

# Meeting Notes

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July 1, 2022

## 1 28.06.2022 Meeting draft

### 1.1 Tridiagonal matrix (Upper)

$n = 2k$

$$\begin{aligned}
 U &= \begin{bmatrix} d_1 & b_1^1 & b_1^2 & & & & \\ & d_2 & b_2^1 & b_2^2 & & & \\ & & d_3 & b_3^1 & b_3^2 & & \\ & & & d_4 & b_4^1 & b_4^2 & \\ & & & & \ddots & \ddots & \ddots \\ & & & & & \ddots & \ddots \\ & & & & & & d_{n-3} & b_{n-3}^1 & b_{n-3}^2 \\ & & & & & & & d_{n-2} & b_{n-2}^1 & b_{n-2}^2 \\ & & & & & & & & d_{n-1} & b_{n-1}^1 \\ & & & & & & & & & d_n \end{bmatrix} \\
 &= \begin{bmatrix} \begin{bmatrix} d_1 & b_1^1 \\ & d_2 \end{bmatrix} & \begin{bmatrix} b_1^2 & \\ b_2^1 & b_2^2 \end{bmatrix} & & & \\ & \begin{bmatrix} d_3 & b_3^1 \\ & d_4 \end{bmatrix} & \begin{bmatrix} b_3^2 & \\ b_4^1 & b_4^2 \end{bmatrix} & & \\ & & \ddots & \ddots & \\ & & & \begin{bmatrix} d_{2k-3} & b_{2k-3}^1 \\ & d_{2k-2} \end{bmatrix} & \begin{bmatrix} b_{2k-3}^2 & \\ b_{2k-2}^1 & b_{2k-2}^2 \end{bmatrix} \\ & & & & \begin{bmatrix} d_{2k-1} & b_{2k-1}^1 \\ & d_{2k} \end{bmatrix} \end{bmatrix} \\
 &= \begin{bmatrix} D_1 & B_1 & & & \\ & D_2 & B_2 & & \\ & & \ddots & \ddots & \\ & & & D_{k-1} & B_{k-1} \\ & & & & D_k \end{bmatrix} \in \mathbb{R}^{2k \times 2k}
 \end{aligned}$$

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_{k-1} \\ X_k \end{bmatrix} \in \mathbb{R}^{2k \times 2} \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_{k-1} \\ Y_k \end{bmatrix} \in \mathbb{R}^{2k \times 2} \quad Y^T = [Y_1^T \ Y_2^T \ \cdots \ Y_{k-1}^T \ Y_k^T] \in \mathbb{R}^{2 \times 2k}$$

$$\begin{aligned}
XY^T &= \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_{k-1} \\ X_k \end{bmatrix} [Y_1^T \ Y_2^T \ \cdots \ Y_{k-1}^T \ Y_k^T] \\
&= \begin{bmatrix} X_1 Y_1^T & X_1 Y_2^T & \cdots & X_1 Y_{k-1}^T & x_1 Y_k^T \\ X_2 Y_1^T & X_2 Y_2^T & \cdots & X_2 Y_{k-1}^T & x_2 Y_k^T \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ X_{k-1} Y_1^T & X_{k-1} Y_2^T & \cdots & X_{k-1} Y_{k-1}^T & X_{k-1} Y_k^T \\ X_k Y_1^T & X_k Y_2^T & \cdots & X_k Y_{k-1}^T & X_k Y_k^T \end{bmatrix} \\
&= X [Y_1^T \ Y_2^T \ \cdots \ Y_{k-1}^T \ Y_k^T] \\
&= [XY_1^T \ XY_2^T \ \cdots \ XY_{k-1}^T \ XY_k^T]
\end{aligned}$$

$$\begin{aligned}
\text{triu}(X_k) &:= X_k \\
\text{triu}(Y_k^T) &:= Y_k^T \\
\text{triu}(X_k Y_k^T) &= X_k Y_k^T
\end{aligned}$$

$$\begin{aligned}
\text{triu}(XY^T) &= \begin{bmatrix} \text{triu}(X_1 Y_1^T) & X_1 Y_2^T & \cdots & X_1 Y_{k-1}^T & X_1 Y_k^T \\ 0_{2 \times 2} & \text{triu}(X_2 Y_2^T) & \cdots & X_2 Y_{k-1}^T & X_2 Y_k^T \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0_{2 \times 2} & 0_{2 \times 2} & \cdots & \text{triu}(X_{k-1} Y_{k-1}^T) & X_{k-1} Y_k^T \\ 0_{2 \times 2} & 0_{2 \times 2} & \cdots & 0_{2 \times 2} & X_k Y_k^T \end{bmatrix} \\
&= \begin{bmatrix} \text{triu}(X_1 Y_1^T) \\ 0_{2(k-1) \times 2} \end{bmatrix} \begin{bmatrix} X_1 Y_2^T \\ \text{triu}(X_2 Y_2^T) \\ 0_{2(k-2) \times 2} \end{bmatrix} \cdots \begin{bmatrix} X_{1:k-2} Y_{k-1}^T \\ \text{triu}(X_{k-1} Y_{k-1}^T) \\ 0_{2 \times 2} \end{bmatrix} XY_k^T
\end{aligned}$$

