Krylov Subspace Iteration Methods

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Set up

- The methods represent iterative techniques for solving large linear systems

$$Ax = b,$$

  where A is non-singular nxn-matrix, b is n-vector, n is large.
- They are based on projection processes onto Krylov subspaces.

Krylov Subspaces

- Krylov subspace generated by an *nxn*-matrix A, and an n-vector b is the subspace spanned by the vectors of the Krylov sequence:

$$K_m = span\{b, Ab, A^2b, ..., A^{m-1}b\}.$$

- The projection method seeks an approximate solution x_m from an affine subspace $x_0 + K_m$ by imposing condition $b - Ax_m \perp L_m$, L_m is another subspace of dimension m, x_0 is an initial guess to the solution. In the case of Krylov subspace methods $K_m = K_m(A, r_0)$, $r_0 = b - Ax_0$ is an n-vector

$$K_m = span\{r_0, Ar_0, A^2r_0, ..., A^{m-1}r_0\}.$$

- **Property 1.** K_m is the subspace of all vectors in R^n which can be written as

$$x = p(A)v,$$

where p is a polynomial of degree not exceeding $m-1$.

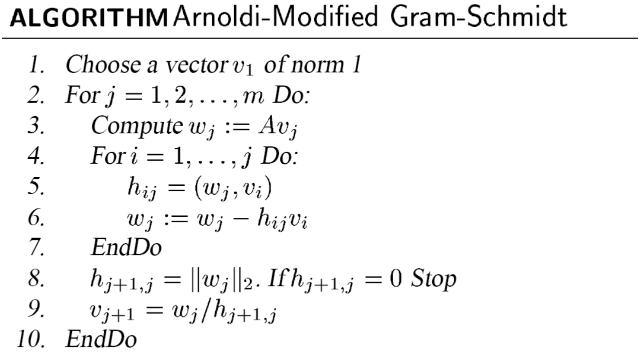
Krylov Subspaces

- The different versions of Krylov subspace methods arise from different choices of the subspace L_m and from the ways in which the system is preconditioned. Two broad choices for L_m give rise to the best-known techniques:

$$\begin{array}{ll} L_m = K_m & \text{FOM} \\ L_m = AK_m & \text{GMRES, MINRES.} \end{array}$$

Arnoldi Modified Gram-Schmidt Method

- This is an algorithm for building an orthogonal basis of the Krylov subspace K_m.



ALGORITHM Arnoldi-Modified Gram-Schmidt

```
Choose a vector $v_1$ of norm 1
For $j = 1, 2, \ldots, m$ Do:
    Compute $w_j := Av_j$
    For $i = 1, \ldots, j$ Do:
        $h_{ij} = (w_j, v_i)$
        $w_j := w_j - h_{ij} v_i$
    EndDo
    $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$ Stop
    $v_{j+1} = w_j / h_{j+1,j}$
EndDo
```

- At each step, the algorithm multiplies Arnoldi vector v_j by A and then orthonormalizes the resulting vector w_j against all previous v_j's by a standard Gram-Schmidt procedure.

Arnoldi's Method

- **Proposition 1.** Assume the Arnoldi Algorithm does not stop before the *m*-th step. Then the vectors $v_1, v_2, ..., v_m$ form an orthonormal basis of the Krylov subspace

$$K_m = span\{v_1, Av_1, ..., A^{m-1}v_1\}.$$

- **Proposition 2.** Projection method onto the subspace K_j will be exact when a breakdown occurs at step j.
- **Proposition 3.** Denote by V_m the nxm matrix with column vectors

  $v_1, ..., v_m$, by $\overline{H}_m$, the $(m+1)xm$ Hessenberg matrix whose nonzero entries h_{ij} are defined by Arnoldi Modified Gram-Schmidt Algorithm and by H_m the matrix obtained from $\overline{H}_m$ by deleting its last row. Then the following relations hold:

$$AV_m = V_m H_m + w_m e_m^T = V_{m+1}\overline{H}_m$$

$$V_m^T A V_m = H_m.$$

Full Orthogonalization Method (FOM)

- Given the initial guess x_0 to the original linear system $Ax = b$, consider the projection method described before, which takes $L_m = K_m(A, r_0)$, where $r_0 = b - Ax_0$. If $v_1 = \frac{r_0}{\|r_0\|_2}$ in Arnoldi's method and set $\beta = \|r_0\|_2$, then

$$\begin{aligned} V_m^T A V_m &= H_m \quad \text{from Proposition 3, and} \\ V_m^T r_0 &= V_m^T(\beta v_1) = \beta e_1. \end{aligned}$$

