Imperial College London

MSc Individual Project

Imperial College London

Department of Mathematics

Preliminary Report

Author:
Zhiwei Zhou

Supervisor:
Dr.Sheehan Olver

July 1, 2022

Chapter 1

Background

1.1 Notation

This report uses Householder notation as following:

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

.

Matrix & Vector

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

Block Matrix & Block Vector

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

Banded Matrix

$$
B = \begin{bmatrix}
\alpha_1 & \beta_1^1 & \beta_1^2 & \cdots & \beta_1^u & & & \\
\beta_1^{-1} & \alpha_2 & \ddots & & & \ddots & & \\
\beta_1^{-2} & \ddots & \ddots & \ddots & & & \ddots & \\
\vdots & & \ddots & & & & & \beta_{n-u}^u \\
\beta_1^{-l} & & & \ddots & & & & \vdots \\
 & \ddots & & & \ddots & & & \beta_{n-2}^2 \\
 & & \ddots & & & \ddots & & \beta_{n-1}^1 \\
 & & & \beta_{n-l}^{-l} & \cdots & \beta_{n-2}^{-2} & \beta_{n-1}^{-1} & \alpha_n
\end{bmatrix},
$$

where $\beta_j^{\pm i}$ is the j-th element on the i-th upper/lower band.

triu($\boldsymbol{A}$)

$$
A = \begin{array}{c}
\begin{array}{ccccc} \phantom{\alpha_{11}} & \overset{2}{\downarrow} & \phantom{\alpha_{1,3}} & \phantom{\alpha_{1,4}} & \phantom{\alpha_{1,5}} \end{array} \\
\begin{bmatrix}
\alpha_{11} & \alpha_{1,2} & \alpha_{1,3} & \alpha_{1,4} & \alpha_{1,5} \\
\alpha_{21} & \alpha_{2,2} & \alpha_{2,3} & \alpha_{2,4} & \alpha_{2,5} \\
\alpha_{31} & \alpha_{3,2} & \alpha_{3,3} & \alpha_{3,4} & \alpha_{3,5} \\
\alpha_{41} & \alpha_{4,2} & \alpha_{4,3} & \alpha_{4,4} & \alpha_{4,5}
\end{bmatrix}
\end{array}
$$

$$
\text{triu}(A, 2) = \begin{array}{c}
\begin{array}{ccccc} & \overset{2}{\downarrow} & \phantom{\alpha_{1,3}} & \phantom{\alpha_{1,4}} & \phantom{\alpha_{1,5}} \end{array} \\
\begin{bmatrix}
0 & 0 & \alpha_{1,3} & \alpha_{1,4} & \alpha_{1,5} \\
0 & 0 & 0 & \alpha_{2,4} & \alpha_{2,5} \\
0 & 0 & 0 & 0 & \alpha_{3,5} \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\end{array}
$$

Chapter 2

Inverse of Upper Banded Matrix

2.1 Task

Given an upper banded matrix U, find X and Y such that $U^{-1} = \mathrm{triu}(XY^{\mathrm{T}})$

2.2 Algorithm

For $U \in \mathbb{R}^{n\times n}$ with banded width u,
if $n = ku$, then

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

otherwise $n = ku + r$, and

$$\begin{aligned} X &\coloneqq U^{-1}E_k; \\ Y_i^{\mathrm{T}} &\coloneqq (D_i X_i)^{-1} \text{ for } i = 1, 2, \ldots, k; \\ \tilde{Y_0}^{\mathrm{T}} &\coloneqq (\tilde{D_0}\tilde{X_0})^{+} = (\tilde{D_0}\tilde{X_0})^{\mathrm{T}}(\tilde{D_0}\tilde{X_0}(\tilde{D_0}\tilde{X_0})^{\mathrm{T}})^{-1}. \end{aligned}$$