$$\begin{aligned}
U^{-1} &= \text{triu}(XY^T) \\
I &= U \text{triu}(XY^T)
\end{aligned}$$

$$E_i = [0 \ \cdots \ 0 \ I_{2 \times 2} \ 0 \ \cdots \ 0]^T$$

$k$ -th block column,

$$\begin{aligned}
E_k &= U \text{triu}(XY^T) E_k \\
&= U X Y_k^T
\end{aligned}$$

$$\begin{aligned}
X &:= U^{-1} E_k \\
E_k &= U X Y_k^T \\
&= U U^{-1} E_k Y_k^T \\
&= E_k Y_k^T \\
Y_k^T &:= I_{2 \times 2}
\end{aligned}$$

$(k-1)$ -th block column,

$$\begin{aligned} E_{k-1} &= U \operatorname{triu}(XY^T)E_{k-1} \\ &= U \begin{bmatrix} X_{1:k-2}Y_{k-1}^T \\ \operatorname{triu}(X_{k-1}Y_{k-1}^T) \\ 0_{2 \times 2} \end{bmatrix} \end{aligned}$$

$(k-1)$ -th block row of  $(k-1)$ -th block column,

$$E_i^T E_j = \begin{cases} I_{2 \times 2}, & \text{if } i = j ; \\ 0_{2 \times 2}, & \text{otherwise.} \end{cases}$$

$$\begin{aligned} E_{k-1}^T E_{k-1} &= I_{2 \times 2} = E_{k-1}^T U \begin{bmatrix} X_{1:k-2}Y_{k-1}^T \\ \operatorname{triu}(X_{k-1}Y_{k-1}^T) \\ 0_{2 \times 2} \end{bmatrix} \\ &= \begin{bmatrix} 0_{2 \times 2(k-2)} & D_{k-1} & B_{k-1} \end{bmatrix} \begin{bmatrix} X_{1:k-2}Y_{k-1}^T \\ \operatorname{triu}(X_{k-1}Y_{k-1}^T) \\ 0_{2 \times 2} \end{bmatrix} \\ &= D_{k-1} \operatorname{triu}(X_{k-1}Y_{k-1}^T) \\ Y_{k-1}^T &:= (D_{k-1}X_{k-1})^{-1} \end{aligned}$$

$$\begin{aligned} D_{k-1} &= \operatorname{triu}(D_{k-1}) \\ D_{k-1}^{-1} &= \operatorname{triu}(D_{k-1}^{-1}) \\ Y_{k-1}^T &:= (D_{k-1}X_{k-1})^{-1} \\ D_{k-1} \operatorname{triu}(X_{k-1}Y_{k-1}^T) &= D_{k-1} \operatorname{triu}(X_{k-1}(D_{k-1}X_{k-1})^{-1}) \\ &= D_{k-1} \operatorname{triu}(X_{k-1}X_{k-1}^{-1}D_{k-1}^{-1}) \\ &= D_{k-1} \operatorname{triu}(D_{k-1}^{-1}) \\ &= D_{k-1}D_{k-1}^{-1} \\ &= I_{2 \times 2} \end{aligned}$$

$$\begin{aligned} X &:= U^{-1}E_k \\ E_k &= UX \\ E_k^T E_k &= I_{2 \times 2} = E_k^T UX \\ &= \begin{bmatrix} 0_{2 \times 2(k-1)} & D_k \end{bmatrix} X \\ &= D_k X_k \\ Y_k^T &:= I_{2 \times 2} \\ &:= (D_k X_k)^{-1} \end{aligned}$$

