Chapter 8

KRYLOV SUBSPACE METHODS

A more readable reference is the book by Lloyd N. Trefethen and David Bau.

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8.1 Krylov Subspaces

Saad, Sections 6.1, 6.2 omitting Proposition 6.3

In a Krylov subspace method

\[ x_i - x_0 \in K_i(A, r_0) = \text{span} \{r_0, Ar_0, \ldots, A^{i-1}r_0\}. \]

We call \( K_i(A, r_0) \) a Krylov subspace. Equivalently,

\[ x_i \in x_0 + \text{span} \{r_0, Ar_0, \ldots, A^{i-1}r_0\}, \]

which we call a linear manifold.

The exact solution \( A^{-1}b = x_0 + A^{-1}r_0 \). The minimal polynomial of \( A \) is the polynomial

\[ p(x) = x^m + c_{m-1}x^{m-1} + \cdots + c_1x + c_0 \]

of lowest degree \( m \) such that \( p(A) = 0 \). If \( A \) is diagonalizable, \( m \) is the number of distinct eigenvalues. To see this, let \( A \) have distinct eigenvalues \( \lambda_1, \lambda_2, \ldots, \lambda_m \), and define

\[ p(\lambda) = (\lambda - \lambda_1)(\lambda - \lambda_2) \cdots (\lambda - \lambda_m) = c_m \lambda^m + \cdots + c_1 \lambda + c_0. \]
Writing $A = X\Lambda X^{-1}$, we have

$$p(A) = X(\Lambda - \lambda_1 I)(\Lambda - \lambda_2 I) \cdots (\Lambda - \lambda_m I)X^{-1} = 0.$$ 

If $A$ has no eigenvalue equal to zero, $A^{-1}$ is a linear combination of $I, A, \ldots, A^{m-1}$,

\[e.g., \begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix}^{-1} = \frac{3}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} - \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}.\]

To see this, write

$$A^{m-1} + c_{m-1}A^{m-2} + \cdots + c_1 I + c_0 A^{-1} = 0.$$ 

Hence $A^{-1}r_0 \in \text{span} \{r_0, Ar_0, \ldots, A^{m-1}r_0\}$, $A^{-1}b \in x_0 + \text{span} \{r_0, Ar_0, \ldots, A^{m-1}r_0\}$, and $x_m = A^{-1}b$. This is the finite termination property. (In practice we do not go this far.)

**Review questions**

1. What is a Krylov subspace?
2. Is $x_0 + \text{span} \{r_0, Ar_0, \ldots, A^{i-1}r_0\}$ a Krylov subspace?
3. Which of the following methods choose their search directions from a Krylov subspace: cyclic coordinate descent? steepest descent? For each that does, what is its Krylov subspace?
4. What is the minimal polynomial of a square matrix $A$?
5. What is the finite termination property?

**Exercise**

1. Use the characteristic polynomial of a nonsingular square matrix $A$ to show that $A^{-1}$ can be expressed as a polynomial of degree at most $n - 1$ in $A$.

**8.2 Arnoldi Orthogonalization**

*Saad, Section 6.3*

For numerical stability we incrementally construct orthonormal bases $\{q_1, q_2, \ldots, q_k\}$ for the Krylov subspaces. However, rather than applying the Gram-Schmidt process to the sequence $r_0, Ar_0, \ldots, A^{k-1}r_0$, we use what is known as the Arnoldi process. It is based on the fact that each Krylov subspace can be obtained from the orthonormal basis of the Krylov subspace of one dimension less using the spanning set $q_1, q_2, \ldots, q_k, Aq_k$. In other words a new direction in the expanded Krylov subspace can be created by multiplying the
most recent basis vector $q_k$ by $A$ rather than by multiplying $A^{k-1}r_0$ by $A$. We remove from this new direction $Aq_k$ its orthogonal projection onto $q_1, q_2, \ldots, q_k$ obtaining the direction

$$v_{k+1} = Aq_k - q_1h_{1k} - q_2h_{2k} - \cdots - q_kh_{kk}$$

where the coefficients $h_{i,k}$ are determined by the orthogonality conditions. This computation should be performed using the modified Gram-Schmidt iteration:

$$t = Aq_k;$$

for $j = 1, 2, \ldots, k$ do {

$/* t = (I - q_jq_j^T)t */$

$h_{jk} = q_j^Tt;$

$t = t - q_jh_{jk};$

}

Normalization produces

$$q_{k+1} = v_{k+1}/h_{k+1,k}.$$ 

The coefficients $h_{ij}$ have been labeled so that we can write

$$AQ_k = Q_{k+1}\bar{H}_k$$

where $Q_k := [q_1, q_2, \ldots, q_k]$ and $\bar{H}_k$ is a $k + 1$ by $k$ upper Hessenberg matrix whose $(i,j)$th element for $j \geq i - 1$ is $h_{ij}$.

