MAT 226B Large Scale Matrix Computation Homework 1

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Problem 1:

(a) Let $A = [a_{j,k}] \in \mathbb{R}^{n \times n} \succ 0$ and $L = [l_{j,k}]$ be its Cholesky factor. Using MATLAB notation, Algorithm ?? shows Cholesky factorization algorithm

Algorithm 1: Cholesky Factorization

```
Input: A = [a_{j,k}] \in \mathbb{R}^{n \times n} \succ 0
Output: L = [l_{j,k}] such that A = LL^T

1 l_{j,k} = a_{j,k}, \forall j \geq k and j, k = 1, 2, \dots, n

2 for k = 1, 2, \dots, n do

3 \begin{vmatrix} l_{k,k} = \sqrt{l_{k,k}} \\ l_{k+1:n,k} = \frac{1}{l_{k,k}} l_{k+1:n,k} \end{vmatrix}

5 \begin{vmatrix} \mathbf{for} \ j = k + 1, k + 2, \dots, n \end{vmatrix} do

6 \begin{vmatrix} l_{j:n,j} = l_{j:n,j} - l_{j:n,k} l_{jk} \\ \mathbf{end} \end{vmatrix} end
```

Line 1 in Algorithm ?? is a memory copy and does not include any flops. Line 3 accounts for n square root operations. On iteration k, Line 4 will account for n-k division operations. Since this loop goes from $k=1,2,\ldots,n$, we get $\sum_{k=1}^{n}(n-k)=\frac{1}{2}n(n-1)$ division operation.

Line 6 does two operations; subtraction and multiplication, each on a vector of length (n - j + 1). Thus, the total cost of the inner loop is

$$\sum_{k=1}^{n} \sum_{j=k+1}^{n} 2(n-j+1) = \frac{1}{3}n(n^2-1)$$

Thus, the total cost of Algorithm ?? is

$$n + \frac{1}{2}n(n-1) + \frac{1}{3}n(n^2 - 1)$$
 flops

- (b) Let A be a banded $n \times n$ matrix with bandwidth 2p + 1, i.e., $a_{jk} = 0$ if |j k| > p. To show that Cholesky factor L has lower bandwidth p, i.e., $l_{jk} = 0$ if j k > p, we need to show the Cholesky factorization does not introduce any fill-in's. Line 3 and 4 in Algorithm ?? do not introduce any fill-in's.
 - At step k, the factor l_{jk} in Line 6 will be non-zero only for $k \le j \le k + p$. Thus, the only possible fill-in's for column j (i.e., at iteration j of the inner loop) is at the first p rows below the diagonal which are already non-zero since A is banded matrix with bandwidth 2p + 1 which means there is p non-zero rows below the diagonal already.
- (c) Cholesky factorization can be re-written more efficiently for banded matrices since it is guaranteed to *not* introduce fill-in such that computation can be skipped for the zero elements. Algorithm ?? shows Cholesky factorization algorithm for banded matrices

Algorithm 2: Cholesky Factorization for Banded Matrices

```
Input: A = [a_{j,k}] \in \mathbb{R}^{n \times n} \succ 0 with bandwidth 2p + 1

Output: L = [l_{j,k}] such that A = LL^T

1 l_{j,k} = a_{j,k}, \forall j \geq k and j, k = 1, 2, \dots, n

2 for k = 1, 2, \dots, n do

3 \begin{vmatrix} l_{k,k} = \sqrt{l_{k,k}} \\ l_{k+1:k+p,k} = \frac{1}{l_{k,k}} l_{k+1:k+p,k} \end{vmatrix}

5 for j = k + 1, k + 2, \dots, k + p do

6 \begin{vmatrix} l_{j:k+p,j} = l_{j:k+p,j} - l_{j:k+p,k} & l_{j,k} \\ end

8 end
```

In the algorithm above, we note the following

- Line 4 now only operates on the first p rows below the diagonal.
- Line 5 only goes through the first p columns after column k (during iteration k) since the factor l_{jk} (Line 6) will be zero for j > k + p
- Line 6 now only operates up to row k + p since the rows below k + p for column k (i.e., at iteration k) will contain zeros.