$$\begin{aligned} X &:= U^{-1}E_k \\ Y_i^T &:= (D_i X_i)^{-1} \end{aligned}$$

$$n = 2k + 1$$

$$U = \begin{bmatrix} [d_1] & \begin{bmatrix} b_1^1 & b_1^2 \\ d_2 & b_2^1 \\ & d_3 \end{bmatrix} & \begin{bmatrix} b_2^2 & \\ b_3^1 & b_3^2 \end{bmatrix} & & \\ & & \ddots & \ddots & \\ & & & \begin{bmatrix} d_{2k-2} & b_{2k-2}^1 \\ & d_{2k-1} \end{bmatrix} & \begin{bmatrix} b_{2k-2}^2 & \\ b_{2k-1}^1 & b_{2k-1}^2 \\ d_{2k} & b_{2k}^1 \\ & d_{2k+1} \end{bmatrix} \end{bmatrix}$$

$$= \begin{bmatrix} \tilde{D}_1 & \tilde{B}_1 & & & \\ & D_2 & B_2 & & \\ & & \ddots & \ddots & \\ & & & D_k & B_k \\ & & & & D_{k+1} \end{bmatrix} \in \mathbb{R}^{(2k+1) \times (2k+1)}$$

$$X := U^{-1} E_{k+1}$$

$$Y_i^T := (D_i X_i)^{-1} \text{ for } i = 2, \dots, k+1$$

$$Y_1^T := (D_1 X_1)^+ = (D_1 X_1)^T (D_1 X_1 (D_1 X_1)^T)^{-1}$$

## 1.2 Banded matrix (Upper)

$$n = ku + r, \quad 0 \leq r < u$$

$$U = \begin{bmatrix} d_1 & b_1^1 & b_1^2 & \cdots & b_1^u & & \\ & d_2 & b_2^1 & b_2^2 & \cdots & b_2^u & \\ & & \ddots & \ddots & \ddots & \cdots & \ddots \\ & & & \ddots & \ddots & \ddots & b_{n-u}^u \\ & & & & \ddots & \ddots & \vdots \\ & & & & & \ddots & b_{n-2}^2 \\ & & & & & & \ddots & b_{n-1}^1 \\ & & & & & & & d_n \end{bmatrix}$$

$$r = 0, \quad n = ku,$$

$$U = \begin{bmatrix} D_1 & B_1 & & & \\ & D_2 & B_2 & & \\ & & \ddots & \ddots & \\ & & & D_{k-1} & B_{k-1} \\ & & & & D_k \end{bmatrix} \in \mathbb{R}^{ku \times ku},$$

$$D_i \in \mathbb{R}^{u \times u}, \quad B_i \in \mathbb{R}^{u \times u} \text{ for } i = 1, 2, \dots, k.$$

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_k \end{bmatrix} \in \mathbb{R}^{ku \times u} \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_k \end{bmatrix} \in \mathbb{R}^{ku \times u} \quad Y^T = [Y_1^T \quad Y_2^T \quad \cdots \quad Y_k^T] \in \mathbb{R}^{u \times ku}$$

$$X_i, Y_i^T \in \mathbb{R}^{u \times u}, \text{ for } i = 1, 2, \dots, k$$

$$X := U^{-1} E_k$$

$$Y_i^T := (D_i X_i)^{-1}$$

$$r \neq 0, \quad n = ku + r,$$

$$U = \begin{bmatrix} \tilde{D}_1 & \tilde{B}_1 & & & \\ & D_2 & B_2 & & \\ & & \ddots & \ddots & \\ & & & D_k & B_k \\ & & & & D_{k+1} \end{bmatrix} \in \mathbb{R}^{(ku+r) \times (ku+r)},$$

$$\tilde{D}_1 \in \mathbb{R}^{r \times r}, \quad \tilde{B}_1 \in \mathbb{R}^{r \times u};$$

$$D_i \in \mathbb{R}^{u \times u}, \quad B_i \in \mathbb{R}^{u \times u} \text{ for } i = 2, \dots, k+1.$$

$$X = \begin{bmatrix} \tilde{X}_1 \\ X_2 \\ \vdots \\ X_{k+1} \end{bmatrix} \in \mathbb{R}^{(ku+r) \times u} \quad Y = \begin{bmatrix} \tilde{Y}_1 \\ Y_2 \\ \vdots \\ Y_{k+1} \end{bmatrix} \in \mathbb{R}^{(ku+r) \times u} \quad Y^T = [\tilde{Y}_1^T \quad Y_2^T \quad \cdots \quad Y_{k+1}^T] \in \mathbb{R}^{u \times (ku+r)}$$

$$\begin{aligned}
&\tilde{X}_1 \in \mathbb{R}^{r \times u} \\
&\tilde{Y}_1^T \in \mathbb{R}^{u \times r} \\
&X_i, Y_i^T \in \mathbb{R}^{u \times u} \text{ for } i = 2, \dots, k+1 \\
&X := U^{-1}E_{k+1} \\
&\tilde{Y}_1^T := (D_1X_1)^+ = (D_1X_1)^T(D_1X_1(D_1X_1)^T)^{-1} \\
&\text{triu}(D_1X_1\tilde{Y}_1^T) = I_{r \times r} \\
&Y_i^T := (D_iX_i)^{-1} \text{ for } i = 2, \dots, k+1
\end{aligned}$$

## 2 28.06.2022 Meeting formal

### 2.1 Notation

This notes use Householder notation and start indexing at one.

