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**NUMERICAL METHODS AND PROGRAMMING**

2024/2025

**Storage and handling of matrices**
**(PROBLEMS 3)**


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1.— We want to calculate the matrix product  $\mathbf{K} = \mathbf{L}\mathbf{U}$  where  $\mathbf{L}$  is a lower triangular matrix and  $\mathbf{U}$  an upper triangular matrix, both of size  $n$ :

- What is the shape of matrix  $\mathbf{K}$ ?
- Design the minimum storage schemes for the three matrices.
- Write a multiplication algorithm adapted to the above storage schemes.
- Describe how does the computational cost grow (measured both in terms of the amount of memory and in terms of the computational time required) as a function of the size of the matrices. Compare it with that which would result from storing the complete matrices and using a multiplication algorithm for full matrices.

Sol. 1.

$$\mathbf{K} = \mathbf{L}\mathbf{U}, \quad \mathbf{L} = \begin{bmatrix} l_{11} & & & \\ l_{21} & l_{22} & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix}, \quad \mathbf{U} = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \cdots & u_{2n} \\ & & \ddots & \vdots \\ & & & u_{nn} \end{bmatrix}$$

a) The product of matrices can be expressed as:

$$\mathbf{K} = [k_{ij}], \quad k_{ij} = \sum_{m=1}^n l_{im} u_{mj}$$

but it has to be considered that:

$$\begin{aligned} l_{im} &= 0 & \text{if } m > i \\ u_{mj} &= 0 & \text{if } m > j \end{aligned}$$

Thus, the product can be obtained as:

$$k_{ij} = \sum_{\substack{m=1, n \\ m \leq i, m \leq j}} l_{im} u_{mj} = \sum_{m=1}^{\min\{i, j\}} l_{im} u_{mj}$$

It can be generally observed that  $k_{ij} \neq 0$ , since there is always a product that adds to element  $k_{ij}$

Then  $\mathbf{K}$  is a full matrix.

b) We store:

$\mathbf{L}$   $\rightarrow$  Row major lower triangular  
 $\mathbf{U}$   $\rightarrow$  Column major upper triangular  
 $\mathbf{K}$   $\rightarrow$  Column major full

So that:

$$l_{ij} \rightsquigarrow vl(lpl) \quad \text{with} \quad lpl = \frac{i(i-1)}{2} + j; \quad j \leq i$$

$$u_{ij} \rightsquigarrow vu(lpu) \quad \text{with} \quad lpu = \frac{j(j-1)}{2} + i; \quad i \leq j$$

$$k_{ij} \rightsquigarrow vk(lpk) \quad \text{with} \quad lpk = (j-1)n + i$$

c)

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do j=1,n
  lpk0=(j-1)*n
  lpu0=(j*(j-1))/2
  do i=1,n
    lpl0=(i*(i-1))/2
    lpk=lpk0+i
    vk(lpk)=0.
    do m=1,min(i,j)
      lpl=lpl0+m
      lpu=lpu0+m
      vk(lpk)=vk(lpk)+vl(lpl)*vu(lpu)
    enddo
  enddo
enddo

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d) The previous algorithm needs:

$$1) \text{ Storage} = \frac{n(n+1)}{2} \quad \text{terms for } \mathbf{L}$$

$$\frac{n(n+1)}{2} \quad \text{terms for } \mathbf{U}$$

$$\frac{n^2}{2} \quad \text{terms for } \mathbf{K}$$

$$\text{Total} = 2n^2 + n \Rightarrow \mathcal{A}(2n^2 + n) \approx \mathcal{A}(2n^2)$$

2) Computing time =

$$\begin{array}{l}
 (2(n-1)+1) \text{ times [1 product and 1 addition]} \rightsquigarrow \begin{bmatrix} \bullet & \bullet & \cdots & \bullet & \bullet \\ \bullet & & & & \\ \vdots & & & & \\ \bullet & & & & \\ \bullet & & & & \\ * & * & \cdots & * & * \\ * & \bullet & \cdots & \bullet & \bullet \\ \vdots & \vdots & & & \\ * & \bullet & & & \\ * & \bullet & & & \end{bmatrix} \\
 \\
 \vdots \qquad \qquad \qquad \vdots \qquad \qquad \qquad \vdots \\
 \\
 (2(n-n)+1) \text{ times [(n) products and (n) additions]} \rightsquigarrow \begin{bmatrix} * & * & \cdots & * & * \\ * & * & \cdots & * & * \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ * & * & \cdots & * & * \\ * & * & \cdots & * & \bullet \end{bmatrix}
 \end{array}$$