(d) Algorithm ?? requires n square root operations. Line 4 requires only p division. Since Line 4 runs for all k values (except for the last p columns but we ignore this corner case assuming $p \ll n$), then the total number of division done by Line 4 is np.

Line 6 costs p subtraction and division (assuming $p \ll n$). Thus the total cost of the whole loop (Line 5-7) is

$$\sum_{k=1}^{n} \sum_{j=k+1}^{k+p} 2p = 2np^2$$

Thus, the total cost of Algorithm ?? is

$$2np^2 + np + n =$$

Problem 2:

(a) Take an example for m=5 to see the pattern of how the non-zero values arise in the Cholesky factor L

$$T_5 = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix} \Longrightarrow L^1 = \begin{bmatrix} d_1 & 0 & 0 & 0 & 0 \\ h_1 & 2 - h_1^2 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 & 0 \\ 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

where $d_1 = \sqrt{2}$ and $h_1 = \frac{-1}{d_1}$

$$L^{2} = \begin{bmatrix} d_{1} & 0 & 0 & 0 & 0 \\ h_{1} & d_{2} & 0 & 0 & 0 \\ 0 & h_{2} & 2 - h_{2}^{2} & 0 & 0 \\ 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

where $d_2 = \sqrt{2 - h_1^2}$ and $h_2 = \frac{-1}{d_2}$

$$L^{3} = \begin{bmatrix} d_{1} & 0 & 0 & 0 & 0 \\ h_{1} & d_{2} & 0 & 0 & 0 \\ 0 & h_{2} & d_{3} & 0 & 0 \\ 0 & 0 & h_{3} & 2 - h_{3}^{2} & 0 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

where
$$d_3 = \sqrt{2 - h_2^2}$$
 and $h_3 = \frac{-1}{d_3}$

Following until the final step, we can see that the diagonal elements of Cholesky factor L are $d_i = \sqrt{2 - h_{i-1}^2}$ and the lower diagonal elements $h_i = \frac{-1}{d_i}$ where $h_0 = 0$.

(b) From the problem description, $T_{m \times m}$ is a banded matrix with bandwidth of 2m + 1. In addition, each row and column in $T_{m \times m}$ has at most 5 nonzero entries.

Let L be the Cholesky factor of $T_{m \times m}$. At the first step of Cholesky factorization (i.e., k=1 in Algorithm $\ref{eq:condition}$) the first column will have the same structure but it will introduce a new fill-in in column 2 at row m+1 because $l_{1,m+1}$ contains non-zero (namely -1) while $l_{2,m+1}$ is zero and the operation $l_{j,2} = l_{j,2} - l_{j,1} * l_{2,1}$ where j=m+1 will result in a nonzero. There is no more fill-in's will be introduce with k=1.

Following with the same process for subsequent columns (i.e., k > 1), it is clear that there is at least a new fill-in will be introduced at entry $l_{m+k,k+1}$ (actually there might be more than one new fill-in due to the fill-in's in previous columns). Thus, the sparsity structure of L is a banded matrix with lower bandwidth of m and all the entries $l_{j,k} \neq 0$ when $k - j \leq m$.

Problem 3:

Given the matrix description, it is possible to find a reordering (symmetric permutation matrix P) that pushes all the non-zero rows to the bottom and all the non-zero columns to the right (except the diagonal entries). The resultant matrix is an *arrow* matrix with m non-zero (dense) rows and columns resides at the bottom-right corner. This is a generalization of the arrow matrix of m=1.

As an example, we take $A \in \mathbb{R}^{n \times n}$, m = 3, n = 10, and $\mathcal{I} = \{2, 6, 8\}$.