Scalars, lower case Greek letters:  $\alpha, \beta, \gamma, \chi, \text{etc.}$

Vectors, lower case Roman letter:  $a, b, c, x, \text{etc.}$

Matrix, upper case Roman letter:  $A, B, C, X, \text{etc.}$

lower case Greek letters:	$\alpha, \beta, \gamma, \chi, \text{etc.}$	for Scalars;
lower case Roman letter:	$a, b, c, x, \text{etc.}$	for Vectors;
upper case Roman letter:	$A, B, C, X, \text{etc.}$	for Matrix.

### 2.2 Repersentation

#### Matrix & Vector

$$x = \begin{bmatrix} \chi_1 \\ \chi_2 \\ \vdots \\ \chi_n \end{bmatrix} \in \mathbb{R}^n$$
$$A = \begin{bmatrix} \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1n} \\ \alpha_{21} & \alpha_{22} & \cdots & \alpha_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \alpha_{m1} & \alpha_{m2} & \cdots & \alpha_{1n} \end{bmatrix}$$
$$= [a_1 \mid a_2 \mid \cdots \mid a_n] \in \mathbb{R}^{m \times n}$$

#### Block Matrix & Block Vector

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{kn}, x_i \in \mathbb{R}^k$$
$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{1n} \end{bmatrix}$$
$$= [A_1 \mid A_2 \mid \cdots \mid A_n] \in \mathbb{R}^{lm \times kn}, A_{ij} \in \mathbb{R}^{l \times k}$$

## 2.3 Algorithm

$$U^{-1} = \text{triu}(XY^T)$$

For  $U \in \mathbb{R}^{n \times n}$ ,  
if  $n = ku$

$$\begin{aligned} X &:= U^{-1}E_k; \\ Y_i^T &:= (D_i X_i)^{-1} \text{ for } i = 1, 2, \dots, k. \end{aligned}$$

if  $n = ku + r$

$$\begin{aligned} X &:= U^{-1}E_k; \\ Y_i^T &:= (D_i X_i)^{-1} \text{ for } i = 2, \dots, k+1; \\ Y_1^T &:= (D_1 X_1)^+ \end{aligned}$$

### 2.3.1 Example

Let

$$U = \begin{bmatrix} D_1 & B_1 & \\ & D_2 & B_2 \\ & & D_3 \end{bmatrix} \in \mathbb{R}^{(2u+r) \times (2u+r)}$$

where  $D_1 \in \mathbb{R}^{r \times r}$ ,  $B_1 \in \mathbb{R}^{r \times u}$ , and  $D_2, B_2, D_3, B_3 \in \mathbb{R}^{u \times u}$ .

By definitions,  $X := U^{-1}E_3$  or  $UX = E_3$ , that is:

$$\begin{array}{c} r \\ u \\ u \end{array} \begin{bmatrix} D_1 & B_1 & 0 \\ 0 & D_2 & B_2 \\ 0 & 0 & D_3 \end{bmatrix} \begin{array}{c} r \\ u \\ u \end{array} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \begin{array}{c} r \\ u \\ u \end{array} \begin{bmatrix} 0 \\ 0 \\ I \end{bmatrix}.$$

Using back-substitution to find  $X$  as following:

$$\begin{aligned} \left[ \begin{array}{c|c|c} 0 & 0 & D_3 \end{array} \right] \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} &= D_3 X_3 = I_{u \times u} & X_3 &= D_3^{-1} \\ \left[ \begin{array}{c|c|c} 0 & D_2 & B_2 \end{array} \right] \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} &= D_2 X_2 + B_2 X_3 = 0_{u \times u} & X_2 &= -D_2^{-1} B_2 X_3 = -D_2^{-1} B_2 D_3^{-1} \\ \left[ \begin{array}{c|c|c} D_1 & B_1 & 0 \end{array} \right] \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} &= D_1 X_1 + B_1 X_2 = 0_{r \times u} & X_1 &= -D_1^{-1} B_1 X_2 = D_1^{-1} B_1 D_2^{-1} B_2 D_3^{-1} \end{aligned}$$