- As a result, the approximate solution using the above $m-$dimensional subspaces is given by

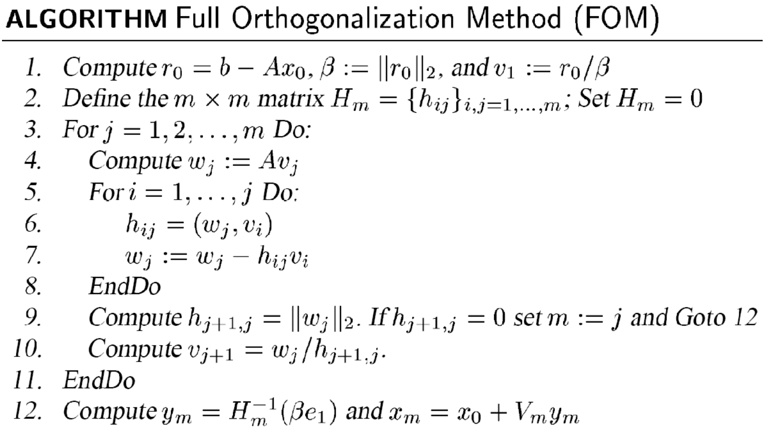
$$x_m = x_0 + V_m y_m, \;\; y_m = H_m^{-1}(\beta e_1)$$

Full Orthogonalization Method (FOM)

- The presented algorithm depends on a parameter m which is the dimension of the Krylov subspace. In practice it is desirable to select m in a dynamic fashion. This would be possible if the residual norm of x_m is available without compution x_m itself.
- **Proposition 4.** The residual vector of the approximate solution x_m computed by the FOM Algorithm is such that

$$\|b - Ax_m\|_2 = h_{m+1,m} \left| e_m^T y_m \right| .$$

Full Orthogonalization Method (FOM)



ALGORITHM Full Orthogonalization Method (FOM)

```
1.  Compute $r_0 = b - Ax_0$, $\beta := \|r_0\|_2$, and $v_1 := r_0/\beta$
2.  Define the $m \times m$ matrix $H_m = \{h_{ij}\}_{i,j=1,\ldots,m}$; Set $H_m = 0$
3.  For $j = 1, 2, \ldots, m$ Do:
4.      Compute $w_j := Av_j$
5.      For $i = 1, \ldots, j$ Do:
6.          $h_{ij} = (w_j, v_i)$
7.          $w_j := w_j - h_{ij}v_i$
8.      EndDo
9.      Compute $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$ set $m := j$ and Goto 12
10.     Compute $v_{j+1} = w_j/h_{j+1,j}$.
11. EndDo
12. Compute $y_m = H_m^{-1}(\beta e_1)$ and $x_m = x_0 + V_m y_m$
```

Generalized Minimum Residual Method (GMRES)

- The method is a projection method based on taking $L_m = AK_m$,in which K_m is the m-th Krylov subspace with $v_1 = r_0 / \left\| r_0 \right\|_{2.}$Such a technique minimizes the residual norm over all vectors in $x_0 + K_m$. The implementation of an algorithm based on this approach is similar to that of the FOM algorithm.
- Any vector x in $x_0 + K_m$ can be written as $x = x_0 + V_m y$, where y is an m-vector.
- Define
$$J(y) = \left\| b - Ax \right\|_2 = \left\| b - A(x_0 + V_m y) \right\|_2 ,$$
- Using relation from Proposition 3
$$\begin{aligned} b - Ax &= b - A(x_0 + V_m y) = r_o - AV_m y = \beta v_1 - V_{m+1} \overline{H}_m y \\ &= V_{m+1}(\beta e_1 - \overline{H}_m y). \end{aligned}$$
- Since the column-vectors of V_{m+1} are orthonormal, then
$$J(y) = \left\| b - A(x_0 + V_m y) \right\|_2 = \left\| \beta e_1 - \overline{H}_m y \right\|_2 .$$

