

[SIMAX] Block Crout Factorizations: An example:

$$\mathbf{B} = \begin{bmatrix} 4 & -1 & 0 & 1 & 4 & 7 \\ 0 & 4 & -1 & 2 & 5 & 8 \\ 0 & 0 & 4 & 3 & 6 & 9 \end{bmatrix}, \quad \mathbf{A} = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

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Assumption: B upper trapezoidal:

$$\mathbf{X} := \begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} = \left[\begin{array}{cccccc|ccc} 2 & -1 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & -1 & 4 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 & -1 & 4 \\ 0 & 0 & -1 & 2 & -1 & 0 & 1 & 2 & 3 \\ 0 & 0 & 0 & -1 & 2 & -1 & 4 & 5 & 6 \\ 0 & 0 & 0 & 0 & -1 & 2 & 7 & 8 & 9 \\ \hline 4 & -1 & 0 & 1 & 4 & 7 & 0 & 0 & 0 \\ 0 & 4 & -1 & 2 & 5 & 8 & 0 & 0 & 0 \\ 0 & 0 & 4 & 3 & 6 & 9 & 0 & 0 & 0 \end{array} \right]$$

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Step 1. Permute: $\mathbf{P} = [\mathbf{e}_1, \mathbf{e}_7, \mathbf{e}_2, \mathbf{e}_8, \mathbf{e}_3, \mathbf{e}_9, \mathbf{e}_4, \mathbf{e}_5, \mathbf{e}_6] \in \mathbb{R}^{9 \times 9}$

$$\mathbf{Y} = \mathbf{P}^T \mathbf{X} \mathbf{P} \quad (\text{Permuted Form})$$

$$= \left[\begin{array}{cc|cc|cc|c|c|c} 2 & 4 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & -1 & 0 & 0 & 0 & 1 & 4 & 7 \\ \hline -1 & -1 & 2 & 4 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & -1 & 0 & 2 & 5 & 8 \\ \hline 0 & 0 & -1 & -1 & 2 & 4 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 3 & 6 & 9 \\ \hline 0 & 1 & 0 & 2 & -1 & 3 & 2 & -1 & 0 \\ 0 & 4 & 0 & 5 & 0 & 6 & -1 & 2 & -1 \\ \hline 0 & 7 & 0 & 8 & 0 & 9 & 0 & -1 & 2 \end{array} \right]$$

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Step 2. Block Crout Factor:

$$\mathbf{Y} = (\mathbf{L}_Y + \mathbf{D}_Y) \mathbf{D}_Y^{-1} (\mathbf{L}_Y + \mathbf{D}_Y)^T \quad (\text{Block Crout Factored Form})$$

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with \mathbf{L}_Y resp. \mathbf{D}_Y

$$\left[\begin{array}{cc|cc|cc|c|c|c} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0.1 & 2 & -0.7 & 3 & 0 & 0 & 0 \\ 0 & 4 & 0.5 & 5 & 0.9 & 6 & 2.3 & 0 & 0 \\ \hline 0 & 7 & 0.9 & 8 & 1.4 & 9 & 5.0 & 3.2 & 0 \end{array} \right], \quad \left[\begin{array}{cc|cc|cc|c|c|c} 2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 1.6 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 1.6 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 4.3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.1 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.2 \end{array} \right]$$

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Step 3. Back permute:

$$\begin{aligned}
& \downarrow \text{Step 3. Back permute:} \\
\mathbf{X} &= \mathbf{PYP}^T = \underbrace{(\mathbf{PL}_Y\mathbf{P}^T)}_{=: \mathbf{L}_X} + \underbrace{(\mathbf{PD}_Y\mathbf{P}^T)}_{=: \mathbf{D}_X} (\mathbf{PD}_Y\mathbf{P}^T)^{-1} (\mathbf{PL}_Y\mathbf{P}^T + \mathbf{PD}_Y\mathbf{P}^T)^T \\
&=: (\mathbf{L}_X + \mathbf{D}_X) \mathbf{D}_X^{-1} (\mathbf{L}_X + \mathbf{D}_X)^T \quad (\text{Saddle point Factored Form}) \\
& \downarrow \text{with } \mathbf{L}_X \text{ resp. } \mathbf{D}_X \\
& \left[\begin{array}{cccccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0.1 & -0.7 & 0 & 0 & 0 & 1 & 2 & 3 \\ 0 & 0.5 & 0.9 & 2.3 & 0 & 0 & 4 & 5 & 6 \\ 0 & 0.9 & 1.4 & 5.0 & 3.2 & 0 & 7 & 8 & 9 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right], \quad \left[\begin{array}{cccccc|cccc} 2 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 1.6 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 1.6 & 0 & 0 & 0 & 0 & 0 & 4 \\ 0 & 0 & 0 & 4.3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5.2 & 0 & 0 & 0 \\ \hline 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right] \\
& \downarrow \text{To determine whether our factors are members of a certain class/family:} \\
\mathbf{X} &= (\mathbf{L}_X + \mathbf{D}_X) \mathbf{D}_X^{-1} (\mathbf{L}_X + \mathbf{D}_X)^T \\
&=: \mathbf{LDL}^T \quad (\text{"Dollar, Gould, Schilders, Wathen" Form}) \\
& \downarrow \text{with } \mathbf{L} := \mathbf{L}_X + \mathbf{D}_X \text{ resp. } \mathbf{D} := (\mathbf{D}_X)^{-1} \\
& \left[\begin{array}{ccc|ccc|ccc} 2 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ -1 & 1.6 & 0 & 0 & 0 & 0 & -1 & 4 & 0 \\ 0 & -1 & 1.6 & 0 & 0 & 0 & 0 & -1 & 4 \\ \hline 0 & 0.1 & -0.7 & 4.3 & 0 & 0 & 1 & 2 & 3 \\ 0 & 0.5 & 0.9 & 2.3 & 5.1 & 0 & 4 & 5 & 6 \\ 0 & 0.9 & 1.4 & 5.0 & 3.2 & 5.2 & 7 & 8 & 9 \\ \hline 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right], \quad \left[\begin{array}{ccc|ccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0.2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.2 \\ \hline 0 & 0 & 0 & 0.2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.2 & 0 & 0 & 0 \\ \hline 0.2 & 0 & 0 & 0 & 0 & 0 & -0.1 & 0 & 0 \\ 0 & 0.2 & 0 & 0 & 0 & 0 & 0 & -0.1 & 0 \\ 0 & 0 & 0.2 & 0 & 0 & 0 & 0 & 0 & -0.1 \end{array} \right]
\end{aligned}$$