Following the definition of  $Y_i^T$ ,

$$\begin{aligned} Y_3^T &= (D_3 X_3)^{-1} = X_3^{-1} D_3^{-1} = D_3 D_3^{-1} = I_{u \times u} \\ Y_2^T &= (D_2 X_2)^{-1} = X_2^{-1} D_2^{-1} = -D_3 B_2^{-1} D_2 D_2^{-1} = -D_3 B_2^{-1} \\ Y_1^T &= (D_1 X_1)^+ = X_1^+ D_1^+ \end{aligned}$$



Note that  $X_3$  and  $Y_3^T$  are upper triangular matrices, then  $\text{triu}(X_3 Y_3^T) = X_3 Y_3^T$ .

$$\begin{aligned}
U \text{triu}(XY^T) &= \begin{bmatrix} D_1 & B_1 & 0 \\ 0 & D_2 & B_2 \\ 0 & 0 & D_3 \end{bmatrix} \left[ \begin{array}{c|c|c} \text{triu}(X_1 Y_1^T) & X_1 Y_2^T & X_1 Y_3^T \\ 0 & \text{triu}(X_2 Y_2^T) & X_2 Y_3^T \\ 0 & 0 & X_3 Y_3^T \end{array} \right] \\
&= \begin{bmatrix} D_1 & B_1 & 0 \\ 0 & D_2 & B_2 \\ 0 & 0 & D_3 \end{bmatrix} \left[ \begin{array}{c|c|c} \text{triu}(D_1^+) & -D_1^{-1} B_1 D_2^{-1} & D_1^{-1} B_1 D_2^{-1} B_2 D_3^{-1} \\ 0 & \text{triu}(D_2^{-1}) & -D_2^{-1} B_2 D_3^{-1} \\ 0 & 0 & D_3^{-1} \end{array} \right] \\
&= \begin{bmatrix} D_1 & B_1 & 0 \\ 0 & D_2 & B_2 \\ 0 & 0 & D_3 \end{bmatrix} \left[ \begin{array}{c|c|c} D_1^{-1} & -D_1^{-1} B_1 D_2^{-1} & D_1^{-1} B_1 D_2^{-1} B_2 D_3^{-1} \\ 0 & D_2^{-1} & -D_2^{-1} B_2 D_3^{-1} \\ 0 & 0 & D_3^{-1} \end{array} \right] \\
&= \begin{bmatrix} D_1 D_1^{-1} & -B_1 D_2^{-1} + B_1 D_2^{-1} & B_1 D_2^{-1} B_2 D_3^{-1} - B_1 D_2^{-1} B_2 D_3^{-1} \\ 0 & D_2 D_2^{-1} & -B_2 D_3^{-1} + B_2 D_3^{-1} \\ 0 & 0 & D_3 D_3^{-1} \end{bmatrix} \\
&= \begin{bmatrix} I_{r \times r} & 0 & 0 \\ 0 & I_{u \times u} & 0 \\ 0 & 0 & I_{u \times u} \end{bmatrix} \\
&= I_{n \times n}
\end{aligned}$$

## 2.4 Content

Consider an upper banded matrix  $U \in \mathbb{R}^{n \times n}$ ,

$$U = \begin{bmatrix} \alpha_1 & \beta_1^1 & \beta_1^2 & \dots & \beta_1^u & & \\ & \alpha_2 & \beta_2^1 & \beta_2^2 & \dots & \beta_2^u & \\ & & \ddots & \ddots & \ddots & \ddots & \\ & & & & & \beta_{n-u}^u & \\ & & & & & \vdots & \\ & & & & & \beta_{n-2}^2 & \\ & & & & & \beta_{n-1}^1 & \\ & & & & & & \alpha_n \end{bmatrix}. \quad (1)$$

Then try to show that its inverse can be represented as the upper triangular part of an outer product, *i.e.*,

$$U^{-1} = \text{triu}(XY^T) \quad (2)$$

Let  $X, Y \in \mathbb{R}^{n \times u}$ , consider the following cases of  $n$ ,

### Case 1, $n = ku$

then (1) can be represented as a block upper bidiagonal matrix,

$$U = \begin{bmatrix} \xrightarrow{u} & \xrightarrow{u} & \dots & \xrightarrow{u} \\ \begin{matrix} \alpha_1 & \dots & \beta_1^{u-1} \\ & \ddots & \vdots \\ & & \alpha_u \end{matrix} & \begin{matrix} \beta_1^u \\ \vdots \\ \beta_u^1 \end{matrix} & & \\ & \begin{matrix} \alpha_{u+1} & \dots & \beta_{u+1}^{u-1} \\ & \ddots & \vdots \\ & & \alpha_{2u} \end{matrix} & \begin{matrix} \beta_{u+1}^u \\ \vdots \\ \beta_{2u}^1 \end{matrix} & & \\ & & \ddots & & & \\ & & & \ddots & & \\ & & & & \begin{matrix} \alpha_{(k-1)u+1} & \dots & \beta_{(k-1)u+1}^{u-1} \\ & \ddots & \vdots \\ & & \alpha_{ku} \end{matrix} \end{bmatrix}$$

