Generalized **M**inimal **Res**idual Method **GMRES**

Summary

1. Introduction to GMRES
2. Method Description
3. Convergence
4. Implementation and Results
5. Arnoldi for eigenvalue
6. Power method for eigenvalue
7. Implementation and Results

GMRES

The generalized minimal residual method (GMRES) is an iterative method for the numerical solution of an indefinite non-symmetric system of linear equations.

The method approximates the solution by the **vector** in a Krylov subspace with minimal residual.

The Arnoldi iteration is used to find this **vector**.

Krylov Subspace

The order-r Krylov subspace generated by an **n-by-n matrix** A and a vector b of dimension n is the linear subspace spanned by the images of b under the first r powers of A.

Starting from:

$$A^0 = I$$

that is:

$$\mathcal{K}_r(A, b) = \operatorname{span}\{b, Ab, A^2b, \ldots, A^{r-1}b\}.$$

Arnoldi Iteration

The Arnoldi iteration is an iterative method for eigenvalues approximation.

Arnoldi finds an approximation to the eigenvalues and eigenvectors of general matrices by constructing an orthonormal basis of the Krylov subspace, which makes it particularly useful when dealing with large sparse matrices.

Generalized minimal residual method

The GMRES method was developed by Yousef Saad and Martin H. Schultz in 1986.

It is a generalization and improvement of the MINRES method due to Paige and Saunders in 1975. The MINRES method requires that the matrix is symmetric, but has the advantage that it only requires handling of three vectors.

Method Description

Denote the Euclidean norm of any vector v by $|v|$. Denote the square system of linear equations to be solved by

$$Ax = b$$

The matrix A is assumed to be invertible of size *m-by-m*. Furthermore, it is assumed that ***b*** is normalized, i.e., that $|b| = 1$

Method Description

The *n-th* Krylov subspace for this problem is

$$K_n = K_n(A, r_0) = \text{span}\{r_0, Ar_0, A^2 r_0, \ldots, A^{n-1} r_0\}$$

where $r_0 = b - Ax_0$ is the initial error given an initial guess x_0. Clearly if $x_0 = 0$, $r_0 = b$.

Method Description

GMRES approximates the exact solution of Ax=b by the vector

$$x_n \in K_n$$

that minimizes the Euclidean norm of the residual

$$r_n = b - Ax_n$$

Method Description

The vectors

$$r_0, Ar_0, \ldots A^{n-1}r_0$$

might be close to linearly dependent, so instead of this basis, the Arnoldi iteration is used to find orthonormal vectors

$$q_1, q_2, \ldots, q_n$$

which form a basis for K_n .

Method Description

Therefore, the vector

$$x_n \in K_n$$

can be written as

$$x_n = x_0 + Q_n y_n$$

with $y_n \in \mathbb{R}^n$, where Q_n

is the m-by-n matrix formed by

$$q_1, \cdots, q_n$$

Method Description

The Arnoldi process also produces an (n+1)-by-n upper Hessenberg matrix $\tilde{H}_n$ with

$$AQ_n = Q_{n+1}\tilde{H}_n.$$

Method Description

Because columns of Q_n are orthonormal, we have

$$\|r_n\| = \|b - Ax_n\| = \|b - A(x_0 + Q_n y_n)\| = \|r_0 - AQ_n y_n\| = \|\beta q_1 - AQ_n y_n\|$$
$$= \|\beta q_1 - Q_{n+1}\tilde{H}_n y_n\| = \|Q_{n+1}(\beta e_1 - \tilde{H}_n y_n)\| = \|\beta e_1 - \tilde{H}_n y_n\|,$$

where

$$e_1 = (1, 0, 0, \ldots, 0)^T$$

is the first vector in the standard basis of $\mathbb{R}^{n+1}$, ...

Method Description

... and

$$\beta = \|r_0\|,$$

r_0 being the first trial vector (usually zero). Hence, x_n can be found by minimizing the Euclidean norm of the residual

$$r_n = \tilde{H}_n y_n - \beta e_1.$$

This is a linear least squares problem of size n.

Method Description

This yields the GMRES method. On the n-th iteration:

1. Calculate q_n with the Arnoldi Iteration;
2. find the y_n which minimizes $||r_n||$;
3. compute $x_n = x_0 + Q_n y_n$;
4. repeat if the residual is not yet small enough

At every iteration, a matrix-vector product $A * q_n$ must be computed. This costs about $2m^2$ floating-point operations for general dense matrices of size ***m***, but the cost can decrease to ***O(m)*** for sparse matrices. In addition to the **matrix-vector product**, ***O(nm)*** floating-point operations must be computed at the **n-th iteration**.

Eigenvalue

Eigenvalues are often introduced in the context of linear algebra or matrix theory.

In linear algebra, an eigenvector or characteristic vector of a linear transformation is a nonzero vector that changes by at most one scalar **(lambda)** factor when that linear transformation is applied.

Arnoldi with eigenvalues

As mentioned earlier GMRES is based on the Arnoldi iteration.

The idea of the Arnoldi iteration as an eigenvalue algorithm is to compute the eigenvalues in the Krylov subspace.

The eigenvalues of H (Hessenberg matrix) are called the Ritz eigenvalues.

It is often observed in practice **that some of the Ritz eigenvalues converge to eigenvalues of A**

Power iteration

The power iteration (also known as the power method) is an another eigenvalue algorithm.

The algorithm will produce a number lambda.

Which is the greatest (in absolute value) eigenvalue of A, and a nonzero vector v, which is a corresponding eigenvector of lambda

Method Description

The power iteration algorithm starts with a vector b0, which may be an approximation to the dominant eigenvector or a random vector.

The method is described by the recurrence relation:

$$b_{k+1} = \frac{Ab_k}{\| Ab_k \|}$$

Method Description

So, at every iteration:

- The vector bk is multiplied by the matrix A
- Next normalized

If we assume A has an eigenvalue that is strictly greater in magnitude than its other eigenvalues and the starting vector b0 has a nonzero component in the direction of an eigenvector associated with the dominant eigenvalue, then a subsequence **bk converges to an eigenvector associated with the dominant eigenvalue.**

Implementation and Results

The project is available at this **GitHub** repo:

https://github.com/CristianCosci/GMRES
https://github.com/ncvescera/GMRES
https://github.com/F-a-b-r-i-z-i-o/GMRES

In the **README** file:

- Other insights about GMRES
- Installation guide
- Code execution guide