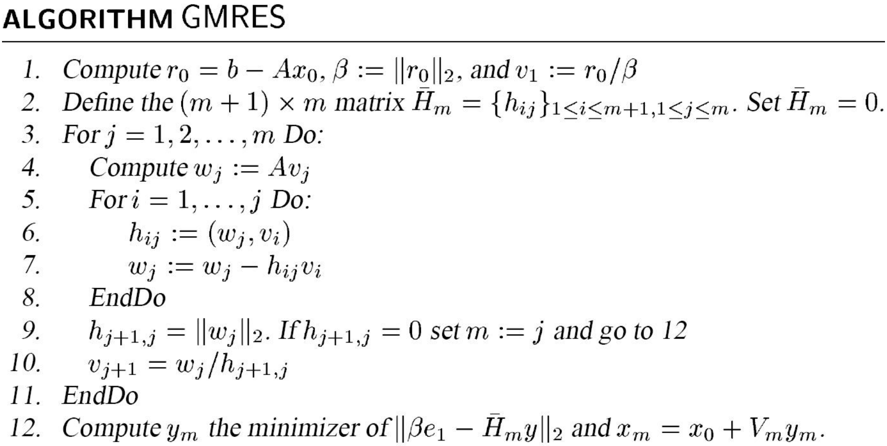
Generalized Minimum Residual Method (GMRES)

- The GMRES approximation is the unique vector of $x_0 + K_m$ which minimizes $J(y)$, i.e.

$$\begin{aligned} x_m &= x_0 + V_m y_m, \textit{where} \\ y_m &= \arg\min_y \left\| \beta e_1 - \overline{H}_m y \right\|_2 \end{aligned}$$

- The minimizer is inexpensive to compute since it requires the solution of an $(m+1)xm$ least-squares problem where m is typically small.

Generalized Minimum Residual Method (GMRES)



ALGORITHM GMRES

```
1.  Compute $r_0 = b - Ax_0$, $\beta := \|r_0\|_2$, and $v_1 := r_0/\beta$
2.  Define the $(m+1) \times m$ matrix $\bar{H}_m = \{h_{ij}\}_{1 \le i \le m+1, 1 \le j \le m}$. Set $\bar{H}_m = 0$.
3.  For $j = 1, 2, \ldots, m$ Do:
4.      Compute $w_j := Av_j$
5.      For $i = 1, \ldots, j$ Do:
6.          $h_{ij} := (w_j, v_i)$
7.          $w_j := w_j - h_{ij} v_i$
8.      EndDo
9.      $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$ set $m := j$ and go to 12
10.     $v_{j+1} = w_j / h_{j+1,j}$
11. EndDo
12. Compute $y_m$ the minimizer of $\|\beta e_1 - \bar{H}_m y\|_2$ and $x_m = x_0 + V_m y_m$.
```

Generalized Minimum Residual Method (GMRES). Practical Implementation issues

- A clear difficulty with GMRES algorithm is that it does not provide the approximate solution x_m explicitly at each step. As a result, it is not easy to determine when to stop. However, there is a solution related to the way in which the least-squares problem is solved.
- In order to solve the least-squares problem $\min \left\| \beta e_1 - \overline{H}_m y \right\|$, it is natural to transform the Hessenberg matrix into upper triangular form by using plane rotations.

Generalized Minimum Residual Method (GMRES). Practical Implementation issues

- **Proposition 5.** Define the rotation matrices to transform $\overline{H}_m$ into upper triangular form

$$\Omega_i = \begin{pmatrix} 1 & & & & & & & \\ & \dots & & & & & & \\ & & 1 & & & & & \\ & & & c_i & s_i & & & \\ & & & -s_i & c_i & & & \\ & & & & & 1 & & \\ & & & & & & \dots & \\ & & & & & & & 1 \end{pmatrix}$$

$$c_i^2 + s_i^2 = 1, \quad s_i = \frac{h_{i+1,i}}{\sqrt{(h_{ii}^{(i-1)})^2 + h_{i+1,i}^2}}, \; c_i = \frac{h_{ii}^{(i-1)}}{\sqrt{(h_{ii}^{(i-1)})^2 + h_{i+1,i}^2}}.$$

Generalized Minimum Residual Method (GMRES). Practical Implementation issues

- Define the product of matrices Ω_i

$$Q_m = \Omega_m \Omega_{m-1} \ldots \Omega_1,$$

- $\overline{R}_m, \overline{g}_m = (\gamma_1, ..., \gamma_{m+1})^T$ the resulting matrix and right-hand side

$$\begin{aligned}\overline{R}_m &= \overline{H}_m^{(m)} = Q_m \overline{H}_m, \\ \overline{g}_m &= Q_m(\beta e_1) = (\gamma_1, ..., \gamma_{m+1})^T.\end{aligned}$$

- Denote by R_m the mxm upper triangular matrix obtained from $\overline{R}_m$ by deleting its last row and by g_m the $m-$dimensional vector obtained from $\overline{g}_m$ by deleting its last component.

