Rome-Moscow school of Matrix Methods and Applied Linear Algebra 2014
A short introduction to Krylov subspaces for linear systems, matrix functions and inexact Newton methods. Plan and exercises.

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Contents

1 Lecture 1. Introduction to Krylov subspace iterative methods for solving linear systems

1.1 Plan of the lecture

1. Krylov subspace methods.
2. $AV_k = V_{k+1}\underline{H}_k$ and $W_k^T AV_k = D_k H_k$.
3. The desire for short-term recursions.
4. $W_k = V_k$, GMRES, FOM (exercise), Arnoldi process (exercise).
5. CG (exercise).
6. Bi-Lanczos process.
7. Ideas for BiCG, CGS and BiCGSTAB.

1.2 Exercises for Lecture 1

The end of each exercise is indicated with $\Diamond$.

Exercise 1.1 Check that the following relation discussed at the lecture indeed defines a basis for $\mathcal{K}(A, r_0)$.

$$h_{k+1,k}v_{k+1} = Av_k - (h_{1,k}v_1 + h_{2,k}v_2 + \cdots + h_{k,k}v_k). \tag{1.1}$$

$\Diamond$

Exercise 1.2 Prove the Arnoldi decomposition, i.e., show that

$$AV_k = V_{k+1}\underline{H}_k, \qquad \text{with} \qquad \mathbb{R}^{(k+1)\times k} \ni \underline{H}_k = \begin{bmatrix} h_{1,1} & h_{1,2} & \dots & h_{1,k} \\ h_{2,1} & h_{2,2} & & \vdots \\ 0 & h_{3,2} & \ddots & \\ \vdots & \ddots & \ddots & h_{k,k} \\ 0 & \dots & 0 & h_{k+1,k} \end{bmatrix}. \tag{1.2}$$

$\Diamond$

Exercise 1.3 Consider a Petrov–Galerkin projection method for which holds

$$W_k^T AV_k = D_k H_k, \qquad W_k^T r_k = 0. \tag{1.3}$$

Finish the derivation of the method for the case $W_k = V_k$, $V_k^T V_k = I$. This method is called FOM, Fully Orthogonal Method. $\Diamond$

Exercise 1.4 Check that the algorithm in Figure 1 (called Arnoldi process) generates V_k such that $V_k^T V_k = I$ and the Arnoldi decomposition (1.2) holds. $\Diamond$

	vector r is given	
1.	define zero matrix $\underline{H}_m \in \mathbb{R}^{(m+1)\times m}$	`H=zeros(m+1,m);`
	and zero matrix $V_{m+1} \in \mathbb{R}^{n\times(m+1)}$	`V=zeros(n,m+1);`
2.	$\beta := \|r\|_2$	`beta=norm(r);`
	$v_1 := r/\beta$	`V(:,1)=(1/beta)*r;`
3.	for $j = 1, 2, \dots, m$ do	`for j=1:m,`
	every loop cycle gives $v_{j+1} =$ `V(:,j+1)` and $(h_{1,j}, \dots, h_{j+1,j})^T =$ `H(1:j+1,j)`	
4.	$w_j := Av_j$	`wj=A*V(:,j);`
5.	for $i = 1, 2, \dots, j$ do	`for i=1:j,`
6.	$h_{ij} := (w_j, v_i)$	`H(i,j)=(V(:,i))'*wj;`
7.	$w_j := w_j - h_{ij}v_i$	`wj=wj-H(i,j)*V(:,i);`
8.	endfor	`end`
9.	$h_{j+1,j} := \|w_j\|_2$.	`H(j+1,j)=norm(wj);`
	If $h_{j+1,j} = 0$ stop.	`if(H(j+1,j)==0), break, end`
10.	$v_{j+1} := w_j/h_{j+1,j}$	`V(:,j+1)=(1/H(j+1,j))*wj;`
11.	endfor	`end`

Figure 1: Arnoldi process (left) and its Matlab implementation (right): modified Gram-Schmidt applied to Krylov subspace $\mathcal{K}_m(A, r)$.

Exercise 1.5 The Arnoldi process shown in Figure 1 is merely the modified Gram-Schmidt process applied to the Krylov subspace. Modify some lines of the algorithm in such a way that the classical Gram-Schmidt process is employed. $\diamondsuit$

Exercise 1.6 (CG method) Below we sketch[1] a derivation of the CG method. Carry out the derivation, filling in the missing parts and answering the questions asked.

