

Some code exercises in Fortran 90

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Interview for the Position:

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Conjugate Gradient for $Ax = b$ (SPD matrix)

Algorithm (Mathematical Form) - **Input:** Initial guess x_0 (approximate or 0).

```
1:  $r_0 := b - Ax_0$ 
2: if  $\|r_0\|$  small then return  $x_0$ 
3: end if
4:  $p_0 := r_0$ 
5:  $k := 0$ 
6: repeat
7:    $\alpha_k := \frac{r_k^\top r_k}{p_k^\top A p_k}$ 
8:    $x_{k+1} := x_k + \alpha_k p_k$ 
9:    $r_{k+1} := r_k - \alpha_k A p_k$ 
10:  if  $\|r_{k+1}\|$  small then break
11:  end if
12:   $\beta_k := \frac{r_{k+1}^\top r_{k+1}}{r_k^\top r_k}$ 
13:   $p_{k+1} := r_{k+1} + \beta_k p_k$ 
14:   $k := k + 1$ 
15: until convergence
16: return  $x_{k+1}$ 
```

Initialization of Conjugate Gradient

Initialization - **Input:** Initial guess x_0 (approximate or 0).

- 1: $r_0 := b - Ax_0$
 - 2: **if** $\|r_0\|$ small **then return** x_0
 - 3: **end if**
 - 4: $p_0 := r_0$
 - 5: $k := 0$
-

```
1 r = b - MATMUL(A, x) ! Initial residual
2 r_norm = SQRT(SUM(r**2))
3 PRINT *, "initial residual norm = ", r_norm
4 p = r
5 k = 0
6 max_iter = 1000
```

Main Loop of Conjugate Gradient

Main loop.

1: repeat

$$2: \quad \alpha_k := \frac{\mathbf{r}_k^T \mathbf{r}_k}{\mathbf{p}_k^T A \mathbf{p}_k}$$

$$3: \quad \mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{p}_k$$

$$4: \quad \mathbf{r}_{k+1} := \mathbf{r}_k - \alpha_k A \mathbf{p}_k$$

5: if $\|\mathbf{r}_{k+1}\|$ small then break

6: end if

$$7: \quad \beta_k := \frac{\mathbf{r}_{k+1}^T \mathbf{r}_{k+1}}{\mathbf{r}_k^T \mathbf{r}_k}$$

$$8: \quad \mathbf{p}_{k+1} := \mathbf{r}_{k+1} + \beta_k \mathbf{p}_k$$

$$9: \quad k := k + 1$$

10: until convergence

11: return \mathbf{x}_{k+1}

```

1 DO k = 1, max_iter ! Main loop
2   alpha = DOT_PRODUCT(r, r) / DOT_PRODUCT(p, MATMUL(A, p))
3   x = x + alpha * p ! Update solution
4   r_new = r - alpha * MATMUL(A, p) ! Update residual
5   r_norm_new = SQRT(SUM(r_new**2)) ! Update residual
6   IF (r_norm_new < 1.0e-6) EXIT ! Go out of the loop
7   beta = DOT_PRODUCT(r_new, r_new) / DOT_PRODUCT(r, r) ! Beta
8   p = r_new + beta * p ! Update search direction
9   r = r_new ! Update residual for next iteration
10  r_norm = r_norm_new ! Update residual for next iteration
11 ENDDO
12 PRINT *, MATMUL(A, x) - b

```

Sparse with COO Matrix, Can also be parallelized using OPENMP

```

1  ! Definition of the hollow matrix (COO)
2  ! 3x3 tridiagonal matrix:
3  ! 4 -1 0
4  ! -1 4 -1
5  ! 0 -1 4
6  VAL = (/ 4.0, -1.0, -1.0, 4.0, -1.0, -1.0, 4.0 /)
7  ROW = (/ 1, 1, 2, 2, 2, 3, 3 /)
8  COL = (/ 1, 2, 1, 2, 3, 2, 3 /)
9  B = (/ 1.0, 2.0, 3.0 /)
10 X = (/ 1.0, 1.0, 1.0 /)

```

```

1  CALL SPMV(N, NNZ, VAL, ROW, COL, P, AP)
2  R = B - AP ! Initialization
3  ALPHA = DOT_PRODUCT(R, R) / DOT_PRODUCT(P, AP) ! Loop