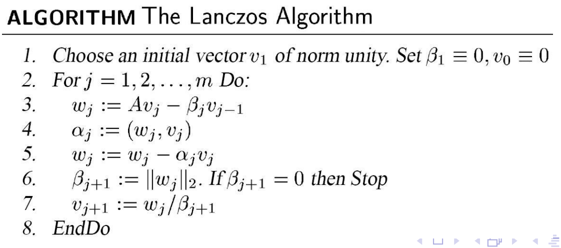
Generalized Minimum Residual Method (GMRES). Practical Implementation issues

- Then,
  1. Vector y_m which minimizes $\left\|\beta e_1 - \overline{H}_m y\right\|_2$ is given by
  $$y_m = R_m^{-1} g_m.$$
  2. The residual vector at step m satisfies
  $$b - Ax_m = V_{m+1}(\beta e_1 - \overline{H}_m y) = V_{m+1} Q_m^T(\gamma_{m+1} e_{m+1})$$ and, as a result,
  $$\left\|b - Ax_m\right\|_2 = \left|\gamma_{m+1}\right|.$$
- This was the process for computing the least-squares solution y_m. The process must be stopped if the residual norm $\left|\gamma_{m+1}\right|$ is small enough. The last rows of $\overline{R}_m$ and $\overline{g}_m$ are deleted and the resulting upper triangular system is solved to obtain y_m. Then the approximate solution $x_m = x_0 + V_m y_m$ is computed.

The Symmetric Lanczos Algorithm

- This algorithm can be viewed as a simplification of Arnoldi's method for the particular case when the matrix is symmetric. When A is symmetric, then the Hessenberg matrix H_m becomes symmetric tridiagonal.

$$\begin{pmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & & \cdots & & \\ & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ & & & \beta_m & \alpha_m \end{pmatrix}$$



ALGORITHM The Lanczos Algorithm

```
1. Choose an initial vector $v_1$ of norm unity. Set $\beta_1 \equiv 0, v_0 \equiv 0$
2. For $j = 1, 2, \ldots, m$ Do:
3.     $w_j := Av_j - \beta_j v_{j-1}$
4.     $\alpha_j := (w_j, v_j)$
5.     $w_j := w_j - \alpha_j v_j$
6.     $\beta_{j+1} := \|w_j\|_2$. If $\beta_{j+1} = 0$ then Stop
7.     $v_{j+1} := w_j / \beta_{j+1}$
8. EndDo
```

The Conjugate Gradient Algorithm

- This algorithm is one of the best known iterative techniques for solving sparse Symmetric Positive Definite linear systems.
- Assume we need to minimize the following function

$$f(x) = \frac{1}{2}x^T Ax - x^T b$$

where A is *nxn*-matrix positive definite and symmetric, b is *n*-vector.

- The minimum value of $f(x)$ is $-b^T A^{-1} b/2$, achieved by setting $x = A^{-1}b$. Therefore, minimizing $f(x)$ and solving $Ax = b$ are equivalent problems if A is symmetric positive definite.

The Conjugate Gradient Algorithm

- The vector x_{j+1} can be expressed as .

$$x_{j+1} = x_j + \alpha_j p_j.$$

- Therefore, the residual vectors must satisfy the recurrence

$$r_{j+1} = r_j - \alpha_j A p_j.$$

- To have r_j's orthogonal it is necessary that

$$(r_j - \alpha_j A p_j, r_j) = 0$$

and, as a result,

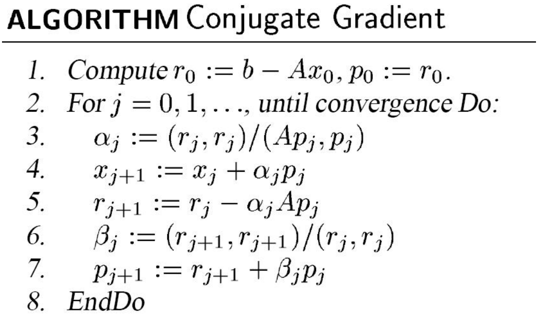
$$\alpha_j = \frac{(r_j, r_j)}{(A p_j, r_j)}.$$

The Conjugate Gradient Algorithm

- The first basis vector p_1 is the gradient of f at x_0, which equals to $Ax_0 - b$. The other vectors in the basis will be conjugate to the gradient . Each next p_{k+1} is defined to be in the direction closest to the gradient r_k under the conjugacy constraint. This direction is given by the projection of r_k onto the space orthogonal to p_k with respect to the inner product induced by A.