We start with FOM (Exercise 1.3) applied to a system with a matrix $A = A^*$. Our aim is to rewrite FOM in an "efficient" form where the solution is obtained by a short-term recurrence. The matrix H_m is tridiagonal. Assume it has an LU factorization $H_m = L_m U_m$.

Explain why the matrix H_m is tridiagonal.

In FOM, the solution after m iterations can be written as

$$x_m = x_0 + z_m = x_0 + V_m y_{\mathsf{fom}} = x_0 + \underline{V_m U_m^{-1}}\ \underline{\underline{L_m^{-1}(\|r_0\|e_1)}} = x_0 + \underline{P_m}\ \underline{\underline{\boldsymbol{\alpha}_m}}, \tag{1.4}$$

where the introduced terms are underlined. What is the size of P_m?

Using your description of FOM obtained in Exercise 1.3, show that the first $m-1$ columns of the matrices P_{m-1} and P_m are, indeed, identical (otherwise we should change the notation, of course). Show that the first $m-1$ entries of the vectors $\boldsymbol{\alpha}_{m-1}$ and $\boldsymbol{\alpha}_m$ are also identical.

Denote columns of P_m by p_j and entries of $\boldsymbol{\alpha}_m$ by α_j, $j = 0, \dots, m-1$:

$$P_m = \begin{bmatrix} p_0\, p_1 \dots p_{m-1} \end{bmatrix}, \qquad \boldsymbol{\alpha}_m = \begin{bmatrix} \alpha_0\, \alpha_1 \dots \alpha_{m-1} \end{bmatrix}^T.$$

Since, as we see from (1.4), the correction vector z_m is a linear combination of vectors p_j, $j = 0, \dots, m-1$, we will call vectors p_j search directions. It follows from relation (1.4) that

$$x_m = x_{m-1} + \alpha_{m-1} p_{m-1} \tag{1.5}$$

[1] The sketch follows the book [3] and Lecture Notes [2].

and, hence,

$$r_m = r_{m-1} - \alpha_{m-1} A p_{m-1}. \tag{1.6}$$

Since $r_m \perp \mathcal{K}_m(A, r_0)$ and $r_m \in \mathcal{K}_{m+1}(A, r_0)$ for $m \geqslant 0$, it follows that r_m is parallel to v_{m+1}. Hence,

$$\begin{aligned}
r_1 \perp \mathcal{K}_1(A, r_0) &= \mathsf{span}\{r_0\} : & & r_1 \perp r_0, \\
r_2 \perp \mathcal{K}_2(A, r_0) &= \mathsf{span}\{r_0, v_2\} = \mathsf{span}\{r_0, r_1\} : & & r_2 \perp r_0, \quad r_2 \perp r_1, \\
& & & \vdots \\
r_m \perp \mathcal{K}_m(A, r_0) &= \mathsf{span}\{r_0, r_1, \ldots, r_{m-2}, v_m\} \\
&= \mathsf{span}\{r_0, r_1, \ldots, r_{m-2}, r_{m-1}\} : & & r_m \perp r_0, \quad r_m \perp r_1, \; \ldots, \; r_m \perp r_{m-1},
\end{aligned}$$

or, simply,

$$r_i \perp r_j, \quad i \neq j. \tag{1.7}$$

Next, we obtain a recurrence for the search directions p_m:

$$P_m = V_m U_m^{-1} \quad \Rightarrow \quad P_m U_m = V_m.$$

The last column in this matrix equality reads:

$$u_{m-1,m} p_{m-2} + u_{m,m} p_{m-1} = v_m,$$

and, since $v_m || r_{m-1}$,

$$u_{m-1,m} p_{m-2} + u_{m,m} p_{m-1} = \xi_m r_{m-1}$$

for some nonzero constant ξ_m. Choosing $u_{m,m} = \xi_m$ (see Exercise 1.6) results in

$$p_{m-1} = r_{m-1} \underline{- \frac{u_{m-1,m}}{u_{m,m}}} p_{m-2} = r_{m-1} + \underline{\beta_{m-2}} p_{m-2},$$

where the scalar parameter β_{m-2} is introduced. The last relation reads:

$$p_m = r_m + \beta_{m-1} p_{m-1}. \tag{1.8}$$

Why can we freely choose the values of $u_{m,m}$? (Hint: these values are diagonal entries of the matrix factor U_m in the LU factorization of H_m.)