2.2.1 Pseudocode

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

`// n = ku + r where 0 <= r < u`
$k \leftarrow$ quotient of n divided by u ; `// floor(n/u)`
$r \leftarrow$ remainder of n divided by u ; `// rem(n,u)`
$E_k \leftarrow$ last block column of $I_{n\times n}$; `// one(U)[:, n-u+1:n]`
$X \leftarrow$ `BackSubstitution`$(U,\ E_k)$
for $i \leftarrow k$ **to** 1 **do**
    $D_i \leftarrow$ i-th diagonal block of U ; `// U[(i-1)*u+r+1:i*u+r, (i-1)*u+r+1:i*u+r]`
    $X_i \leftarrow$ i-th block of X ; `// X[(i-1)*u+r+1:i*u+r, :]`
    $Y_i^{\mathrm{T}} \leftarrow (D_i X_i)^{-1}$, i-th block of Y^{T} ; `// Yt[:,(i-1)*u+r+1:i*u+r]`
end
if $r = 0$ **then return** $U^{-1} := \mathrm{triu}(XY^{\mathrm{T}})$, X, Y
else need find $\tilde{Y}_0^{\mathrm{T}}$ using Moore-Penrose right inverse
    $\tilde{D}_0 \in \mathbb{R}^{r\times r} \leftarrow$ first diagonal block of U ; `// U[1:r, 1:r]`
    $\tilde{X}_0 \in \mathbb{R}^{r\times u} \leftarrow$ first block of X ; `// X[1:r, :]`
    $\tilde{Y}_0^{\mathrm{T}} \in \mathbb{R}^{u\times r} \leftarrow (\tilde{D}_0\tilde{X}_0)^{+} = (\tilde{D}_0\tilde{X}_0)^{\mathrm{T}}(\tilde{D}_0\tilde{X}_0(\tilde{D}_0\tilde{X}_0)^{\mathrm{T}})^{-1}$, first block of Y^{T}
end
return $U^{-1} := \mathrm{triu}(XY^{\mathrm{T}})$, X, Y

Algorithm 1: Inverse of banded matrix in outer product form

2.2.2 Example

Let $U \in \mathbb{R}^{n\times n}$ and $n = 2u + r$, *i.e.*, $k = 2$,

$$U = \begin{bmatrix} \tilde{D}_0 & \tilde{B}_0 & \\ & D_1 & B_1 \\ & & D_2 \end{bmatrix} \in \mathbb{R}^{(2u+r)\times(2u+r)}$$

where $\tilde{D}_0 \in \mathbb{R}^{r\times r}$, $\tilde{B}_0 \in \mathbb{R}^{r\times u}$, and D_1, B_1, D_2, B_2, $\in \mathbb{R}^{u\times u}$.
By definitions, $X := U^{-1}E_2$ with $I = \left[\begin{array}{c|c|c} \tilde{E}_0 & E_1 & E_2 \end{array}\right]$, that is:

$$UX = E_2$$

$$\begin{array}{c} \\ r \\ u \\ u \end{array}\begin{array}{c} \begin{array}{ccc} r & u & u \end{array} \\ \left[\begin{array}{ccc} \tilde{D}_0 & \tilde{B}_0 & 0 \\ \hline 0 & D_1 & B_1 \\ \hline 0 & 0 & D_2 \end{array}\right] \end{array} \begin{array}{c} \\ r \\ u \\ u \end{array}\begin{array}{c} u \\ \left[\begin{array}{c} \tilde{X}_0 \\ X_1 \\ X_2 \end{array}\right] \end{array} = \begin{array}{c} \\ r \\ u \\ u \end{array}\begin{array}{c} u \\ \left[\begin{array}{c} 0 \\ 0 \\ I \end{array}\right] \end{array}.$$

Using back-subsitution to find X as following:

$$\left[\begin{array}{c|c|c} 0 & 0 & D_2 \end{array}\right] \left[\begin{array}{c} \tilde{X}_0 \\ \hline X_1 \\ \hline X_2 \end{array}\right] = D_2X_2 = I_{u\times u} \qquad X_2 = D_2^{-1}$$

$$\left[\begin{array}{c|c|c} 0 & D_1 & B_1 \end{array}\right] \left[\begin{array}{c} \tilde{X}_0 \\ \hline X_1 \\ \hline X_2 \end{array}\right] = D_1X_1 + B_1X_2 = 0_{u\times u} \quad X_1 = -D_1^{-1}B_1X_2 = -D_1^{-1}B_1D_2^{-1}$$

$$\left[\begin{array}{c|c|c} \tilde{D}_0 & \tilde{B}_0 & 0 \end{array}\right] \left[\begin{array}{c} \tilde{X}_0 \\ \hline X_1 \\ \hline X_2 \end{array}\right] = \tilde{D}_0\tilde{X}_0 + \tilde{B}_0X_1 = 0_{r\times u} \quad \tilde{X}_0 = -\tilde{D}_0^{-1}\tilde{B}_0X_1 = \tilde{D}_0^{-1}\tilde{B}_0D_1^{-1}B_1D_2^{-1}$$