$$= \begin{bmatrix} D_1 & B_1 & & & \\ & D_2 & B_2 & & \\ & & \ddots & \ddots & \\ & & & D_{k-1} & B_{k-1} \\ & & & & D_k \end{bmatrix} \in \mathbb{R}^{ku \times ku}, D_i, B_i \in \mathbb{R}^{u \times u} \text{ for } i = 1, 2, \dots, k. \quad (3)$$

Represent the  $n$ -dimensional identity matrix  $I_{n \times n}$  in block form,

$$I_{n \times n} = I_{ku \times ku} = \text{diag}(\underbrace{I_{u \times u}, I_{u \times u}, \dots, I_{u \times u}}_k) = [E_1 \mid E_2 \mid \dots \mid E_k].$$

then, its block columns  $E_i$  for  $i = 1, 2, \dots, k$  satisfies

$$E_i \in \mathbb{R}^{ku \times u}$$

$$E_i^T E_j = \begin{cases} I_{u \times u}, & \text{if } i = j; \\ 0_{u \times u}, & \text{otherwise.} \end{cases}$$

To find  $X$  and  $Y$  such that (2) holds, let

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_{k-1} \\ X_k \end{bmatrix} \in \mathbb{R}^{ku \times u}, Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_{k-1} \\ Y_k \end{bmatrix} \in \mathbb{R}^{ku \times u}, X_i, Y_i \in \mathbb{R}^{u \times u} \text{ for } i = 1, 2, \dots, k,$$

and let  $X_k$  and  $Y_k^T$  be upper triangular matrix, then  $\text{triu}(X_k Y_k^T) = X_k Y_k^T$ .  
For the outer product form,

$$\begin{aligned} Y^T &= [Y_1^T \mid Y_2^T \mid \dots \mid Y_{k-1}^T \mid Y_k^T] \in \mathbb{R}^{u \times ku} \\ XY^T &= \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_{k-1} \\ X_k \end{bmatrix} [Y_1^T \mid Y_2^T \mid \dots \mid Y_{k-1}^T \mid Y_k^T] \\ &= \begin{bmatrix} X_1 Y_1^T & X_1 Y_2^T & \dots & X_1 Y_{k-1}^T & X_1 Y_k^T \\ X_2 Y_1^T & X_2 Y_2^T & \dots & X_2 Y_{k-1}^T & X_2 Y_k^T \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ X_{k-1} Y_1^T & X_{k-1} Y_2^T & \dots & X_{k-1} Y_{k-1}^T & X_{k-1} Y_k^T \\ X_k Y_1^T & X_k Y_2^T & \dots & X_k Y_{k-1}^T & X_k Y_k^T \end{bmatrix} \\ &= X [Y_1^T \mid Y_2^T \mid \dots \mid Y_{k-1}^T \mid Y_k^T] \\ &= [XY_1^T \mid XY_2^T \mid \dots \mid XY_{k-1}^T \mid XY_k^T] \in \mathbb{R}^{ku \times ku}, \end{aligned}$$

and its the upper triangular component,

$$\begin{aligned} \text{triu}(XY^T) &= \begin{bmatrix} \text{triu}(X_1 Y_1^T) & X_1 Y_2^T & \dots & X_1 Y_{k-1}^T & X_1 Y_k^T \\ 0_{u \times u} & \text{triu}(X_2 Y_2^T) & \dots & X_2 Y_{k-1}^T & X_2 Y_k^T \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0_{u \times u} & 0_{u \times u} & \dots & \text{triu}(X_{k-1} Y_{k-1}^T) & X_{k-1} Y_k^T \\ 0_{u \times u} & 0_{u \times u} & \dots & 0_{u \times u} & X_k Y_k^T \end{bmatrix} \\ &= \begin{bmatrix} \text{triu}(X_1 Y_1^T) & X_1 Y_2^T & \dots & X_{1:k-2} Y_{k-1}^T & X_1 Y_k^T \\ 0_{(k-2)u \times u} & \text{triu}(X_2 Y_2^T) & \dots & \text{triu}(X_{k-1} Y_{k-1}^T) & X_2 Y_k^T \\ 0_{u \times u} & 0_{(k-2)u \times u} & \dots & 0_{u \times u} & X_k Y_k^T \end{bmatrix}. \end{aligned} \quad (4)$$