where no entry has been rounded to 0.

Alternative: An extra step after 2:

$$\begin{array}{l}
\downarrow \text{Step 2. Block Crout Factor:} \\
\mathbf{Y} = (\mathbf{L}_Y + \mathbf{D}_Y) \mathbf{D}_Y^{-1} (\mathbf{L}_Y + \mathbf{D}_Y)^T \quad (\text{Block Crout Factored Form}) \\
\downarrow \text{with } \mathbf{L}_Y \text{ resp. } \mathbf{D}_Y \\
\left[\begin{array}{cc|cc|cc|c|c|c} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0.1 & 2 & -0.7 & 3 & 0 & 0 & 0 \\ 0 & 4 & 0.5 & 5 & 0.9 & 6 & 2.3 & 0 & 0 \\ 0 & 7 & 0.9 & 8 & 1.4 & 9 & 5.0 & 3.2 & 0 \end{array} \right], \left[\begin{array}{cc|cc|cc|c|c|c} 2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 1.6 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 1.6 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 4.3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.2 \end{array} \right] \\
\downarrow \text{Step 2b. Block diagonal} \rightarrow \text{Diagonal:}
\end{array}$$

Note that each step $\mathbf{S}_k := \mathbf{S}_k - (\mathbf{L}_k + \mathbf{D}_k) \mathbf{D}_k^{-1} (\mathbf{D}_k + \mathbf{U}_k)$ where

$$(\mathbf{L}_k + \mathbf{D}_k) \mathbf{D}_k^{-1} (\mathbf{D}_k + \mathbf{U}_k) = [\mathbf{D}_k; \mathbf{L}_k] \mathbf{D}_k^{-1} [\mathbf{D}_k, \mathbf{U}_k].$$

If each diagonal block \mathbf{D}_k can be factored:

$$\mathbf{D}_k = (d_k + u_k) d_k^{-1} (l_k + d_k) \implies \mathbf{D}_k^{-1} = (d_k + u_k)^{-1} d_k (l_k + d_k)^{-1}$$

then

$$\begin{aligned}
(\mathbf{L}_k + \mathbf{D}_k) \mathbf{D}_k^{-1} (\mathbf{D}_k + \mathbf{U}_k) &= [\mathbf{D}_k; \mathbf{L}_k] \mathbf{D}_k^{-1} [\mathbf{D}_k, \mathbf{U}_k] \\
&= [(l_k + d_k) d_k^{-1} (d_k + u_k); L] (d_k + u_k)^{-1} d_k (l_k + d_k)^{-1} [(l_k + d_k) d_k^{-1} (d_k + u_k), U] \\
&= [(l_k + d_k); L (d_k + u_k)^{-1} d_k] d_k^{-1} d_k (l_k + d_k)^{-1} [(l_k + d_k) d_k^{-1} (d_k + u_k), U] \\
&= [(l_k + d_k); L (d_k + u_k)^{-1} d_k] d_k^{-1} [(d_k + u_k), d_k (l_k + d_k)^{-1} U].
\end{aligned}$$

leads to a **new** LDU type factorization

$$\mathbf{Y} = (\hat{\mathbf{L}} + \hat{\mathbf{D}}) \hat{\mathbf{D}}^{-1} (\hat{\mathbf{D}} + \hat{\mathbf{U}})$$

where \mathbf{L}, \mathbf{U} are strictly lower respectively upper triangular and where \mathbf{D} is diagonal (not anylonger block-diagonal).