Following the definition of Y_i^{T},

$$
\begin{aligned}
Y_2^{\mathrm{T}} &= (D_2X_2)^{-1} = X_2^{-1}D_2^{-1} = D_2D_2^{-1} = I_{u\times u} \\
Y_1^{\mathrm{T}} &= (D_1X_1)^{-1} = X_1^{-1}D_1^{-1} = -D_2B_1^{-1}D_1D_1^{-1} = -D_2B_1^{-1} \\
\tilde{Y}_0^{\mathrm{T}} &= (\tilde{D}_0\tilde{X}_0)^{+} = \tilde{X}_0^{+}\tilde{D}_0^{+}
\end{aligned}
$$

Note that X_2 and Y_2^{T} are upper triangular matrices, then $\mathrm{triu}(X_2Y_2^{\mathrm{T}}) = X_2Y_2^{\mathrm{T}}$.

$$
\begin{aligned}
U\,\mathrm{triu}(XY^{\mathrm{T}}) &= \left[\begin{array}{ccc} \tilde{D}_0 & \tilde{B}_0 & 0 \\ \hline 0 & D_1 & B_1 \\ \hline 0 & 0 & D_2 \end{array}\right]\left[\begin{array}{c|c|c} \mathrm{triu}(\tilde{X}_0\tilde{Y}_0^{\mathrm{T}}) & \tilde{X}_0Y_1^{\mathrm{T}} & \tilde{X}_0Y_2^{\mathrm{T}} \\ 0 & \mathrm{triu}(X_1Y_1^{\mathrm{T}}) & X_1Y_2^{\mathrm{T}} \\ 0 & 0 & X_2Y_2^{\mathrm{T}} \end{array}\right] \\
&= \left[\begin{array}{ccc} \tilde{D}_0 & \tilde{B}_0 & 0 \\ \hline 0 & D_1 & B_1 \\ \hline 0 & 0 & D_2 \end{array}\right]\left[\begin{array}{c|c|c} \mathrm{triu}(\tilde{D}_0^{+}) & -\tilde{D}_0^{-1}\tilde{D}_0D_1^{-1} & \tilde{D}_0{}^{-1}\tilde{B}_0D_1^{-1}B_1D_2^{-1} \\ 0 & \mathrm{triu}(D_1^{-1}) & -D_1^{-1}B_1D_2^{-1} \\ 0 & 0 & D_2^{-1} \end{array}\right] \\
&= \left[\begin{array}{ccc} \tilde{D}_0 & \tilde{B}_0 & 0 \\ \hline 0 & D_1 & B_1 \\ \hline 0 & 0 & D_2 \end{array}\right]\left[\begin{array}{c|c|c} \tilde{D}_0^{-1} & -\tilde{D}_0^{-1}\tilde{D}_0D_1^{-1} & \tilde{D}_0{}^{-1}\tilde{B}_0D_1^{-1}B_1D_2^{-1} \\ 0 & D_1^{-1} & -D_1^{-1}B_1D_2^{-1} \\ 0 & 0 & D_2^{-1} \end{array}\right] \\
&= \left[\begin{array}{c|c|c} \tilde{D}_0\tilde{D}_0^{-1} & -\tilde{B}_0D_1^{-1} + \tilde{B}_0D_1^{-1} & \tilde{B}_0D_1^{-1}B_1D_2^{-1} - \tilde{B}_0D_1^{-1}B_1D_2^{-1} \\ 0 & D_1D_1^{-1} & -B_1D_2^{-1} + B_1D_2^{-1} \\ 0 & 0 & D_2D_2^{-1} \end{array}\right] \\
&= \left[\begin{array}{c|c|c} I_{r\times r} & 0 & 0 \\ 0 & I_{u\times u} & 0 \\ 0 & 0 & I_{u\times u} \end{array}\right] \\
&= I_{n\times n}
\end{aligned}
$$