From (2),

$$I_{n \times n} = U \text{triu}(XY^T). \quad (5)$$

For  $X$  and  $Y_k$ , from (4), the  $k$ -th block column of (5) can be written as,

$$\begin{aligned}
E_k &= U \operatorname{triu}(XY^T)E_k \\
E_k &= UXY_k^T
\end{aligned} \tag{6}$$

Define that

$$X := U^{-1}E_k; \tag{7}$$

$$Y_k^T := I_{u \times u}, \tag{8}$$

which can be shown that (6) holds for the defined (7) and (8) through

$$\begin{aligned}
UXY_k^T &= UU^{-1}E_k I_{u \times u} \\
&= I_{n \times n} E_k I_{u \times u} \\
&= E_k I_{u \times u} \\
&= E_k, \text{ as required.}
\end{aligned}$$

Then, for  $Y_{k-1}$ , forming the  $(k-1)$ -th block column of (5) from (4) first,

$$\begin{aligned}
E_{k-1} &= U \operatorname{triu}(XY^T)E_{k-1} \\
&= U \begin{bmatrix} X_{1:k-2}Y_{k-1}^T \\ \operatorname{triu}(X_{k-1}Y_{k-1}^T) \\ 0_{u \times u} \end{bmatrix}.
\end{aligned}$$

Focusing on the  $(k-1)$ -th block row of  $(k-1)$ -th block column,

$$\begin{aligned}
E_{k-1}^T E_{k-1} &= E_{k-1}^T U \begin{bmatrix} X_{1:k-2}Y_{k-1}^T \\ \operatorname{triu}(X_{k-1}Y_{k-1}^T) \\ 0_{u \times u} \end{bmatrix} \\
I_{u \times u} &= \begin{bmatrix} 0_{u \times (k-2)u} & D_{k-1} & B_{k-1} \end{bmatrix} \begin{bmatrix} X_{1:k-2}Y_{k-1}^T \\ \frac{\operatorname{triu}(X_{k-1}Y_{k-1}^T)}{0_{u \times u}} \end{bmatrix} \\
I_{u \times u} &= D_{k-1} \operatorname{triu}(X_{k-1}Y_{k-1}^T).
\end{aligned} \tag{9}$$

Define that

$$Y_{k-1}^T := (D_{k-1}X_{k-1})^{-1}, \tag{10}$$

and notice that  $D_{k-1} \in \mathbb{R}^{u \times u}$  is a upper triangular, therefore

$$\begin{aligned}
D_{k-1} &= \operatorname{triu}(D_{k-1}); \\
D_{k-1}^{-1} &= \operatorname{triu}(D_{k-1}^{-1}).
\end{aligned} \tag{11}$$

With the fact (11), (9) holds for the defined (10) as,

$$\begin{aligned}
D_{k-1} \text{triu}(X_{k-1} Y_{k-1}^T) &= D_{k-1} \text{triu}(X_{k-1} (D_{k-1} X_{k-1})^{-1}) \\
&= D_{k-1} \text{triu}(X_{k-1} X_{k-1}^{-1} D_{k-1}^{-1}) \\
&= D_{k-1} \text{triu}(D_{k-1}^{-1}) \\
&= D_{k-1} D_{k-1}^{-1} \\
&= I_{u \times u}, \text{ as required.}
\end{aligned}$$

Similar ideas can be use to redefine  $Y_k^T$  in (8), from (7),

$$\begin{aligned}
E_k &= UX \\
E_k^T E_k &= E_k^T UX \\
I_{u \times u} &= E_k^T UX \\
&= \begin{bmatrix} 0_{u \times (k-1)u} & D_k \end{bmatrix} \begin{bmatrix} X_{1:k-1} \\ X_k \end{bmatrix} \\
&= D_k X_k \\
I_{u \times u} &= (D_k X_k)^{-1},
\end{aligned}$$

following that

$$\begin{aligned}
Y_k^T &:= I_{u \times u} \\
&:= (D_k X_k)^{-1}.
\end{aligned}$$