Given the basis $q_1, q_2, \ldots, q_k$, we can express any element of the $k$th dimensional Krylov subspace as $Q_ky$ for some $k$-vector $y$.

**Review questions**

1. In the Arnoldi process for orthogonalizing a Krylov subspace $K_i(A, r_0)$, how is each new basis vector $q_{k+1}$ produced?

2. The relationship among the first $k + 1$ vectors produced by the Arnoldi process for $K_i(A, r_0)$ can be summarized as

$$AQ_k = Q_{k+1}\bar{H}_k$$

where $Q_k$ is composed of the first $k$ vectors. What are dimensions of $\bar{H}_k$ and what other property does it have? What is $Q_k^TAQ_k$ in terms of $\bar{H}_k$?

3. Let $Q_k$ be composed of the first $k$ vectors of the Arnoldi process for $K_i(A, r_0)$. What is $r_0$ in terms of $Q_k$ and $\|r_0\|$?
8.3 Generalized Minimal Residual Method

Saad, Sections 6.5.1, 6.5.3–6.5.5.

GMRES, “generalized minimal residuals,” is a popular iterative method for nonsymmetric matrices $A$. It is based on the principle of minimizing the norm of the residual $\|b - Ax\|_2$, since the energy norm is available only for an s.p.d. matrix. It is, however, not a gradient method; rather it chooses for the correction $x_k - x_0$ that element of the Krylov subspace $\text{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}$ which minimizes the 2-norm of the residual.

For numerical stability we construct orthonormal bases $\{q_1, q_2, \ldots, q_k\}$ for the Krylov subspaces using the Arnoldi process. We can express any element of the $k$th dimensional Krylov subspace as $Q_k y$ for some $k$-vector $y$. Thus, the minimization problem becomes

$$\min_y \|b - A(x_0 + Q_k y)\|_2.$$ 

This is a linear least squares problem involving $k+1$ unknowns and $n$ equations. The number of equations can be reduced to $k+1$ by using eq. (8.1) to get

$$\|b - A(x_0 + Q_k y)\|_2 = \|r_0 - AQ_k y\|_2$$

$$= \|\rho q_1 - AQ_k y\|_2 \quad \text{where } \rho = \|r_0\|$$

$$= \|Q_{k+1}(\rho e_1 - H_k y)\|_2$$

$$= \|\rho e_1 - H_k y\|_2.$$ 

Review questions

1. For GMRES applied to $Ax = b$, where $A$ is $n$ by $n$, from what subset of $\mathbb{R}^n$ does one choose the approximation $x_k$ given an initial guess $x_0$?

2. How many matrix–vector multiplications are required for each iteration of GMRES?

3. What is the optimality property of GMRES?

4. For the GMRES solution from a $k$-dimensional subspace, one solves a least squares problem of reduced dimension. What are the dimensions of the coefficient matrix in this problem, and what is its special property?

8.4 Conjugate Gradient Method

Saad, Sections 6.7.1, 6.11.3.

Considered here is the case where $A$ is symmetric. Let $H_k$ be all but the last row of $\bar{H}_k$. Then $Q_k^T AQ_k = H_k$, which is square and upper Hessenberg. Since $A$ is symmetric, $H_k$ is tridiagonal, and we write

$$\bar{H}_k = \bar{T}_k, \quad H_k = T_k.$$
Clearly, it is unnecessary to compute elements of $T_k$ known to be zero, thus reducing the cost from $O(k^2)$ to $O(k)$.