2.3 Derivation

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

$$
U = \begin{bmatrix} \alpha_1 & \beta_1^1 & \beta_1^2 & \cdots & \beta_1^u & & & \\ & \alpha_2 & \beta_2^1 & \beta_2^2 & \cdots & \beta_2^u & & \\ & & \ddots & \ddots & & \ddots & \ddots & \\ & & & & & & & \beta_{n-u}^u \\ & & & & \ddots & \ddots & & \vdots \\ & & & & & & & \beta_{n-2}^2 \\ & & & & & & & \beta_{n-1}^1 \\ & & & & & & & \alpha_n \end{bmatrix}. \tag{2.1}
$$

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

$$
U^{-1} = \mathrm{triu}(XY^{\mathrm{T}}) \tag{2.2}
$$

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

Case 1, $n = ku$

then (2.1) can be repersent as a block upper bidiagonal matrix,

$$
\begin{array}{cc}
 & \begin{array}{cccc} \overset{u}{\longleftrightarrow} & \overset{u}{\longleftrightarrow} & \cdots\cdots & \overset{u}{\longleftrightarrow} \end{array} \\
U = \begin{array}{c} u\updownarrow \\ u\updownarrow \\ \vdots \\ u\updownarrow \end{array} &
\left[\begin{array}{cccccccccc}
\alpha_1 & \cdots & \beta_1^{u-1} & \beta_1^{u} & & & & & & \\
 & \ddots & \vdots & \vdots & \ddots & & & & & \\
 & & \alpha_u & \beta_u^{1} & \cdots & \beta_u^{u} & & & & \\
 & & & \alpha_{u+1} & \cdots & \beta_{u+1}^{u-1} & \beta_{u+1}^{u} & & & \\
 & & & & \ddots & \vdots & \vdots & \ddots & & \\
 & & & & & \alpha_{2u} & \beta_{2u}^{1} & \cdots & \beta_{2u}^{u} & \\
 & & & & & & \ddots & \ddots & \ddots & \ddots \\
 & & & & & & & \alpha_{(k-1)u+1} & \cdots & \beta_{(k-1)u+1}^{u-1} \\
 & & & & & & & & \ddots & \vdots \\
 & & & & & & & & & \alpha_{ku}
\end{array}\right]
\end{array}
$$

$$
= \begin{bmatrix} D_1 & B_1 & & & \\ & D_2 & B_2 & & \\ & & \ddots & \ddots & \\ & & & D_{k-1} & B_{k-1} \\ & & & & D_k \end{bmatrix} \in \mathbb{R}^{ku\times ku},\ D_i,\ B_i \in \mathbb{R}^{u\times u} \text{ for } i = 1,\, 2,\, \ldots,\, k. \tag{2.3}
$$

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

$$
I_{n\times n} = I_{ku\times ku} = \mathrm{diag}(\underbrace{I_{u\times u},\ I_{u\times u},\ \cdots,\ I_{u\times u}}_{k}) = \left[\begin{array}{c|c|c|c} E_1 & E_2 & \cdots & E_k \end{array}\right].
$$

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

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

To find X and Y such that (2.2) holds, let

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

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

$$
\begin{aligned}
Y^{\mathrm{T}} &= \left[\begin{array}{c|c|c|c|c} Y_1^{\mathrm{T}} & Y_2^{\mathrm{T}} & \cdots & Y_{k-1}^{\mathrm{T}} & Y_k^{\mathrm{T}} \end{array}\right] \in \mathbb{R}^{u\times ku} \\
XY^{\mathrm{T}} &= \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_{k-1} \\ X_k \end{bmatrix} \left[\begin{array}{c|c|c|c|c} Y_1^{\mathrm{T}} & Y_2^{\mathrm{T}} & \cdots & Y_{k-1}^{\mathrm{T}} & Y_k^{\mathrm{T}} \end{array}\right] \\
&= \left[\begin{array}{c|c|c|c|c} X_1Y_1^{\mathrm{T}} & X_1Y_2^{\mathrm{T}} & \cdots & X_1Y_{k-1}^{\mathrm{T}} & x_1Y_k^{\mathrm{T}} \\ X_2Y_1^{\mathrm{T}} & X_2Y_2^{\mathrm{T}} & \cdots & X_2Y_{k-1}^{\mathrm{T}} & x_2Y_k^{\mathrm{T}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ X_{k-1}Y_1^{\mathrm{T}} & X_{k-1}Y_2^{\mathrm{T}} & \cdots & X_{k-1}Y_{k-1}^{\mathrm{T}} & X_{k-1}Y_k^{\mathrm{T}} \\ X_kY_1^{\mathrm{T}} & X_kY_2^{\mathrm{T}} & \cdots & X_kY_{k-1}^{\mathrm{T}} & X_kY_k^{\mathrm{T}} \end{array}\right] \\
&= X\left[\begin{array}{c|c|c|c|c} Y_1^{\mathrm{T}} & Y_2^{\mathrm{T}} & \cdots & Y_{k-1}^{\mathrm{T}} & Y_k^{\mathrm{T}} \end{array}\right] \\
&= \left[\begin{array}{c|c|c|c|c} XY_1^{\mathrm{T}} & XY_2^{\mathrm{T}} & \cdots & XY_{k-1}^{\mathrm{T}} & XY_k^{\mathrm{T}} \end{array}\right] \in \mathbb{R}^{ku\times ku},
\end{aligned}
$$