In summary, for  $U \in \mathbb{R}^{ku \times ku}$ , (2) holds the following definitions of  $X$  and  $Y$ :

$$\begin{aligned}
X &:= U^{-1} E_k \\
Y_i^T &:= (D_i X_i)^{-1}
\end{aligned}$$

### 3 Test

$$\left[ \begin{array}{cccccc} & \underbrace{b_1^1 \quad b_1^2 \quad \cdots \quad b_1^u}_{\text{bandwidth} = u} & & & & \\ d_1 & & & & & \\ & d_2 & b_2^2 & b_2^2 & \cdots & b_2^u \\ & & \ddots & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots & \ddots \\ & & & & \ddots & \ddots \\ & & & & & b_{n-u}^u \\ & & & & & \vdots \\ & & & & & b_{n-2}^2 \\ & & & & & b_{n-1}^1 \\ & & & & & d_n \end{array} \right]$$

The diagram shows a large square matrix partitioned into blocks. The diagonal blocks are labeled  $d_1, d_2, d_3, d_4, \dots, d_{2k-3}, d_{2k-2}, d_{2k-1}, d_{2k}$ . The off-diagonal blocks are labeled  $b_{i,j}^1$  and  $b_{i,j}^2$ . The blocks are arranged in a staircase pattern, with the diagonal blocks being square and the off-diagonal blocks being rectangular. The blocks are connected by dashed lines, indicating the partitioning of the matrix.

The diagram shows a sequence of points arranged in a grid-like pattern. The points are labeled as follows:

- $d_1$ ,  $b_1^{r-1}$ , ...,  $d_r$
- $b_1^r$ , ...,  $b_r^u$
- $b_{1+r}^1$ , ...,  $b_{1+r}^{u-1}$
- $d_{1+r}$ , ...,  $b_{u+r}^1$ , ...,  $b_{u+r}^u$
- $d_{u+r}$
- $d_{n-u+1}$ ,  $b_{n-u+1}^u$ , ...,  $d_n$

Horizontal arrows indicate distances  $r$  and  $u$ . Vertical arrows indicate distances  $r$  and  $u$ .

$$\begin{array}{c}
\begin{array}{c} \xleftarrow{u} \\ \hline \end{array} \\
\begin{array}{c} \xleftarrow{l} \\ \hline \end{array} \\
\left[ \begin{array}{ccccccc}
d_1 & b_1^1 & b_1^2 & \dots & b_1^u & & \\
b_1^{-1} & d_2 & & & & & \\
b_1^{-2} & & & & & & \\
\vdots & & & & & & \\
b_1^{-l} & & & & & & \\
& & & & & & b_{n-u}^u \\
& & & & & & \vdots \\
& & & & & & b_{n-2}^2 \\
& & & & & & b_{n-1}^1 \\
& & & & b_{n-l}^{-l} & \dots & b_{n-2}^{-2} & b_{n-1}^{-1} & d_n
\end{array} \right]
\end{array}$$

**Input** : An upper banded matrix  $U \in \mathbb{R}^{n \times n}$  and its bandwidth  $u$ .

**Output**: Its inverse  $U^{-1}$  and  $X, Y \in \mathbb{R}^{n \times u}$  such that  $U^{-1} = \text{triu}(XY^T)$ .

```

1 // n = ku + r where 0 <= r < u
2 k ← quotient of n divided by u ;                               // floor(n/u)
3 r ← remainder of n divided by u ;                               // rem(n,u)
4  $E_k \leftarrow$  last block column of  $I_{n \times n}$  ;                   // one(U)[:, n-u+1:n]
5  $X \leftarrow \text{BackSubstitution}(U, E_k)$ 
6 for i ← k to 1 do
7    $D_i \leftarrow$  i-th diagonal block of U ;                       // U[(i-1)*u+r+1:i*u+r, (i-1)*u+r+1:i*u+r]
8    $X_i \leftarrow$  i-th block of X ;                                 // X[(i-1)*u+r+1:i*u+r, :]
9    $Y_i^T \leftarrow (D_i X_i)^{-1}$ , i-th block of  $Y^T$  ;           // Yt[:, (i-1)*u+r+1:i*u+r]
10 end
11 if r = 0 then return  $U^{-1} := \text{triu}(XY^T)$ , X, Y
12 else need find  $Y_0^T$  using Moore-Penrose right inverse
13    $D_0 \in \mathbb{R}^{r \times r} \leftarrow$  first diagonal block of U ;       // U[1:r, 1:r]
14    $X_0 \in \mathbb{R}^{r \times u} \leftarrow$  first block of X ;               // X[1:r, :]
15    $Y_0^T \in \mathbb{R}^{u \times r} \leftarrow (D_0 X_0)^+ = (D_0 X_0)^T (D_0 X_0 (D_0 X_0)^T)^{-1}$ , first block of  $Y^T$ 
16 end
17 return  $U^{-1} := \text{triu}(XY^T)$ , X, Y

```

**Algorithm 1:** Inverse of banded matrix in outer product form