$$\begin{aligned}
 \text{Total} &= \sum_{d=1}^n (2(n-d)+1) [ (d) \text{ “products”} + (d) \text{ “additions”} ] \\
 &= \sum_{d=1}^n (2(n-d)+1) (2d) \quad \text{FPO (Floating Point Operations)} \\
 &= \left( \sum_{d=1}^n 2d(2n+1) - \sum_{d=1}^n (2d)^2 \right) \text{FPO} = \left( (2n+1)(n+1)n - \frac{2}{3}(2n+1)(n+1)n \right) \text{FPO} \\
 &= \left( \frac{2n^3}{3} + \frac{3n^2}{3} + \frac{n}{3} \right) \text{FPO} \Rightarrow T \left( \frac{2n^3}{3} + \frac{3n^2}{3} + \frac{n}{3} \right) \approx T \left( \frac{2n^3}{3} \right)
 \end{aligned}$$

If we would have used full matrices then:

$$3n^2 \text{ terms for } \mathbf{L}, \mathbf{U}, \mathbf{K} \Rightarrow \mathcal{A}(3n^2)$$

$$2n^3 \text{ FPO to obtain } \mathbf{K} \Rightarrow T(2n^3)$$

Thus, it is saved approximately  $\begin{cases} 1/3 \text{ in memory} \\ 2/3 \text{ in computing time} \end{cases}$

2.— Repeat the previous problem when the matrices  $\mathbf{L}$  and  $\mathbf{U}$  have half-bandwidths  $l$  and  $u$  respectively, with  $l \ll n$ , and  $u \ll n$ .

Sol. 2.

$$\mathbf{L} = \begin{bmatrix} l_{11} & & & & & & \\ l_{21} & l_{22} & & & & & \\ \vdots & \vdots & \ddots & & & & \\ l_{l+1,1} & l_{l+1,2} & \cdots & l_{l+1,l+1} & & & \\ & & \ddots & \ddots & & & \\ & & & l_{i,i-l} & l_{i,i-l+1} & & l_{i,i} \\ & & & & \ddots & \ddots & \ddots \\ & & & & & l_{n,n-l} & l_{n,n-l+1} & \cdots & l_{n,n} \end{bmatrix}$$

$$\mathbf{U} = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1,u+1} & & & & \\ & u_{22} & \cdots & u_{2,u+1} & \ddots & & & \\ & & \ddots & \vdots & \ddots & u_{j-u,j} & & \\ & & & u_{u+1,u+1} & u_{j-u+1,j} & \ddots & & \\ & & & & \ddots & \vdots & \ddots & u_{n-u,n} \\ & & & & & u_{j,j} & u_{n-u+1,n} \\ & & & & & & \ddots & \vdots \\ & & & & & & & u_{n,n} \end{bmatrix}$$

a)  $\mathbf{K} = [k_{ij}]$ ;  $k_{ij} = \sum_{m=1}^n l_{im}u_{mj}$

however

$$\begin{aligned} l_{im} &= 0 && \text{if } m > i & \text{ or } & m < i - l \\ u_{mj} &= 0 && \text{if } m > j & \text{ or } & m < j - u \end{aligned}$$

So that:

$$K_{ij} = \sum_{\substack{m=1, n \\ i-l \leq m \leq i \\ j-u \leq m \leq j}} l_{im}u_{mj} = \sum_{m=\max\{i-l, j-u, 1\}}^{\min\{i, j\}} l_{im}u_{mj}$$

Thus whenever  $\min\{i, j\} < \max\{i - l, j - u, 1\}$  there will be no products adding terms to  $k_{ij}$ . Therefore, only coefficient  $k_{ij}$  such that  $\min\{i, j\} \geq \max\{i - l, j - u, 1\}$  would be non-zero, a priori, so those that  $i \geq i - l, i \geq j - u, j \geq i - l, j \geq j - u$ .