Show that

$$(A p_i, p_j) = 0, \quad i \neq j. \tag{1.9}$$

This reveals *conjugacy of the search directions* p_i. (Hint: consider the matrix $P_m^* A P_m$.)

The recurrences (1.5), (1.6), (1.8) obtained respectively for x_m, r_m and p_m contain two scalar parameters α_{m-1} and β_{m-1}. They can be defined from the requirements of orthogonality (1.7) and conjugacy (1.9), respectively. We first determine α_{m-1}:

$$0 = (r_m, r_{m-1}) = (r_{m-1}, r_{m-1}) - \alpha_{m-1}(A p_{m-1}, r_{m-1}),$$

so that

$$\alpha_{m-1} = \frac{(r_{m-1}, r_{m-1})}{(A p_{m-1}, r_{m-1})}. \tag{1.10}$$

Using recurrence (1.8), show that (1.10) can be rewritten as

$$\alpha_{m-1} = \frac{(r_{m-1}, r_{m-1})}{(Ap_{m-1}, p_{m-1})}.$$

To determine β_{m-1} we use the conjugacy relation (1.9):

$$0 = (p_m, Ap_{m-1}) = (r_m, Ap_{m-1}) + \beta_{m-1}(p_{m-1}, Ap_{m-1}),$$

$$\text{hence} \quad \beta_{m-1} = -\frac{(r_m, Ap_{m-1})}{(p_{m-1}, Ap_{m-1})} \tag{1.11}$$

Show that (1.11) can be rewritten as

$$\beta_{m-1} = \frac{(r_m, r_m)}{(r_{m-1}, r_{m-1})}$$

(Hint: find Ap_{m-1} from (1.6), use the expression obtained for α_{m-1}.)
Answer the following two questions:

(1) α_{m-1} is chosen such that $(r_m, r_{m-1}) = 0$. Do we still have that $(r_i, r_j) = 0$, $i \neq j$?

(2) β_{m-1} is chosen such that $(p_m, Ap_{m-1}) = 0$. Do we still have that $(Ap_i, p_j) = 0$, $i \neq j$?

We have just derived the conjugate gradient (CG) method:

for $m = 1, 2, \ldots,$

$$\alpha_{m-1} = \frac{(r_{m-1}, r_{m-1})}{(Ap_{m-1}, p_{m-1})}$$
$$x_m = x_{m-1} + \alpha_{m-1} p_{m-1}$$
$$r_m = r_{m-1} - \alpha_{m-1} A p_{m-1}$$
$$\beta_{m-1} = \frac{(r_m, r_m)}{(r_{m-1}, r_{m-1})}$$
$$p_m = r_m + \beta_{m-1} p_{m-1}$$

endfor

How much storage (number of vectors) do we need for CG? How much is computational work (number of flops) per iteration?

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2 Lecture 2. Basic preconditioners for Krylov subspace iterative methods

2.1 Plan of the lecture

1. An example "Preconditioning is needed".
2. A classification table of the Krylov subspace methods from Lecture 1.
3. Residual polynomials, basic convergence estimates for $A = A^T$, Chebyshev polynomials.
4. Elman's convergence estimate. Other estimates.
5. Preconditioning. General idea.
6. Preconditioning. Example 1: saddle-point problem with a positive real $(1, 1)$ block.
7. Preconditioning. Example 2: M-matrices, regular splitting.
8. Preconditioning. Example 3: geometric multigrid.

2.2 Exercises for Lecture 2

Exercise 2.1 Consider the example "Preconditioning is needed". Convince yourself that, indeed, at least n steps are needed to converge (with n being the size of A). ♢

Exercise 2.2 Let X and Y be the matrices in the iteration matrix $\mathcal{G}$ of the preconditioned saddle point system. Derive expressions for X and Y in terms of the matrices P, B, C. ♢

Exercise 2.3 Check that the matrix $P - A$, as appeared in the preconditioned saddle point system, is symmetric. ♢

Exercise 2.4 (a) Let $M \in \mathbb{R}^{n \times n}$ be a nonnegative real matrix, i.e., $\forall\, x \in \mathbb{R}^n$ $(Mx, x) \geqslant 0$. Show that $\|(I + M)^{-1}\|_2 \leqslant 1$.

(b) Let M be the matrix appeared in the preconditioned saddle point system. Derive an expression for M in terms of B, C, $P_H \equiv \frac{1}{2}(P + P^T)$ and $P_S \equiv \frac{1}{2}(P - P^T)$.