and its the upper triangular componnent,

$$
\begin{aligned}
\operatorname{triu}(XY^{\mathrm{T}}) &= \left[\begin{array}{c|c|c|c|c} \operatorname{triu}(X_1Y_1^{\mathrm{T}}) & X_1Y_2^{\mathrm{T}} & \cdots & X_1Y_{k-1}^{\mathrm{T}} & X_1Y_k^{\mathrm{T}} \\ 0_{u\times u} & \operatorname{triu}(X_2Y_2^{\mathrm{T}}) & \cdots & X_2Y_{k-1}^{\mathrm{T}} & X_2Y_k^{\mathrm{T}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0_{u\times u} & 0_{u\times u} & \cdots & \operatorname{triu}(X_{k-1}Y_{k-1}^{\mathrm{T}}) & X_{k-1}Y_k^{\mathrm{T}} \\ 0_{u\times u} & 0_{u\times u} & \cdots & 0_{u\times u} & X_kY_k^{\mathrm{T}} \end{array}\right] \\
&= \left[\begin{array}{c|c|c|c|c} \operatorname{triu}(X_1Y_1^{\mathrm{T}}) & X_1Y_2^{\mathrm{T}} & & X_{1:k-2}Y_{k-1}^{\mathrm{T}} & \\ 0_{(k-2)u\times u} & \operatorname{triu}(X_2Y_2^{\mathrm{T}}) & \cdots & \operatorname{triu}(X_{k-1}Y_{k-1}^{\mathrm{T}}) & XY_k^{\mathrm{T}} \\ 0_{u\times u} & 0_{(k-2)u\times u} & & 0_{u\times u} & \end{array}\right].
\end{aligned} \tag{2.4}
$$

From (2.2),

$$
I_{n\times n} = U \operatorname{triu}(XY^{\mathrm{T}}). \tag{2.5}
$$

For X and Y_k, from (2.4), the k-th block column of (2.5) can be written as,

$$
\begin{aligned}
E_k &= U \operatorname{triu}(XY^{\mathrm{T}})E_k \\
E_k &= UXY_k^{\mathrm{T}}
\end{aligned} \tag{2.6}
$$

Define that

$$
X := U^{-1}E_k; \tag{2.7}
$$

$$
Y_k^{\mathrm{T}} := I_{u\times u}, \tag{2.8}
$$

which can be shown that (2.6) holds for the defined (2.7) and (2.8) through

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

Then, for Y_{k-1}, forming the $(k-1)$-th block column of (2.5) from (2.4) first,

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

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

$$\begin{aligned} E_{k-1}^{\mathrm{T}}E_{k-1} &= E_{k-1}^{\mathrm{T}}U \begin{bmatrix} X_{1:k-2}Y_{k-1}^{\mathrm{T}} \\ \mathrm{triu}(X_{k-1}Y_{k-1}^{\mathrm{T}}) \\ 0_{u\times u} \end{bmatrix} \\ I_{u\times u} &= \left[\begin{array}{c|c|c} 0_{u\times(k-2)u} & D_{k-1} & B_{k-1} \end{array}\right] \left[\begin{array}{c} X_{1:k-2}Y_{k-1}^{\mathrm{T}} \\ \hline \mathrm{triu}(X_{k-1}Y_{k-1}^{\mathrm{T}}) \\ \hline 0_{u\times u} \end{array}\right] \\ I_{u\times u} &= D_{k-1}\,\mathrm{triu}(X_{k-1}Y_{k-1}^{\mathrm{T}}). \end{aligned} \tag{2.9}$$