Since  $i \geq i - l$  and  $j \geq j - u$  are always satisfied:

$$k_{ij} \text{ might be non-zero} \iff \begin{cases} i \geq j - u \Rightarrow \text{uper bandwidth (u)} \\ j \geq i - l \Rightarrow \text{lower bandwidth (l)} \end{cases}$$

Then  $\mathbf{K}$  is a banded matrix with lower bandwidth that of  $\mathbf{L}$  and upper bandwidth that of  $\mathbf{U}$ .

$$\mathbf{K} = \left[ \begin{array}{cccccccc}
 \ddots & * & \dots & * & & & & \\
 * & \ddots & * & \dots & * & & & \\
 \vdots & * & \ddots & * & \dots & * & & \\
 \vdots & \vdots & * & \ddots & * & \dots & * & \\
 * & \vdots & \vdots & * & \ddots & * & \dots & * \\
 & * & \vdots & \vdots & * & \ddots & * & \dots & * \\
 & & * & \vdots & \vdots & * & \ddots & * & \dots & * \\
 & & & * & \vdots & \vdots & * & \ddots & * & \dots & * \\
 & & & & * & \vdots & \vdots & * & \ddots & * & \vdots \\
 & & & & & * & \vdots & \vdots & * & \ddots & * \\
 & & & & & & * & \vdots & \vdots & * & \ddots & * \\
 & & & & & & & * & \vdots & \vdots & * & \ddots & * \\
 & & & & & & & & * & \dots & \dots & * & \ddots \\
 & & & & & & & & & * & \dots & \dots & * & \ddots \\
 & & & & & & & & & & * & \dots & \dots & * & \ddots
 \end{array} \right]$$

$l$   $\left\{ \begin{array}{l} \dots \\ \dots \\ \dots \\ \dots \\ \dots \end{array} \right.$ 
}  $u$

b) We store matrices  $\mathbf{L}$ ,  $\mathbf{U}$ ,  $\mathbf{K}$  banded (by diagonals)

$$\begin{aligned}
 l_{ij} &\rightsquigarrow vl(lp_l) && \text{with } lp_l = (j - i + l)n + i; && i - l \leq j \leq i \\
 u_{ij} &\rightsquigarrow vu(lp_u) && \text{with } lp_u = (j - i)n + i; && j - u \leq i \leq j \\
 k_{ij} &\rightsquigarrow vk(lp_k) && \text{with } lp_k = (j - i + l)n + i; && \begin{cases} i - l \leq j \leq i \\ j - u \leq i \leq j \end{cases}
 \end{aligned}$$

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c)      do j=1,n
         do i=max(1,j-u), min(n,j+1)
           lpk=(j-i+1)*n+i
           vk(lp_k)=0.d+00
           do k=max(i-1,j-u,1), min(i,j)
             lpl=(k-i+1)*n+i
             lpu=(j-k)*n+k
             vk(lp_k)=vk(lp_k)+v1(lpl)*vu(lpu)
           enddo
         enddo
       enddo

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d) The algorithm requires:

1) Storage =	$n(l + 1)$	elements for $\mathbf{L}$
	$n(u + 1)$	elements for $\mathbf{U}$
	$n(l + 1 + u)$	elements for $\mathbf{K}$

$$\text{Total} = 2n(l + 1 + u) + n \Rightarrow \mathcal{A}(2n(l + 1 + u) + n) = \mathcal{A}(2n(l + u + 1, 5))$$

## 2) Computing time

The exact computation is difficult to obtain, however we know that  $l \ll n$  and  $u \ll n$

If we assume that, what happens on the central rows and columns is of application for the rest (which is reasonable since the only irregular ones would be the  $(1+l)$  first rows and the  $(1+u)$  last columns) then we can proceed as follows.

To obtain the  $(l+1+u)$  elements of row  $i$  we need:

$$\left\{ \begin{array}{l} (1) \text{ product} + (1) \text{ addition} \\ (2) \text{ products} + (2) \text{ additions} \\ \vdots \\ (\min(l, u)+1) \text{ products} + (\min(l, u)+1) \text{ additions} \\ \vdots \\ (\min(l, u)+1) \text{ products} + (\min(l, u)+1) \text{ additions} \\ \vdots \\ (2) \text{ products} + (2) \text{ additions} \\ (1) \text{ product} + (1) \text{ addition} \end{array} \right.$$

Therefore the number of operations per row is:

$$(l+1+u - \min(l, u)) \ 2(\min(l, u) + 1) \ \text{OCF}$$

$$2(\max(l, u) + 1) (\min(l, u) + 1) \ \text{OCF}$$

$$2(l+1)(u+1) \ \text{OCF}$$

So the total computing complexity will be approximately  $T(2n(l+1)(u+1))$

Remember that if full matrices were considered then:

$$\left\{ \begin{array}{l} 3n^2 \text{ elements for } \mathbf{L}, \mathbf{U}, \mathbf{K} \implies \mathcal{A}(3n^2) \\ 2n^3 \text{ OCF to obtain } \mathbf{K} \implies T(2n^3) \end{array} \right.$$

Thus, when  $l \ll n$  and  $u \ll n$  the reduction in storage and computing time is very significant (specially in time).

