega U)x_k + \omega b$$

or as

$$x_{k+1} = x_k + \omega(D + \omega L)^{-1}(b - Ax_k)$$

With $\omega = 1$ we get the method of Gauss-Seidel back. In general the optimal value of ω is not known.

Iterative refinement

Last week we saw direct methods. For numerical stability it is necessary to perform partial pivoting. However, this goes at the expense of the efficiency.
If the LU-factors are inaccurate, such that $A = LU - R$, they can still be used as *preconditioner* for the process

$$x_{i+1} = x_i + (LU)^{-1}(b - Ax_i)$$

This is called *iterative refinement* and is used to improve the accuracy of the direct solution.

One-step projection methods

The convergence of Richardson's method is not guaranteed and if the method converges, convergence is often very slow.

We now introduce two methods that are guaranteed to converge for wide classes of matrices. The two methods take special linear combinations of the vectors r_k and Ar_k to construct a new iterate x_{k+1} that satisfies a local optimality property.

Steepest descent

Let A be symmetric positive definite. Define the function

$$f(x_k) = \|x_k - x\|_A^2 = (x_k - x)^T A(x_k - x)$$

Let $x_{k+1} = x_k + \alpha_k r_k$ Then the choice

$$\alpha_k = \frac{r_k^T r_k}{r_k^T A r_k}$$

minimizes $f(x_{k+1})$.

Minimal residual

Let A be general square. Define the function

$$g(x_k) = \|b - Ax_k\|_2^2 = r_k^T r_k$$

Let $x_{k+1} = x_k + \alpha_k r_k$ Then the choice

$$\alpha_k = \frac{r_k^T A r_k}{r_k^T A^T A r_k}$$

minimizes $g(x_{k+1})$.

Orthogonality properties

The optimality properties of the steepest descent method and the minimal residual method are equivalent with the following orthogonality properties:

For steepest descent

$$\alpha_k = \frac{r_k^T r_k}{r_k^T A r_k} \Rightarrow r_{k+1} \perp r_k$$

For the minimal residual method

$$\alpha_k = \frac{r_k^T A r_k}{r_k^T A^T A r_k} \Rightarrow r_{k+1} \perp A r_k \ .$$

Concluding remarks

During the next lessons the steepest decent method and the minimal residual method will be generalised.

This will ultimately give rise to a class of optimal methods.

Moreover, we will see that these methods are closely linked to eigenvalue method (as the simple iterative methods are to the Power method).