Assuming $A$ is also positive definite, we choose $x_k$ to be that element of $x_0 + \mathcal{K}_k(A,r_0)$ which is closest to $A^{-1}b$ in energy norm. Hence, each iterate $x_k$ has the following optimality property:

$$|||x_k - A^{-1}b||| = \min\{|||x - A^{-1}b||| : x \in x_0 + \mathcal{K}_k(A,r_0)\}.$$ 

In Section 7.3 this is shown to be equivalent to making the residual $b - Ax_k$ orthogonal to $\mathcal{K}_k(A,r_0) = \mathcal{R}(Q_k)$. Writing $x_k = x_0 + Q_k y$, this becomes

$$0 = Q_k^T(b - Ax_k)$$
$$= Q_k^T(r_0 - AQ_k y)$$
$$= Q_k^T(\rho q_1 - AQ_k y)$$
$$= \rho e_1 - T_k y,$$

a tridiagonal system to solve for $y$.

Although the conjugate gradient method can be derived from the Lanczos orthogonalization described above, it is more usual to start from method of steepest descent. The conjugate gradient method constructs direction $p_i$ from the gradients $r_0, r_1, r_2, \ldots$. These directions are conjugate

$$p_i^T A p_j = 0 \text{ if } i \neq j,$$

or orthogonal in the energy inner product. We skip the details and simply state the result:

$$x_0 = \text{initial guess;}$$
$$r_0 = b - Ax_0;$$
$$p_0 = r_0;$$

for $i = 0, 1, 2, \ldots$ do 

$$\alpha_i = \frac{r_i^T r_i}{p_i^T A p_i};$$
$$x_{i+1} = x_i + \alpha_i p_i;$$
$$r_{i+1} = r_i - \alpha_i A p_i;$$
$$p_{i+1} = r_{i+1} + \frac{r_{i+1}^T r_{i+1}}{r_i^T r_i} p_i;$$

The cost per iteration is

1 matrix · vector $A p_i$
2 vector · vector $r_{i+1}^T r_{i+1}, p_i^T (A p_i)$
3 vector + scalar · vector
for a total cost of 1 matrix–vector product and $5n$ multiplications. For
\[
\begin{pmatrix}
-1 & -1 \\
4 & 1 \\
\end{pmatrix}
\]
the cost of matrix-vector is $2.5n$ “multiplications.”

We note that $r_i \in K_i(A, r_0)$ and $p_i \in K_i(A, r_0)$. Moreover, it can be shown that the
gradients \( \{r_0, r_1, \ldots, r_{i-1}\} \) constitute an orthogonal basis for the Krylov subspace.

**convergence rate**

\[
\|x_k - A^{-1}b\| \leq \left( \frac{\sqrt{\kappa_2(A)} - 1}{\sqrt{\kappa_2(A)} + 1} \right)^k \|x_0 - A^{-1}b\|
\]

To reduce **energy norm** of error by \( \varepsilon \) requires $\approx \frac{\sqrt{\kappa_2(A)}}{2} \log \frac{1}{\varepsilon}$ iterations, e.g., \( \frac{n^{1/2}}{\pi} \log \frac{1}{\varepsilon} \).

**Review questions**

1. What does it mean for the directions of the conjugate gradient method to be conjugate?
2. What is the optimality property of the conjugate gradient method?
3. How many matrix–vector multiplications are required for each iteration of CG?
4. On what property of the matrix does the rate of convergence of conjugate gradient depend?

**Exercises**

1. Given $x_i, r_i, p_i$, one conjugate gradient iteration is given by

\[
\alpha_i = r_i^T r_i / (p_i^T A p_i) \quad r_{i+1} = r_i - \alpha_i A p_i \\
x_{i+1} = x_i + \alpha_i p_i \quad p_{i+1} = r_{i+1} + \frac{r_{i+1}^T r_{i+1}}{r_i^T r_i} p_i
\]

where $A$ is assumed to be symmetric positive definite. Suppose you are given

```java
static void ax(float[] x, float[] y) {
    int n = x.length;
    // Given x this method returns y where
    // y[i] = a[i][0]*x[0] +...+ a[i][n-1]*x[n-1]
    ...
}
```

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You should complete the following method which performs one conjugate gradient iteration, overwriting the old values of $x_i, r_i, r_i^T r_i$, and $p_i$ with the new values. Your method must use no temporary arrays except for one float array of dimension $n$ and it must do a minimum amount of floating-point arithmetic.