We can permute A with the following permutation matrix

And the result will be

The Cholesky factor L of P^TAP will thus has the same sparsity structure as P^TAP as shown in Figure $\ref{eq:thm2}$ for arbitrary n and m. Thus, the upper bound of the $nnz(L)=(n-m)+m(n-m)+\frac{1}{2}m^2$; where n-m accounts for the diagonal elements (orange line), m(n-m) is the blue rectangle, and $\frac{1}{2}m^2$ is the red triangle.

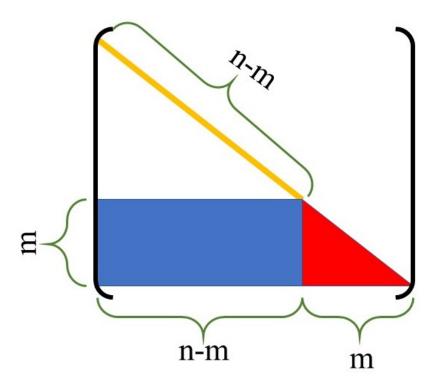


Figure 1: Sparsity structure of Cholesky factor L

It is however possible to eliminate the non-zero in the red rectangle due to cancellation. This will give the lower bound of nnz(L) to be (n-m)+m(n-m).

Problem 4:

Figure ?? shows the associated graph G(A) of matrix A along with the steps of the minimum degree algorithm. From these steps, the reordering of the nodes will be 2,4,5,3,6,7,1,8,9

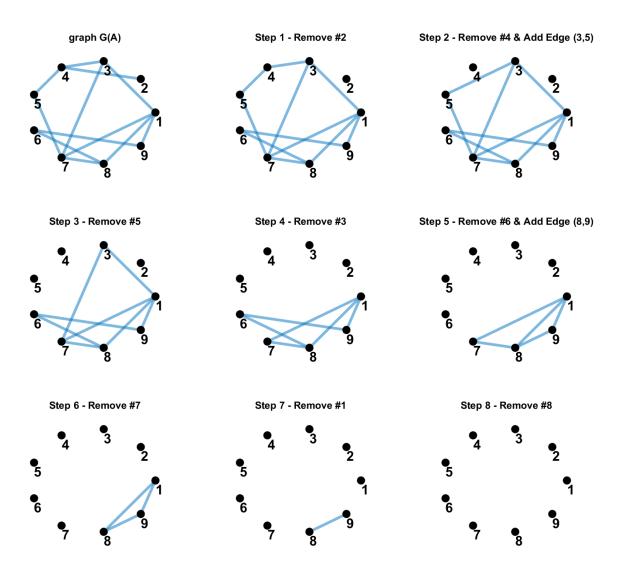


Figure 2: Graph G(A) along with the 8 steps of the minimum degree algorithm applied on it.

From the reordering above, the permutation matrix can be constructed such that

From which, we can compute P^TAP to be

Applying Cholesky factorization to P^TAP we get the following lower triangular matrix where the fill-in elements are shown with +

Problem 5:

(a) The number of nonzero entries in L=80

Nonzero entries in L at column 4:

Nonzero entries in L at column 7:

$$L(:,7) = \begin{bmatrix} L_{7,7} = & 1.921537845661046e + 00 \\ L_{8,7} = & -4.003203845127178e - 02 \\ L_{9,7} = & -4.003203845127178e - 02 \\ L_{11,7} = & -8.006407690254357e - 02 \\ L_{12,7} = & -5.604485383178049e - 01 \\ L_{15,7} = & -8.006407690254357e - 02 \\ L_{16,7} = & -5.604485383178049e - 01 \end{bmatrix}$$

Nonzero entries in L at column 10:

$$L(:,10) = \begin{bmatrix} L_{10,10} = & 1.9317955145497680e + 00 \\ L_{11,10} = & -5.581787456852771e - 01 \\ L_{12,10} = & -5.821358759653915e - 03 \\ L_{13,10} = & -2.238984138328429e - 04 \\ L_{14,10} = & -1.388170165763626e - 01 \\ L_{15,10} = & -4.097340973141025e - 02 \\ L_{16,10} = & -6.269155587319600e - 03 \end{bmatrix}$$

