Chapter 8

KRYLOV SUBSPACE METHODS

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

8.1 Krylov Subspaces

Saad, Sections 6.1, 6.2 omitting Proposition 6.3

In a Krylov subspace method

$$x_i - x_0 \;\in\; \mathcal{K}_i(A, r_0) = \text{ span } \{r_0, Ar_0, \ldots, A^{i-1}r_0\}.$$

We call $\mathcal{K}_i(A, r_0)$ 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 λ_1, λ_2, ..., λ_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 is no eigenvalue equal to zero, A^{-1} is a linear combination of $I, A, \ldots, A^{m-1}$,

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

To see this, write

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

Hence $A^{-1}r_0 \in$ span $\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$, $A^{-1}b \in x_0 +$ 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 $x_0 +$ 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, ..., $A^{k-1}r_0$, 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, ..., 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, ..., q_k obtaining the direction

$$v_{k+1} = Aq_k - q_1 h_{1k} - q_2 h_{2k} - \cdots - q_k h_{kk}$$

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** {
    $/* \ t = (I - q_j q_j^\mathsf{T})t \ */$
    $h_{jk} = q_j^\mathsf{T} t$;
    $t = t - q_j h_{jk}$;
}

Normalization produces

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

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

$$AQ_k = Q_{k+1}\bar{H}_k \tag{8.1}$$

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, ..., q_k, we can express any element of the kth dimensional Krylov subspace as $Q_k\, y$ for some k-vector y.

Review questions

1. In the Arnoldi process for orthogonalizing a Krylov subspace $\mathcal{K}_i(A, r_0)$, 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 $\mathcal{K}_i(A, r_0)$ 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 $Q_k^\mathsf{T} A Q_k$ in terms of $\bar{H}_k$?

3. Let Q_k be composed of the first k vectors of the Arnoldi process for $\mathcal{K}_i(A, r_0)$. 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 kth 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

$$\begin{aligned} \|b - A(x_0 + Q_k\, y)\|_2 &= \|r_0 - AQ_k\, y\|_2 \\ &= \|\rho q_1 - AQ_k\, y\|_2 \quad \text{where } \rho = \|r_0\| \\ &= \|Q_{k+1}(\rho e_1 - \bar{H}_k y)\|_2 \\ &= \|\rho e_1 - \bar{H}_k y\|_2. \end{aligned}$$

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 $Q_k^{\mathsf{T}} A Q_k = H_k$, 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 $\mathcal{O}(k^2)$ to $\mathcal{O}(k)$.

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

$$\begin{aligned} 0 &= Q_k^{\mathsf{T}}(b - Ax_k) \\ &= Q_k^{\mathsf{T}}(r_0 - AQ_k\, y) \\ &= Q_k^{\mathsf{T}}(\rho q_1 - AQ_k\, y) \\ &= \rho e_1 - T_k y, \end{aligned}$$

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

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

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

$x_0 =$ initial guess;
$r_0 = b - Ax_0$;
$p_0 = r_0$;
for $i = 0, 1, 2, \ldots$ **do** {

$$\alpha_i = \frac{r_i^{\mathsf{T}} r_i}{p_i^{\mathsf{T}} A p_i};$$

$$x_{i+1} = x_i + \alpha_i p_i;$$

$$r_{i+1} = r_i - \alpha_i A p_i;$$

$$p_{i+1} = r_{i+1} + \frac{r_{i+1}^{\mathsf{T}} r_{i+1}}{r_i^{\mathsf{T}} r_i} p_i;$$

}

The cost per iteration is

1	matrix · vector	Ap_i
2	vector · vector	$r_{i+1}^{\mathsf{T}} r_{i+1}$, $p_i^{\mathsf{T}}(Ap_i)$
3	vector + scalar · vector	

for a total cost of 1 matrix–vector product and $5n$ multiplications. For $\begin{bmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{bmatrix}$ the cost of matrix·vector is $2.5n$ "multiplications."

We note that $r_i \in \mathcal{K}_i(A, r_0)$ and $p_i \in \mathcal{K}_i(A, r_0)$. 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 *enery norm* of error by ε 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

$$\alpha_i = r_i^\mathsf{T} r_i / (p_i^\mathsf{T} A p_i) \qquad r_{i+1} = r_i - \alpha_i A p_i$$
$$x_{i+1} = x_i + \alpha_i p_i \qquad p_{i+1} = r_{i+1} + \frac{r_{i+1}^\mathsf{T} r_{i+1}}{r_i^\mathsf{T} r_i} p_i$$

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

```
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]
   ...
}
```

You should complete the following method which performs one conjugate gradient iteration, overwriting the old values of $x_i, r_i, r_i^\mathsf{T} r_i$, 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.

```
static void cg(float[] x, float[] r, float rTr, 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 $Q^\mathsf{T} AQ = T$ is tridiagonal. And that for a general matrix one can get an upper Hessenberg matrix $Q^\mathsf{T} AQ = H$. 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 $W^\mathsf{T} = V^{-1}$, we can write this as two conditions:

$$W^\mathsf{T} AV = T, \quad W^\mathsf{T} V = I.$$

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

$$v_i^\mathsf{T} w_j = \delta_{ij}.$$

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

$$W_k^\mathsf{T} AV_k = T_k, \quad W_k^\mathsf{T} V_k = I.$$

These relations can be exploited to obtain an approximate solution:

$$\tilde{x} = x_0 + V_k y \text{ such that } \quad W_k^\mathsf{T} (b - Ax) = 0,$$

which simplifies to the tridiagonal system

$$T_k y = W_k^\mathsf{T} r_0.$$

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 $\mathcal{K}_k(A^\mathsf{T}, w_1)$.

The method just described can be shown to be equivalent to the *biconjugate gradient* method, which is given below, without a derivation:

$x_0 =$ initial guess;
$r_0 = b - Ax_0$; choose r'_0 so that $r_0^\mathsf{T} r'_0 \neq 0$;
$p_0 = r_0$; $p'_0 = r'_0$;
for $i = 0, 1, 2, \ldots$ **do** {

$$\alpha_i = \frac{r_i^\mathsf{T} r'_i}{(Ap_i)^\mathsf{T} p'_i};$$
$$x_{i+1} = x_i + \alpha_i p_i;$$
$$r_{i+1} = r_i - \alpha_i A p_i;$$
$$r'_{i+1} = r'_i - \alpha_i A^\mathsf{T} p'_i;$$
$$\beta_i = \frac{r_{i+1}^\mathsf{T} r'_{i+1}}{r_i^\mathsf{T} r'_i};$$
$$p_{i+1} = r_{i+1} + \beta_i p_i;$$
$$p'_{i+1} = r'_{i+1} + \beta_i p'_i;$$

}

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 is 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 by 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.