Define that

$$Y_{k-1}^{\mathrm{T}} \coloneqq (D_{k-1}X_{k-1})^{-1}, \tag{2.10}$$

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

$$\begin{aligned} D_{k-1} &= \mathrm{triu}(D_{k-1}); \\ D_{k-1}^{-1} &= \mathrm{triu}(D_{k-1}^{-1}). \end{aligned} \tag{2.11}$$

With the fact (2.11), (2.9) holds for the defined (2.10) as,

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

Similar ideas can be use to redefine Y_k^{T} in (2.8), from (2.7),

$$\begin{aligned} E_k &= UX \\ E_k^{\mathrm{T}}E_k &= E_k^{\mathrm{T}}UX \\ I_{u\times u} &= E_k^{\mathrm{T}}UX \\ &= \left[\begin{array}{c|c} 0_{u\times(k-1)u} & D_k \end{array}\right] \left[\begin{array}{c} X_{1:k-1} \\ \hline X_k \end{array}\right] \\ &= D_kX_k \\ I_{u\times u} &= (D_kX_k)^{-1}, \end{aligned}$$

following that

$$\begin{aligned} Y_k^{\mathrm{T}} &\coloneqq I_{u\times u} \\ &\coloneqq (D_kX_k)^{-1}. \end{aligned}$$

In summary, for $U \in \mathbb{R}^{ku\times ku}$, (2.2) holds the following definitions of X and Y:

$$\begin{aligned} X &\coloneqq U^{-1}E_k \\ Y_i^{\mathrm{T}} &\coloneqq (D_iX_i)^{-1} \end{aligned} \tag{2.12}$$

Case 2, $n = ku + r$

In this case, (2.1) can still be repersent as a block upper bidiagonal matrix,

$$
U = \begin{bmatrix}
d_1 & \cdots & b_1^{r-1} & b_1^{r} & \cdots & b_1^{u} & & & & & & \\
 & \ddots & \vdots & \vdots & & \ddots & & & & & & \\
 & & d_r & b_r^{1} & \cdots & b_r^{u} & & & & & & \\
 & & & d_{1+r} & \cdots & b_{1+r}^{u-1} & b_{r+1}^{u} & & & & & \\
 & & & & \ddots & \vdots & \vdots & \ddots & & & & \\
 & & & & & d_{u+r} & b_{u+r}^{1} & \cdots & b_{u+r}^{u} & & & \\
 & & & & & & & \ddots & & \ddots & & \\
 & & & & & & & & & d_{n-u+1} & \cdots & b_{n-u+1}^{u} \\
 & & & & & & & & & & \ddots & \vdots \\
 & & & & & & & & & & & d_n
\end{bmatrix}
$$

$$
= \begin{bmatrix}
\tilde{D}_0 & \tilde{B}_0 & & & \\
 & D_1 & B_1 & & \\
 & & \ddots & \ddots & \\
 & & & D_{k-1} & B_{k-1} \\
 & & & & D_k
\end{bmatrix} \in \mathbb{R}^{(ku+r)\times(ku+r)},
$$

where $\tilde{D}_0 \in \mathbb{R}^{r\times r}$, $\tilde{B}_0 \in \mathbb{R}^{r\times u}$, D_i, $B_i \in \mathbb{R}^{u\times u}$ for $i = 1, 2, \ldots, k$.
Then the partitions of X, Y, and $I_{n\times n}$ changed as n cannot be divided by u,

$$
X = \begin{bmatrix} \tilde{X}_0 \\ X_1 \\ \vdots \\ X_k \end{bmatrix} \in \mathbb{R}^{(ku+r)\times u},\ Y = \begin{bmatrix} \tilde{Y}_0 \\ Y_1 \\ \vdots \\ Y_k \end{bmatrix} \in \mathbb{R}^{(ku+r)\times u},\ \tilde{X}_0, \tilde{Y}_0 \in \mathbb{R}^{r\times u},\ X_i, Y_i \in \mathbb{R}^{u\times u} \text{ for } i = 1, 2, \ldots, k,
$$

and

$$
I_{n\times n} = I_{(ku+r)\times(ku+r)} = \operatorname{diag}(I_{r\times r}, \underbrace{I_{u\times u}, \cdots, I_{u\times u}}_{k}) = \left[\ \tilde{E}_0 \ \middle|\ E_1 \ \middle|\ \cdots \ \middle|\ E_k \ \right].
$$