\[
\text{static void cg(float[]} x, \text{ float[]} r, \text{ float } rTr, \text{ float[]} p)\\
\]

2. Solve the following system using the conjugate gradient method with $x_1 = 0$.

\[
\begin{bmatrix}
4 & -1 & 0 \\
-1 & 4 & -1 \\
0 & -1 & 4
\end{bmatrix} x = 
\begin{bmatrix}
2 \\
6 \\
2
\end{bmatrix}
\]

### 8.5 Biconjugate Gradient Method

*Saad, Section 7.3.1*

Recall that for a symmetric matrix $A$ one can find by means of a direct calculation an orthogonal similarity transformation such that $Q^T AQ = T$ is tridiagonal. And that for a general matrix one can get an upper Hessenberg matrix $Q^T AQ = H$. In fact, for a general matrix it is possible to find by means of a direct calculation a similarity transformation such that $V^{-1} AV = T$ is tridiagonal if one requires only that $V$ be nonsingular. Letting $W^T = V^{-1}$, we can write this as two conditions:

\[W^T AV = T, \quad W^T V = I.\]

The columns of $V = [v_1 v_2 \cdots v_n]$ and $W = [w_1 w_2 \cdots w_n]$ are said to form a biorthogonal system in that

\[v_i^T w_j = \delta_{ij}.\]

Lanczos orthogonalization incrementally builds up the relations $Q_k^T AQ_k = T_k$, which if carried to completion would yield $Q^T AQ = T$. Similarly, Lanczos biorthogonalization incrementally constructs $V_k, W_k, T_k$ such that

\[W_k^T AV_k = T_k, \quad W_k^T V_k = I.\]

These relations can be exploited to obtain an approximate solution:

\[\tilde{x} = x_0 + V_k y\]

such that

\[W_k^T (b - Ax) = 0,\]

which simplifies to the tridiagonal system

\[T_k y = W_k^T r_0.\]

The columns of $V_k$ are a basis for $\mathcal{K}_k(A, v_1)$, and the columns of $W_k$ are a basis for $\mathcal{K}_k(A^T, w_1)$.

The method just described can be shown to be equivalent to the *biconjugate gradient* method, which is given below, without a derivation:
\[ x_0 = \text{initial guess}; \]
\[ r_0 = b - Ax_0; \text{ choose } r_0' \text{ so that } r_0^Tr_0' \neq 0; \]
\[ p_0 = r_0; p_0' = r_0'; \]
\[ \text{for } i = 0, 1, 2, \ldots \text{ do } \{
\]
\[ \alpha_i = \frac{r_i^Tr_i'}{(Ap_i)^Tp_i'}; \]
\[ x_{i+1} = x_i + \alpha_ip_i; \]
\[ r_{i+1} = r_i - \alpha_iAp_i; \]
\[ r_{i+1}' = r_i' - \alpha_iA^Tp_i'; \]
\[ \beta_i = \frac{r_{i+1}^Tr_{i+1}'}{r_i^Tr_i'}; \]
\[ p_{i+1} = r_{i+1} + \beta_ip_i; \]
\[ p_{i+1}' = r_{i+1}' + \beta_ip_i'; \]
\[ \} \]

Convergence of BiCG is slower and more erratic than GMRES. Also there is the possibility of breakdown when a denominator becomes zero.

**Review questions**

1. How close can one come to diagonalizing a general matrix by a similarity transformation with a finite number of arithmetic operations?

2. What does it mean for the columns of \( V = [v_1 v_2 \cdots v_n] \) and \( W = [w_1 w_2 \cdots w_n] \) to form a biorthogonal system?

3. Lanczos biorthogonalization applied to an \( n \times n \) matrix \( A \) incrementally constructs matrices \( V_k, W_k \) of dimension \( n \) by \( k \) and \( T_k \) of dimension \( k \) by \( k \). What relations are satisfied by these matrices? and what is special about \( T_k \)?

4. How many matrix–vector multiplications are required for each iteration of BiCG applied to a general system \( Ax = b \)? and with which matrices?

5. How does the convergence of BiCG compare to that of GMRES?

### 8.6 Biconjugate Gradient Stabilized Method

*Saad, Section 7.4.2*

BiCGSTAB has significantly smoother convergence rate than BiCG.

**Review question**

1. How does BiCGSTAB compare to BiCG? Be precise.