$$\begin{array}{l}
\downarrow \text{Step 2b. Block diagonal} \leftrightarrow \text{Diagonal:} \\
\mathbf{Y} = (\hat{\mathbf{L}}_Y + \hat{\mathbf{D}}_Y) \hat{\mathbf{D}}_Y^{-1} (\hat{\mathbf{L}}_Y + \hat{\mathbf{D}}_Y)^T \quad (\text{Modified Block Crout Factored Form}) \\
\downarrow \text{with } \hat{\mathbf{L}}_Y \text{ resp. } \hat{\mathbf{D}}_Y \\
\left[\begin{array}{ccc|ccc|c|c|c} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 4 & -8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline -1 & 2 & 4 & -8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & 4 & -8 & 0 & 0 & 0 \\ \hline 0 & 1 & 0.2 & 1.8 & -0.4 & 4.4 & 4.8 & 0 & 0 \\ 0 & 4 & 1 & 4 & 1.5 & 4.5 & 3.1 & 5.0 & 0 \\ 0 & 7 & 1.8 & 6.2 & 2.4 & 6.6 & 6.2 & 2.7 & 4.5 \end{array} \right], \left[\begin{array}{ccc|ccc|c|c|c} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & -8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -8 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 4.8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4.5 \end{array} \right]
\end{array}$$

Our Constrained Factored Form is an element of family 10 (from [DGSW] Table4.2):

1. $\mathbf{C} = \mathbf{0}$
2. $[\mathbf{L}_{13}; \mathbf{L}_{23}] = \mathbf{B}^T$
3. All non-zero blocks of \mathbf{L} correctly positioned
4. $\mathbf{L}_{31} = \mathbf{D}_{31}^{-T}$.

The Block Crout Factorization is a straight forward simple recursive process. However, proper termination (existence of factors \mathbf{L}_Y and \mathbf{D}_Y) depends on properties of \mathbf{A} and \mathbf{B} . Paper [LAA] only does:

1. Step 2b. An existence proof for the Crout block Factorization Step 2 for
 - \mathbf{A} symmetric positive definite
 - \mathbf{B} lower trapezoidal and
 - \mathbf{B} of maximal rank

The obtained Crout block Factorization *can not be used for the construction of a (inexact) preconditioner* because related \mathbf{L} does not contain blocks together form \mathbf{B} :

$$\mathbf{B} = \begin{bmatrix} 4 & 0 & 0 & 1 & 4 & 7 \\ -1 & 4 & 0 & 2 & 5 & 8 \\ 0 & -1 & 4 & 3 & 6 & 9 \end{bmatrix} \rightarrow \mathbf{L}_X + \mathbf{D}_X = \left[\begin{array}{ccc|ccc|ccc} 2 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ -1 & 2 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 0 & -1 & 2 & 0 & 0 & 0 & 0 & 0 & 4 \\ \hline 0 & 0.2 & -0.4 & 4.8 & 0 & 0 & 1 & 2.2 & 3.6 \\ 0 & 1 & 1.5 & 3.1 & 5.0 & 0 & 4 & 6 & 7.5 \\ 0 & 1.8 & 2.4 & 6.2 & 2.7 & 4.5 & 7 & 9.8 & 11.4 \\ \hline 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right]$$

But it is an efficient factorization because $\text{tril}(\mathbf{A}_{11})$ is an unaltered part of \mathbf{L} .

Paper [SIMAX] introduces several novelties:

1. Step 2b. A (required!) different existence proof for the Crout block Factorization Step 2 for
 - \mathbf{A} symmetric positive definite
 - \mathbf{B} upper trapezoidal and
 - \mathbf{B} of maximal rank
2. Step 3. Modified Incomplete Block Factorization
3. Step 3a. Such that existence can be proven

4. Step 3b. And such that the factorization $(\mathbf{L}_\mathbf{X} + \mathbf{D}_\mathbf{X})\mathbf{D}_\mathbf{X}^{-1}(\mathbf{L}_\mathbf{X} + \mathbf{D}_\mathbf{X})^\mathbf{T}$ is a constrained preconditioner.
5. Step 4. Comparison against an existing method

Suddenly we have an algorithm which generates an exact factorization member of family 10 – and in addition an inexact preconditioner.

[SIMAX] and [LAA] papers both set up the Block Crout factorization. Apart from that [SIMAX] is not related to [LAA] but as mentioned based on ideas by [SHILDERS] who presents an algorithm to calculate a constrained factored form preconditioner.

[SIMAX] opens the road for the construction of algorithms for various incomplete constrained factored form preconditioners. And: Solution of systems $\mathbf{X}\mathbf{u} = \mathbf{b}$ can be done very efficiently with the use of $(\mathbf{L}_\mathbf{Y} + \mathbf{D}_\mathbf{Y})\mathbf{D}_\mathbf{Y}^{-1}(\mathbf{L}_\mathbf{Y} + \mathbf{D}_\mathbf{Y})^\mathbf{T}(\mathbf{P}^\mathbf{T}\mathbf{u}) = \mathbf{P}^\mathbf{T}\mathbf{b}$.