Following the above statement, (2.12) cannot be defined for case $i = 0$ as $\tilde{D}_0\tilde{X}_0$ is a rectangular matrix which cannot be invertible. However, this can be solved easily by the introduction of the Moore-Penrose as follows:

$$
\begin{aligned}
\tilde{Y}_0^{\mathrm{T}} &\coloneqq (\tilde{D}_0\tilde{X}_0)^{+} \\
&\coloneqq (\tilde{D}_0\tilde{X}_0)^{\mathrm{T}}(\tilde{D}_0\tilde{X}_0(\tilde{D}_0\tilde{X}_0)^{\mathrm{T}})^{-1} \\
\tilde{D}_0 \operatorname{triu}(\tilde{X}_0\tilde{Y}_0^{\mathrm{T}}) &= \tilde{D}_0 \operatorname{triu}(\tilde{X}_0(\tilde{D}_0\tilde{X}_0)^{+}) \\
&= \tilde{D}_0 \operatorname{triu}(\tilde{X}_0\tilde{X}_0^{+}\tilde{D}_0)^{+}) \\
&= \tilde{D}_0 \operatorname{triu}(\tilde{D}_0^{+}) \\
&= \tilde{D}_0 \operatorname{triu}(\tilde{D}_0^{-1}) \\
&= \tilde{D}_0\tilde{D}_0^{-1} \\
&= I_{r\times r}, \text{ as required.}
\end{aligned}
$$

In conclusion, X and Y can be defined as following,

$$
\begin{aligned}
X &\coloneqq U^{-1}E_k; \\
Y_i^{\mathrm{T}} &\coloneqq \begin{cases} (D_iX_i)^{-1} \text{ for } i = 1,\, 2,\, \ldots,\, k, & \text{if } n = ku \ ; \\ \begin{cases} (D_iX_i)^{-1} & \text{if } i = 1,\, 2,\, \ldots,\, k; \\ (\tilde{D}_0\tilde{X}_0)^{+} & \text{otherwise.} \end{cases} & \text{otherwise.} \end{cases}
\end{aligned}
$$

Chapter 3

Ongoing work

As the above algorithm has now been found to be unstable under `Float64` type, the current use of `BigFloat` type to avoid floating point overflow problems needs to be improved. There are currently two ideas for storing the numbers generated midway through the process to improve the floating point computing performance:

- **Idea 1:** Use the fact that there are infinity pairs of x and y and the difference between them are only a constant multiple, *i.e.,* let $\tilde{x}$, $\tilde{y}$, and $\tilde{c}$ such that

$$\begin{aligned} x &= \operatorname{diag}(c)\tilde{x} \text{ or } x_i = c_i\tilde{x}_i \\ y &= (\operatorname{diag}(c))^{-1}\tilde{y} \text{ or } y_j = c_j^{-1}\tilde{y}_j \\ \text{and, } U^{-1} &= \operatorname{triu}(xy^{\mathrm{T}}) \text{ holds.} \end{aligned}$$

  Then,

$$\begin{aligned} U^{-1} &= \operatorname{triu}(xy^{\mathrm{T}}) \\ e_i^{\mathrm{T}}U^{-1}e_j &= x_i y_j \\ &= c_i\tilde{x}_i c_j^{-1}\tilde{y}_j \\ &= \frac{c_i}{c_j}\tilde{x}_i\tilde{y}_j \end{aligned}$$

  which provides the operation of re-scaling for (possible) improving the floating point problem.