(c) Does $\|(I + M)^{-1}\|_2 \leqslant 1$ hold if C is *nonnegative* definite?

♢

Exercise 2.5 Let A be an M-matrix. Prove that $A^{-1} \geqslant 0$. Hint: use the von Neumann matrix series: $\sum_{k=0}^{N} C^k$ converges, as $N \to \infty$, to the inverse of $I - C$ if and only if $\rho(C) < 1$. ♢

Exercise 2.6 Let G be the iteration matrix of the preconditioned linear system with an M-matrix. Show that $\rho(G) < 1$ provided that $\alpha \leqslant (\max_i n_{ii})^{-1}$. ♢

Exercise 2.7 Consider the fixed point iteration for the Laplacian. As we discussed in the lecture, the components of the residual corresponding to the high frequency components will converge relatively well. With approximately which factor? More precisely, let $\tilde{r}_k$ be the residual at iteration k and $\tilde{\cdot}$ indicates that it is the residual in the eigenvector basis (in this basis the system matrix is diagonal and contains the eigenvalues). Assume the iteration parameter α is chosen optimally for the high frequency components. Then for the component i of the residual holds $(\tilde{r}_{k+1})_i \leqslant q(\tilde{r}_k)_i$. Estimate the value of q. ♢

3 Lecture 3. Inexact Newton-Krylov methods for solving large nonlinear systems

3.1 Plan of the lecture

1. Newton method. Smoothness assumptions.
2. Newton and preconditioned fixed-point iterations.
3. Convergence, important Lemma.
4. The important lemma, residual, error. A stopping criterion.
5. Saving work in the Newton method. Inexact Newton methods.
6. Convergence of inexact Newton methods.
7. Jacobian evaluations. Matrix-free methods.
8. Choice of the linear solver. CGS.

3.2 Exercises for Lecture 3

Exercise 3.1 Prove the important Lemma using the Banach lemma and the following result (see, e.g. [1]).

If A is nonsingular and $r \equiv \|A^{-1}E\|_p < 1$, then $A + E$ is nonsingular and

$$\|(A+E)^{-1} - A^{-1}\| \leqslant \frac{\|E\|_p \, \|A^{-1}\|_p}{1-r}.$$

$\diamondsuit$

Exercise 3.2 We solve linear system $Ax = b$ and write it as $F(x) = 0$, where $F(x) = b - Ax$. Consider the fixed-point iteration for $K(x) = F(x) + x$ and write it down in terms of A, x, and b. Does this method look familiar to you? $\diamondsuit$

Exercise 3.3 Write down the fixed-point iteration for $K(x) = x - F(x)$ and compare it with the Newton method. What if $F'(x_c) = I$? $\diamondsuit$

Exercise 3.4 Let r_m be the residual of the Jacobian linear system in the inexact Newton method, with m being the linear iteration number. Assume that the inner iterative linear solver has zero initial guess $s_0 = 0$. What does the stopping criterion of the linear solver discussed at the lecture mean $\|r_m\|$ and $\|r_0\|$? $\diamondsuit$

Exercise 3.5 Write down the first two terms of the Taylor expansion of $F(x_c + \delta w)$ around the point x_c. Do you see a connection to the directional difference evaluations of the Jacobian action? Can you propose a more accurate directional difference approximation? $\diamondsuit$

4 Lecture 4. Computing actions of the matrix exponential and other matrix functions for large matrices

4.1 Plan of the lecture

1. Matrix functions, definitions.
2. Krylov subspace for computing actions of matrix functions. The case $f(x) = 1/x$.
3. A need for a residual concept. Matrix exponential residual. Galerkin projection.
4. Shift-and-invert acceleration. Inner-outer iterations.
5. Chebyshev polynomials.
6. ODE systems $y' = -Ay$ and $y' = -Ay + g(t)$. Exponential block Krylov subspace method.

5 References

[1] G. H. Golub and C. F. Van Loan. *Matrix Computations.* The Johns Hopkins University Press, Baltimore and London, third edition, 1996.

[2] H. A. van der Vorst. Iterative methods for large linear systems. Lecture Notes, June 2002. http://www.staff.science.uu.nl/~vorst102/lecture.html.

[3] H. A. van der Vorst. *Iterative Krylov methods for large linear systems.* Cambridge University Press, 2003.