$$\begin{aligned}
p_{j+1} &= r_{j+1} + \beta_j p_j, \\
(Ap_j, r_j) &= (Ap_j, p_j - \beta_{j-1} p_{j-1}) = (Ap_j, p_j) \\
\alpha_j &= \frac{(r_j, r_j)}{(Ap_j, p_j)}, \ \beta_j = \frac{(r_{j+1,} Ap_j)}{(p_j, Ap_j)} \\
Ap_j &= -\frac{1}{\alpha_j}(r_{j+1} - r_j), \beta_j = \frac{1}{\alpha_j}\frac{(r_{j+1,}(r_{j+1} - r_j))}{(Ap_j, p_j)} = \frac{(r_{j+1}, r_{j+1})}{(r_j, r_j)}
\end{aligned}$$

The Conjugate Gradient Algorithm



ALGORITHM Conjugate Gradient

```
Compute $r_0 := b - Ax_0$, $p_0 := r_0$.
For $j = 0, 1, \ldots$, until convergence Do:
    $\alpha_j := (r_j, r_j)/(Ap_j, p_j)$
    $x_{j+1} := x_j + \alpha_j p_j$
    $r_{j+1} := r_j - \alpha_j Ap_j$
    $\beta_j := (r_{j+1}, r_{j+1})/(r_j, r_j)$
    $p_{j+1} := r_{j+1} + \beta_j p_j$
EndDo
```

- The process stops if r_{j+1} is "sufficiently small".

Convergence Analysis

- One of the main tool used in the analysis of convergence behavior is Chebyshev polynomials.
- **Lemma 1.** Let x_m be the approximate solution obtained from the $m-$th step of the CG algorithm, and let $d_m = x_* - x_m$, where x_* is the exact solution. Then x_m is of the form

  $$x_m = x_0 + q_m(A) r_0,$$

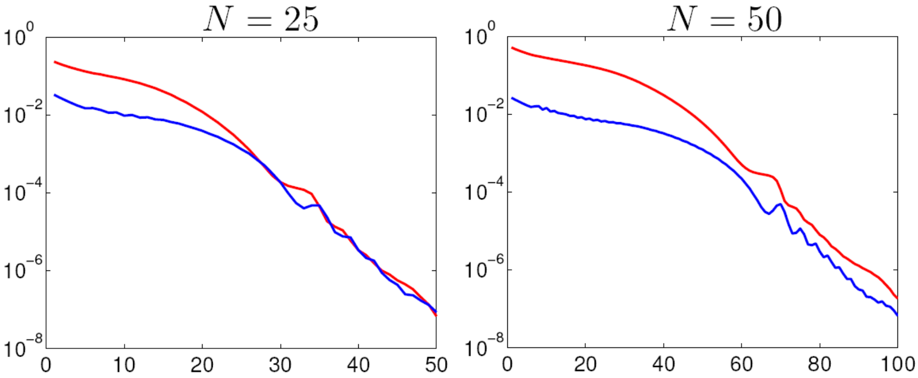
  where q_m is a polynomial of degree $m-1$ such that

  $$\left\| (I - A q_m(A)) d_0 \right\|_A = \min_{q \in P_{m-1}} \left\| (I - A q(A)) d_0 \right\|_A .$$

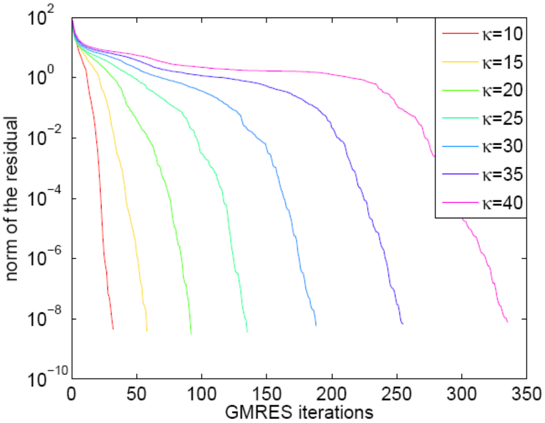
- **Theorem 2.** Let x_m be the approximate solution obtained from the $m-$th step of the CG algorithm, and x_* is the exact solution. Then

  $$\left\| x_* - x_m \right\|_A \leq 2 \left[\frac{\sqrt{k} - 1}{\sqrt{k} + 1} \right]^m \left\| x_* - x_0 \right\|_A .$$

Convergence Analysis



Convergence Analysis



GMRES residual norms show a period of stagnation followed by rapid convergence. The above plots are for $\kappa = 10, 15, \ldots, 40$.