- 3.— Of the matrix  $\mathbf{L}$  it is known that it is lower triangular and that all its elements are null except for those located on the main diagonal (which are always nonzero) and those in the row  $\alpha$  (which in general will be nonzero, but not necessarily), this is:

$$\mathbf{L} = \begin{bmatrix} l_{11} & & & & & & & \\ & l_{22} & & & & & & \\ & & \ddots & & & & & \\ l_{\alpha 1} & l_{\alpha 2} & \cdots & l_{\alpha \alpha} & & & & \\ & & & & \ddots & & & \\ & & & & & l_{\beta\beta} & & \\ & & & & & & \ddots & \\ & & & & & & & l_{nn} \end{bmatrix}.$$

In order to obtain the matrix product  $\mathbf{A} = \mathbf{L}\mathbf{L}^T$ .

- Is  $\mathbf{A}$  going to be symmetric? And positive definite? Why?
- What is the general shape of matrix  $\mathbf{A}$ ?
- Develop the storage schemes that are considered the most suitable for the two matrices. As matrix  $\mathbf{A}$  is being computed, is it possible to store its coefficients in the place occupied by the corresponding coefficients of the matrix  $\mathbf{L}$  matrix to save memory space? Why?
- Develop an algorithm suited to perform the matrix product with the storage schemes described in the previous section.
- How does the computational time necessary to obtain  $\mathbf{A}$  grow as the size of the matrix increases?

**Sol. 3.**

- a)  $\mathbf{A} = \mathbf{L}\mathbf{L}^T$  with  $\det(\mathbf{L}) = \prod_{i=1}^n l_{ii} \neq 0$  is

$$\left\{ \begin{array}{l} 1) \text{ Symmetric, because } \mathbf{A}^T = (\mathbf{L}\mathbf{L}^T)^T = (\mathbf{L}^T)^T \mathbf{L}^T = \mathbf{L}\mathbf{L}^T = \mathbf{A} \\ 2) \text{ positive semidefinite, because } \mathbf{v}^T \mathbf{A} \mathbf{v} = \mathbf{v}^T (\mathbf{L}\mathbf{L}^T) \mathbf{v} = \\ \quad (\mathbf{v}^T \mathbf{L})(\mathbf{L}^T \mathbf{v}) = \underbrace{(\mathbf{L}^T \mathbf{v})^T}_{\mathbf{w}^T} \underbrace{(\mathbf{L}^T \mathbf{v})}_{\mathbf{w}} = \mathbf{w}^T \mathbf{w} \geq 0 \\ 3) \text{ positive definite, because } \mathbf{v}^T \mathbf{A} \mathbf{v} = 0 \iff \mathbf{w} = \mathbf{L}^T \mathbf{v} = \mathbf{0} \xrightarrow{\det(\mathbf{L}) \neq 0} \mathbf{v} = \mathbf{0} \end{array} \right.$$

b)

$$\mathbf{L} = \begin{bmatrix} l_{11} & & & & & & & \\ & l_{22} & & & & & & \\ & & \ddots & & & & & \\ l_{\alpha 1} & l_{\alpha 2} & \cdots & l_{\alpha \alpha} & & & & \\ & & & & \ddots & & & \\ & & & & & l_{nn} & & \end{bmatrix} \quad \mathbf{L}^T = \begin{bmatrix} l_{11} & & & l_{\alpha 1} & & & & \\ & l_{22} & & l_{\alpha 2} & & & & \\ & & \ddots & \vdots & & & & \\ & & & l_{\alpha \alpha} & & & & \\ & & & & \ddots & & & \\ & & & & & l_{nn} & & \end{bmatrix}$$