```

```

1  SUBROUTINE SPMV(N, NNZ, VAL, ROW, COL, V, RES)
2    INTEGER, INTENT(IN) :: N, NNZ
3    REAL(KIND=KIND(0.D0)), INTENT(IN) :: VAL(NNZ), V(N)
4    INTEGER, INTENT(IN) :: ROW(NNZ), COL(NNZ)
5    REAL(KIND=KIND(0.D0)), INTENT(OUT) :: RES(N)
6    INTEGER :: I
7
8    RES = 0.0
9    DO I = 1, NNZ
10     RES(ROW(I)) = RES(ROW(I)) + VAL(I) * V(COL(I))
11   END DO
12 END SUBROUTINE SPMV

```

Lanczos Algorithm for Hermitian A

Input: Hermitian $A \in \mathbb{C}^{n \times n}$, v_1 unit norm, max steps m (default: $m = n$).

```
1:  $v_1 \in \mathbb{C}^n$  such that  $\|v_1\| = 1$ 
2:  $w'_1 := Av_1$ 
3:  $\alpha_1 := v_1^* w'_1$ 
4:  $w_1 := w'_1 - \alpha_1 v_1$ 
5: for  $j = 2$  to  $m$  do
6:    $\beta_j := \|w_{j-1}\|$ 
7:   if  $\beta_j = 0$  then
8:     choose  $v_j$  orthogonal to  $v_1, \dots, v_{j-1}$  with  $\|v_j\| = 1$ 
9:   else
10:     $v_j := w_{j-1} / \beta_j$ 
11:  end if
12:   $w'_j := Av_j - \beta_j v_{j-1}$ 
13:   $\alpha_j := v_j^* w'_j$ 
14:   $w_j := w'_j - \alpha_j v_j$ 
15: end for
16: return  $V = [v_1, \dots, v_m]$ ,  $T = V^* AV$  (real symmetric tridiagonal)
```

Initialization of the Lanczos Algorithm

Initialization.

- 1: $v_1 \in \mathbb{C}^n$ such that $\|v_1\| = 1$
 - 2: $w'_1 := Av_1$
 - 3: $\alpha_1 := v_1^* w'_1$
 - 4: $w_1 := w'_1 - \alpha_1 v_1$
-

```
1 ! Initial vector (random, then normalized)
2 CALL RANDOM_NUMBER(V(:,1))
3 norm = SQRT(SUM(V(:,1)**2))
4 V(:,1) = V(:,1) / norm
5
6 ! Initial step
7 w_prime = MATMUL(A, V(:,1))
8 alpha(1) = DOT_PRODUCT(w_prime, V(:,1))
9 w = w_prime - alpha(1) * V(:,1)
```


Main Loop of the Lanczos Algorithm

Main loop.

```

1: for  $j = 2$  to  $m$  do
2:    $\beta_j := \|w_{j-1}\|$ 
3:   if  $\beta_j = 0$  then
4:     choose  $v_j$  orthogonal to  $v_1, \dots, v_{j-1}$  with  $\|v_j\| = 1$ 
5:   else
6:      $v_j := w_{j-1} / \beta_j$ 
7:   end if
8:    $w'_j := Av_j - \beta_j v_{j-1}$ 
9:    $\alpha_j := v_j^* w'_j$ 
10:   $w_j := w'_j - \alpha_j v_j$ 
11: end for
12: return  $V = [v_1, \dots, v_m]$ ,  $T = V^*AV$  (real symmetric tridiagonal)

```

```

1 DO j = 2, m
2   beta(j) = SQRT(SUM(w**2))
3   IF (beta(j) /= 0.0D0) THEN
4     V(:,j) = w / beta(j)
5   ELSE
6     PRINT *, 'beta(', j, ') = 0. Lanczos stops. Because Gram-
7       Schmidt requires too much computation.'
8     EXIT
9   END IF
10  w_prime = MATMUL(A, V(:,j)) - beta(j) * V(:,j-1)
11  alpha(j) = DOT_PRODUCT(w_prime, V(:,j))
12  w = w_prime - alpha(j) * V(:,j)
13 END DO

```

Construction of the Tridiagonal Matrix

Construction of the Tridiagonal Matrix.

