Generalized Minimal Residual Method (GMRES)

History:

In 1986, GMRES was developed by Yousef Saad and Martin H. Schultz. It is a generalization and improvement of the MINRES method. Shockingly, for how early it was developed, it is a very powerful tool still used today. Over the last 38 years, there have been many refinements to the algorithm for different use cases. Still further developments are begin made.

Given a linear system $Ax = b$, where A is an invertible matrix, consider the sequence of vectors:

$$b, Ab, A^2b, \ldots, A^n b, \ldots$$

Among these vectors, $n+1$ vectors can be written as:

$$\alpha_0 b + \alpha_1 Ab + \alpha_2 A^2 b + \cdots + \alpha_n A^n b = 0$$

for some nonzero coefficients $\{\alpha_i\}$. Since $n+1$ n-dimensional vectors are linearly dependent, let k ($k \leq n$) be the smallest integer such that $\alpha_k \neq 0$.

The inverse of A acting on b can be written as:

$$A^{-1}b = -\frac{1}{\alpha_k}(\alpha_{k+1}b + \cdots + \alpha_n A^{n-k-1}b),$$

which is known as the **Weak-Cayley Hamilton Theorem**.

The inverse of A acting on b can be computed using only matrix-vector products. The vectors $b, Ab, A^2b, \ldots, A^n b$ form a subspace for the solution.

Krylov Subspace

For a matrix A and vector b, the r-th Krylov subspace is defined as:

$$K_r(A, b) := \text{span}\{b, Ab, \ldots, A^{r-1}b\}.$$

Arnoldi Process

The Arnoldi process is an algorithm, similar to the Gram-Schmidt algorithm, that constructs an orthonormal basis for the Krylov subspace $K_r(A, b) := \text{span}\{b, Ab, \ldots, A^{r-1}b\}$.

Algorithm:

- Choose a v_1 such that $\|v_1\| = 1$.
- For $j = 1, 2, \ldots$
  - $h_{i,j} = (Av_j)^T v_i, \quad i = 1, 2, \ldots, j$ (forming H_k)
  - $\hat{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{i,j} v_i$
  - $h_{j+1,j} = \|\hat{v}_{j+1}\|$
  - $v_{j+1} = \frac{\hat{v}_{j+1}}{h_{j+1,j}}$ (forming V_k)

This algorithm produces matrices V_k and H_k, where:

- V_k contains the orthonormal basis for the Krylov subspace.
- H_k is an upper Hessenberg matrix.

Solving $Ax = f$ Using GMRES

1. Choose an initial guess x_0 and compute the residual $r_0 = f - Ax_0$.
2. Set $v_1 = \frac{r_0}{\|r_0\|}$.
3. Apply the Arnoldi process to compute V_k and H_k.
4. Update the solution as:
$$x_k = x_0 + z_k, \quad z_k = V_k y_k,$$
where y_k minimizes:
$$\| \|r_0\| e_1 - H_k y \|,$$
with e_1 being the first column of the $(k+1) \times (k+1)$ identity matrix.

This is a simple version of GMRES. Many refined versions, such as GMRES(m), exist.

GMRES Further Developments

GMRES(m)

In GMRES(m), the algorithm restarts after every m iterations, preventing the memory and computational cost from growing indefinitely. This makes it more efficient for problems where m is chosen to balance accuracy and computational expense.

Preconditioned GMRES (PGMRES)

To improve convergence, preconditioners can be applied. These modify the system as $M^{-1}Ax = M^{-1}b$, where M is a preconditioner matrix chosen such that $M^{-1}A$ has better spectral properties, leading to faster convergence. Examples include ILU (Incomplete LU), Jacobi, and SSOR.

Flexible GMRES (FGMRES)

Flexible GMRES allows for changing preconditioners or using nonlinear preconditioning during iterations. This is particularly useful for complex systems where the preconditioning strategy evolves.

Generalized Block GMRES (BGMRES)

Block GMRES simultaneously solves systems with multiple right-hand sides $Ax = B$ by building Krylov subspaces for all right-hand vectors in parallel.

Recycling GMRES

Recycling GMRES methods reuse Krylov subspaces across multiple linear systems (e.g., when solving parameter-dependent systems or in time-stepping schemes). This reduces computational effort.

Complexity: The computational complexity is generally less than $O(n^2)$. Different variants offer trade-offs between computational cost, memory usage, and convergence rate.

Applications

GMRES is widely used in various fields, including:

- **Engineering and Computational Fluid Dynamics**
- **Financial Engineering and Risk Analysis**
- **Physics and Material Science**
- **Environmental Modeling**
- **Weather Prediction and Geophysical Exploration**
- **Machine Learning Optimization**

- **Biomedical Engineering**
- **Robotics and Control Systems**