Then





- 4.— Of the matrices  $L$  and  $U$  it is known that they are lower and upper triangular respectively, and that all their elements are null except for those located on the main diagonal, in the row  $\alpha$  of  $L$  and in the  $\beta$  column of  $U$ . This is:

$$\mathbf{L} = \begin{bmatrix} l_{11} & & & & & & & \\ & l_{22} & & & & & & \\ & & \dots & & & & & \\ l_{\alpha 1} & l_{\alpha 2} & \dots & l_{\alpha \alpha} & & & & \\ & & & & \dots & & & \\ & & & & & l_{\beta \beta} & & \\ & & & & & & \dots & \\ & & & & & & & l_{nn} \end{bmatrix}, \mathbf{U} = \begin{bmatrix} u_{11} & & & & & & & & & \\ & u_{22} & & & & & & & & u_{1\beta} \\ & & \dots & & & & & & & u_{2\beta} \\ & & & \dots & & & & & & \vdots \\ & & & & u_{\alpha \alpha} & & & & & \vdots \\ & & & & & \dots & & & & \vdots \\ & & & & & & & & & u_{\beta \beta} \\ & & & & & & & & & \dots \\ & & & & & & & & & & u_{nn} \end{bmatrix}$$

- a) what is the general shape of the product matrix  $A = LU$ ?
- b) Design storage schemes suited for the three matrices
- c) Write a specific algorithm including the storage schemes described for the matrix product.

**Sol. 4.**

- a) It is a special case of product of two skyline matrices.

We know that  $A = LU$  shares the same row profile as  $L$  and the same column profile as  $U$ , so the only non-zero elements of  $A$  will be:

$$\begin{aligned}
 a_{ii}; & \quad i = 1, \dots, n \\
 a_{\alpha j}; & \quad j = 1, \dots, \alpha - 1 \\
 a_{i\beta}; & \quad i = 1, \dots, \beta - 1
 \end{aligned}$$

The the resulting matrix of the product will have the following shape:

$$\left\{ \begin{array}{l}
 \text{Case } \alpha < \beta \rightsquigarrow \mathbf{A} = \begin{bmatrix} \dots & & & & \vdots \\ \dots & \dots & & & \vdots \\ & & \dots & & \vdots \\ & & & \dots & \vdots \\ \dots & & & & \dots \end{bmatrix} \\
 \\
 \text{Case } \alpha = \beta \rightsquigarrow \mathbf{A} = \begin{bmatrix} \dots & & & & \vdots \\ \dots & \dots & & & \vdots \\ \dots & \dots & \dots & & \vdots \\ \dots & \dots & \dots & \dots & \vdots \\ \dots & & & \dots & \dots \end{bmatrix} \\
 \\
 \text{Case } \alpha > \beta \rightsquigarrow \mathbf{A} = \begin{bmatrix} \dots & & & & \vdots \\ \dots & \dots & & & \vdots \\ \dots & \dots & \dots & & \vdots \\ \dots & \dots & \dots & \dots & \vdots \\ \dots & & & \dots & \dots \end{bmatrix}
 \end{array} \right.$$

- b) In order to store matrices  $\mathbf{L}$  and  $\mathbf{U}$  we need to arrays of  $(n + (\alpha - 1))$  and  $(n + (\beta - 1))$  elements respectively:

$$\begin{aligned}\mathbf{vl} &= (l_{11}, l_{22}, \dots, l_{\alpha-1, \alpha-1}, l_{\alpha 1}, l_{\alpha 2}, \dots, l_{\alpha, \alpha}, l_{\alpha+1, \alpha+1}, \dots, l_{nn}) \\ \mathbf{vu} &= (u_{11}, u_{22}, \dots, u_{\beta-1, \beta-1}, u_{1\beta}, u_{2\beta}, \dots, u_{\beta\beta}, u_{\beta+1, \beta+1}, \dots, u_{nn})\end{aligned}$$

To store matrix  $\mathbf{A}$  we need a vector of  $(n + (\alpha - 1) + (\beta - 1))$  elements.

We may, for example, arrange the data as:

$$\mathbf{va} = (a_{11}, a_{22}, \dots, a_{nn}, a_{\alpha 1}, \dots, a_{\alpha, \alpha-1}, a_{1\beta}, \dots, a_{\beta-1, \beta})$$

- c) This problem can be solve similarly to the previous one.

We need to multiply  $\mathbf{LU}$  and identify the values of the elements of  $\mathbf{A}$ .

Considering the three possible cases ( $\alpha < \beta$ ,  $\alpha = \beta$ ,  $\alpha > \beta$ ).

Finally, the elements  $l_{ik}$ ,  $u_{kj}$  y  $a_{ij}$  are substituted by their indexes according to the storage scheme of the previous problem.