Nonzero entries in L at column 13:

$$L(:,13) = \begin{bmatrix} L_{13,13} = & 1.9314855917443310e + 00 \\ L_{14,13} = & -5.180834914653560e - 01 \\ L_{15,13} = & -1.515180286251492e - 01 \\ L_{16,13} = & -2.197481923194983e - 02 \end{bmatrix}$$

Nonzero entries in L at column 16:

$$L(:,16) = [L_{16,16} = 1.717283221311613e+00]$$

The relative error is

$$\frac{\parallel A - LL^T \parallel_2}{\parallel L \parallel_2} = 3.513060e - 16$$

(b) $medium_ex1.mat$ ($A \in \mathbb{R}^{1600 \times 1600}$)

No ordering:

- nnz(L) = 64039
- flag = 0
- k = 1600
- Ten largest entries in $l_{j,1000} =$

_	
	1.818644e+00
$L_{1040,1000} =$	$5.498601e{-01}$
$L_{1039,1000} =$	$1.903980e{-01}$
$L_{1038,1000} =$	7.649394e - 02
$L_{1037,1000} =$	3.549975e - 02
$L_{1036,1000} =$	$1.867330e{-02}$
$L_{1035,1000} =$	$1.086313e{-02}$
$L_{1034,1000} =$	$6.832166e{-03}$
$L_{1033,1000} =$	$4.562541\mathrm{e}{-03}$
$L_{1032,1000} =$	$3.192202e{-03}$

Reordering with symamd

- nnz(L) = 20296
- flag = 0
- k = 1600
- Ten largest entries in $l_{j,1000} =$

```
1.657056e + 00
L_{1000,1000} =
                  3.344285e{-01}
L_{1064,1000} =
L_{1067,1000} =
                  3.344285e - 01
                  2.225333e-01
L_{1066,1000} =
L_{1061,1000} =
                  2.225333e-01
L_{1068,1000} =
                  1.508700e - 01
L_{1011,1000} =
                  3.897475e{-02}
L_{1062,1000} =
                  3.897475e{-02}
                  2.514500e{-02}
L_{1012,1000} =
                  2.514500e - 02
L_{1063,1000} =
```

Reordering with colamd

- nnz(L) = 32451
- flag = 0
- k = 1600
- Ten largest entries in $l_{j,1000} =$

 $L_{1000,1000} =$ 1.793525e+006.537247e - 01 $L_{1001,1000} =$ $5.575611e{-01}$ $L_{1003,1000} =$ $L_{1002,1000} =$ $2.364628e{-01}$ $3.913581e{-02}$ $L_{1005,1000} =$ $L_{1007,1000} =$ $3.178591e{-02}$ $L_{1032,1000} =$ 2.481432e - 02 $2.367906e{-02}$ $L_{1036,1000} =$ $1.416474\mathrm{e}{-02}$ $L_{1034,1000} =$ $9.514311e{-03}$ $L_{1038,1000} =$

Reordering with symrcm

- nnz(L) = 45020
- flag = 0
- k = 1600
- Ten largest entries in $l_{j,1000} =$

1.792960e + 00 $L_{1000,1000} =$ $6.331742e{-01}$ $L_{1034,1000} =$ $5.577368e{-01}$ $L_{1035,1000} =$ $L_{1001,1000} =$ $2.420380e{-01}$ 1.009250e - 01 $L_{1033,1000} =$ $L_{1002,1000} =$ $4.826873e{-02}$ $L_{1032,1000} =$ 3.746352e - 02 $L_{1003,1000} =$ 1.954431e - 02 $1.865257\mathrm{e}{-02}$ $L_{1031,1000} =$ 1.080417e - 02 $L_{1030,1000} =$