1: **return** $V = [v_1, \dots, v_m]$, $T = V^*AV$ (real symmetric tridiagonal)

```
1 ! BUILD TRIDIAGONAL MATRIX T
2 T = 0.0D0
3 DO i = 1, m
4     T(i,i) = alpha(i)
5     IF (i < m) THEN
6         T(i,i+1) = beta(i+1)
7         T(i+1,i) = beta(i+1)
8     END IF
9 END DO
```

Givens QR Factorization without Explicit Q

Input: $A \in \mathbb{R}^{m \times n}$

```
1: Initialize:  $indexI = 0$ ,  $indexJ = 0$ ,  $C = 0$ ,  $S = 0$ 
2: for  $i = 1$  to  $n$  do
3:   for  $j = i + 1$  to  $m$  do
4:      $c := \frac{A(i,i)}{\sqrt{A(i,i)^2 + A(j,i)^2}}$ 
5:      $s := \frac{A(j,i)}{\sqrt{A(i,i)^2 + A(j,i)^2}}$ 
6:      $A(i,:) := cA(i,:) + sA(j,:)$ 
7:      $A(j,:) := -sA(i,:) + cA(j,:)$ 
8:      $indexI(j, i) := i$ ,  $indexJ(j, i) := j$ 
9:      $C(j, i) := c$ ,  $S(j, i) := s$ 
10:   end for
11: end for
12: return  $R = A$ ,  $indexI$ ,  $indexJ$ ,  $C$ ,  $S$ 
```

Explicit Construction of Q

Input: $indexI$, $indexJ$, C , S

```
1: Initialize  $Q = I$ 
2: for  $i = 1$  to  $n$  do
3:   for  $j = i + 1$  to  $m$  do
4:     if  $indexI(j, i) > 0$  then
5:        $c := C(j, i)$ ,  $s := S(j, i)$ 
6:        $Q(:, i) := cQ(:, i) + sQ(:, j)$ 
7:        $Q(:, j) := -sQ(:, i) + cQ(:, j)$ 
8:     end if
9:   end for
10: end for
11: return  $Q$ 
```

Iterative QR with Givens Rotations

Iterative QR algorithm with convergence check.

```
1: Initialize:  $A$ ,  $tol$ ,  $max\_iter$ ,  $Q = I$ 
2: for  $iter = 1$  to  $max\_iter$  do
3:   Compute Givens QR:  $A = R$ , store  $indexI$ ,  $indexJ$ ,  $C$ ,  $S$ 
4:   Construct  $Q$  using stored rotations
5:    $A := RQ$ 
6:   Compute  $\|A - \text{diag}(A)\|_F^2$ 
7:   if off-diagonal norm  $< tol$  then
8:     return approximate eigenvalues  $A(i, i)$ 
9:   end if
10: end for
```

Iterative QR with Givens Rotations

```

1 DO iter = 1, max_iter
2   R = A
3   Q = 0.0D0
4   Q(i,i) = 1.0D0
5   DO i = 1, n ! QR by Givens
6     DO j = i+1, n
7       denom = SQRT(R(i,i)**2 + R(j,i)**2)
8       cc = R(i,i)/denom
9       ss = R(j,i)/denom
10      tmp_row = cc*R(i,:) + ss*R(j,:)
11      R(j,:) = -ss*R(i,:) + cc*R(j,:)
12      R(i,:) = tmp_row
13      ! Store rotation
14      indexI(j,i)=i; indexJ(j,i)=j
15      C(j,i)=cc; S(j,i)=ss
16    END DO
17  END DO
18  DO i = 1, n ! Apply rotations to Q
19    DO j = i+1, n
20      IF (indexI(j,i) > 0) THEN
21        tmp_row = cc*Q(:,i) + ss*Q(:,j)
22        Q(:,j) = -ss*Q(:,i) + cc*Q(:,j)
23        Q(:,i) = tmp_row
24      END IF
25    END DO
26  END DO
27  A = MATMUL(R, Q)
28  norm_offdiag = 0.0D0
29  DO i = 1, n
30    DO j = 1, n
31      IF (i /= j) norm_offdiag += A(i,j)**2
32    END DO
33  END DO
34  IF (SQRT(norm_offdiag) < tol) EXIT ! Check convergence
35 END DO

```

Symmetric QR Algorithm with Givens Rotations for tridiagonal matrixs

Can be also optimized for tridiagonal matrixs.