- **Idea 2:** Rewrite the x and y in exponential form, *i.e.,* let $\tilde{x}$, $\tilde{y}$, s^x, and s^y such that

$$\begin{aligned} x_i &= s_i^x e^{\tilde{x}_i} \text{ where } \tilde{x}_i = \log(|x_i|), s_i^x = sign(x_i) \\ y_j &= s_j^y e^{\tilde{y}_j} \text{ where } \tilde{y}_j = \log(|y_i|), s_j^y = sign(y_i) \end{aligned}$$

  using the factor that $\mathcal{O}(\log n)$ growth slower $\mathcal{O}(n)$ for (possible) improving the floating point problem.
  Starting form upper bidiagonal matrix as the back-substitution process for upper bidiagonal matrix does not involve addition and the multiplication operation can keep this exponential form intact as $x_i y_j = s_i^x s_j^y e^{\tilde{x}_i+\tilde{y}_j}$

The efficiency of the algorithm can also be tested, ref. [3, 6]

- Time complexity $(\underbrace{u\mathcal{O}(n)}_{X} + \underbrace{k\mathcal{O}(u^3)}_{Y} + \underbrace{0.5\mathcal{O}(n^2)}_{\operatorname{triu}(XY^{\mathrm{T}}})$

- Space complexity

- Benchmark test

- *etc.*

Chapter 4

Future work

- Fix the stability problem (if possible) ref. [3, 5]
- Learn different definition of semi-separable matrix and its properties ref. [9–11]
- Learn Laplacian matrix $\boldsymbol{\Delta}$ (1D first) in the finite difference method, which is a tridiagonal matrix, and try to find a application of the above algorithm on its LU decomposition as

  $$\Delta = \begin{bmatrix} \times & \times & & \\ \times & \ddots & \ddots & \\ & \ddots & \ddots & \times \\ & & \times & \times \end{bmatrix} = \begin{bmatrix} \times & & & \\ \times & \ddots & & \\ & \ddots & \ddots & \\ & & \times & \times \end{bmatrix} \begin{bmatrix} \times & \times & & \\ & \ddots & \ddots & \\ & & \ddots & \times \\ & & & \times \end{bmatrix} = LU \quad (\text{or } LL^{\mathrm{T}} \text{ if } \Delta \text{ is posi. def.})$$

  Then, if Δ has Cholesky factorization,

  $$\Delta^{-1} = L^{-\mathrm{T}} L^{-1} = \mathrm{tril}(xy^{\mathrm{T}})\,\mathrm{triu}(yx^{\mathrm{T}}) = \mathrm{tril}(\tilde{X}\tilde{Y}^{\mathrm{T}}) + \mathrm{triu}(\tilde{Y}\tilde{X}^{\mathrm{T}})$$

- As inverse of upper bidiagonal and block upper bidiagonal matrices have solved, try to explore for block upper tridiagonal or triangular matrices
- 2D Laplacian matrix for PDE, $\Delta \otimes I + I \otimes \Delta$ (if possible)

All references [1–11]

Bibliography

[1] E. Asplund, *Inverses of matrices {a ij} which satisfy a ij= 0 for j> i+ p*, Mathematica Scandinavica, (1959), pp. 57–60.

[2] S. Chandrasekaran and M. Gu, *Fast and stable eigendecomposition of symmetric banded plus semi-separable matrices*, Linear Algebra and Its Applications, 313 (2000), pp. 107–114.

[3] G. H. Golub and C. F. Van Loan, *Matrix computations*, JHU press, 2013.

[4] N. Higham, *Cholesky factorization*, Wiley Interdisciplinary Reviews: Computational Statistics, 1 (2009), pp. 251 – 254.

[5] N. J. Higham, *Accuracy and stability of numerical algorithms*, SIAM, 2002.

[6] R. Hunger, *Floating point operations in matrix-vector calculus*, vol. 2019, Munich University of Technology, Inst. for Circuit Theory and Signal ..., 2005.

[7] J. Jain, H. Li, C.-K. Koh, and V. Balakrishnan, *O (n) algorithms for banded plus semiseparable matrices*, in Numerical methods for structured matrices and applications, Springer, 2010, pp. 347–358.

[8] P. Rózsa, R. Bevilacqua, F. Romani, and P. Favati, *On band matrices and their inverses*, Linear Algebra and Its Applications, 150 (1991), pp. 287–295.

[9] R. Vandebril, M. V. Barel, G. Golub, and N. Mastronardi, *A bibliography on semiseparable matrices*, Calcolo, 42 (2005), pp. 249–270.

[10] R. Vandebril, M. Van Barel, and N. Mastronardi, *A note on the representation and definition of semiseparable matrices*, Numerical Linear Algebra with Applications, 12 (2005), pp. 839–858.

[11] ——, *Matrix computations and semiseparable matrices: linear systems*, vol. 1, JHU Press, 2007.