Reordering with colperm

- nnz(L) = 169301
- flag = 0
- k = 1600
- Ten largest entries in $l_{j,1000} =$

Γ	$L_{1000,1000} =$	1.792811e+00
	$L_{1001,1000} =$	$6.493278e{-01}$
	$L_{1038,1000} =$	5.577833e - 01
	$L_{1037,1000} =$	$2.018610e{-01}$
İ	$L_{1036,1000} =$	$8.587340e{-02}$
	$L_{1035,1000} =$	4.232677e - 02
	$L_{1002,1000} =$	$4.206819e{-02}$
	$L_{1034,1000} =$	2.337139e - 02
i	$L_{1003,1000} =$	2.248362e - 02
	$L_{1033,1000} =$	1.386363e - 02

$\mathtt{medium_ex2.mat}$ ($A \in \mathbb{R}^{1728 \times 1728}$)

No ordering:

- nnz(L) = 231419
- flag = 0
- k = 1728
- Ten largest entries in $l_{j,1000} =$

	2.314829e+00
$L_{1001,1000} =$	$4.761016e{-01}$
$L_{1144,1000} =$	$4.319974e{-01}$
$L_{1132,1000} =$	$9.419033e{-02}$
$L_{1143,1000} =$	8.877675e - 02
$L_{1131,1000} =$	$4.015705e{-02}$
$L_{1120,1000} =$	$2.484508e{-02}$
$L_{1133,1000} =$	2.205327e - 02
$L_{1142,1000} =$	$2.035099e{-02}$
$L_{1119,1000} =$	$1.557268e{-02}$

Reordering with symamd

- nnz(L) = 76723
- flag = 0
- k = 1728
- Ten largest entries in $l_{j,1000} =$

```
2.155675e + 00
L_{1000,1000} =
L_{1002,1000} =
                   2.348857e - 01
                   2.300113e{-01}
L_{1005,1000} =
L_{1485,1000} =
                   1.991918e - 01
L_{1001,1000} =
                   1.615753e - 01
                   1.054859e{-01}
L_{1490,1000} =
                   5.035958e{-02}
L_{1533,1000} =
L_{1003,1000} =
                   4.928256\mathrm{e}{-02}
L_{1532,1000} =
                   3.999123e{-02}
                   3.973150e - 02
L_{1006,1000} =
```

Reordering with colamd

- nnz(L) = 145731
- flag = 0
- k = 1728
- Ten largest entries in $l_{j,1000} =$

 $L_{1000,1000} =$ 2.414184e + 00 $4.267708e{-01}$ $L_{1117,1000} =$ 4.142187e - 01 $L_{1001,1000} =$ $L_{1002,1000} =$ 4.142187e - 01 $L_{1165,1000} =$ 4.142187e - 01 $L_{1006,1000} =$ $7.322048e{-02}$ $L_{1012,1000} =$ 7.322048e - 027.112846e-02 $L_{1004,1000} =$ $1.255208\mathrm{e}{-02}$ $L_{1119,1000} =$ 4.184027e - 03 $L_{1044,1000} =$

Reordering with symrcm

- nnz(L) = 143595
- flag = 0
- k = 1728
- Ten largest entries in $l_{j,1000} =$

2.371271e+00 $L_{1000,1000} =$ $L_{1098,1000} =$ $4.362329e{-01}$ $4.217148e{-01}$ $L_{1109,1000} =$ $L_{1110,1000} =$ $4.217148e{-01}$ $9.197598e{-02}$ $L_{1001,1000} =$ $L_{1012,1000} =$ 8.871207e - 02 $L_{1011,1000} =$ 8.117340e - 02 $L_{1099,1000} =$ 1.654299e - 02 $1.568771e{-02}$ $L_{1088,1000} =$ 8.948869e - 03 $L_{1013,1000} =$

Reordering with colperm

- nnz(L) = 337092
- flag = 1
- k = 682
- Four largest entries (the rest is all zero) in $l_{j,1000}=$

$$\begin{bmatrix} L_{1000,1000} = & 6.000000 \text{e} + 00 \\ L_{1001,1000} = & 1.000000 \text{e} + 00 \\ L_{1010,1000} = & 1.000000 \text{e} + 00 \\ L_{1100,1000} = & 1.000000 \text{e} + 00 \end{bmatrix}$$