

Micro-/macro-block factorizations for regularized saddle point systems

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April 17, 2012

Micro-/Macro-block factorizations

for regularized saddle-point problems

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Introduction

Any symmetric matrix \mathbf{X} , positive definite or not, can be factored:

$$\mathbf{Q}^T \mathbf{X} \mathbf{Q} = \mathbf{L} \mathbf{D} \mathbf{L}^T$$

where

- 1 \mathbf{L} is a unit lower triangular matrix, and

See [3, Section 4.4, page 115].

For \mathbf{X} without special structure: Use Bunch-Kaufman-Parlett algorithm in [7].

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- 3 \mathbf{D} is a micro-block diagonal with 1x1 or 2x2 micro blocks

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Regularized saddle-point problems: Definition

Structure of indefinite \mathbf{X} from regularized saddle point problems:

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & -\mathbf{C} \end{bmatrix}.$$

- 1 \mathbf{A} n by n symmetric positive definite;

Goal: Construct a preconditioner or implicit/[explicit factorization](#).

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- ② $\mathbf{C} \neq \mathbf{0}$ (**regularized saddle point problem**): occurs for instance in electronic circuit simulation [11].

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Regularized saddle-point problems: Preconditioners

Are for instance based on:

- ① (Block-) diagonal approximations of \mathbf{A} ;
- ② (Block-) diagonal approximations of \mathbf{C} ;
- ③ Schur-complement based approaches;
- ④ Explicit/**implicit Micro-block factorizations**.

See for instance Axelsson, Gould, Keller, Schilders, Simoncini, Trefethen, Wathen [1, 5, 6, 12, 4, 2, 8]. Example approach from [5]: Factor $\mathbf{C} = \mathbf{LDL}^T$ and introduce $\mathbf{x}_3 = -\mathbf{DL}^T \mathbf{x}_2$:

$$\begin{bmatrix} \mathbf{A} & \mathbf{0} & \mathbf{B}^T \\ \mathbf{0} & \mathbf{D}^{-1} & \mathbf{L}^T \\ \mathbf{B} & \mathbf{L} & \mathbf{0} \end{bmatrix}.$$

Schilders' factorization/preconditioner for **C = 0**

Schilder's in [12] exploits more structure:

$$\mathbf{X} = \begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} = \left[\begin{array}{c|c|c} \square & \begin{array}{c} | \\ | \\ | \end{array} & \begin{array}{c} \triangle \\ \triangle \\ \triangle \end{array} \\ \hline \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} & \begin{array}{c} \square \\ \square \\ \square \end{array} & \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \\ \hline \begin{array}{c} \triangle \\ \triangle \\ \triangle \end{array} & \begin{array}{c} | \\ | \\ | \end{array} & \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \end{array} \right]$$

- 1 **A** n by n symmetric positive definite;

Sufficient condition is maximal row rank for **B**.

The new **C** ≠ **0** factorization [9] borrows two key concepts from [12].

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- 1 \mathbf{A} n by n symmetric positive definite;
- 2 $\mathbf{B} = [\mathbf{B}_1, \mathbf{B}_2] = \begin{bmatrix} \square & \text{||} \\ \text{||} & \text{||} \end{bmatrix}$ m by n upper trgl., max. row rank;

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- 3 $\mathbf{C} = \mathbf{0}$, m by m - diagonal matrix.

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The new $\mathbf{C} \neq \mathbf{0}$ factorization [9] borrows two key concepts from [12].

Schilders' I: The micro-block matrix $Y = Q^T X Q$ [12] proposes the pivot-explicit micro-block matrix $Y = Q^T X Q$

1	a_{11} b_{11}	b_{11} $-c_{11}$	a_{12} b_{12}	0 0	a_{13} b_{13}	0 0	m a_{14} b_{41}	0 0	$m+1$ a_{15} b_{15}	a_{16} b_{16}	n a_{17} b_{17}
	a_{21} 0	b_{12} 0	a_{22} b_{22}	b_{22} $-c_{22}$	a_{23} b_{23}	0 0	a_{24} b_{24}	0 0	a_{25} b_{25}	a_{26} b_{26}	a_{27} b_{27}
	a_{31} 0	b_{13} 0	a_{32} 0	b_{23} 0	a_{33} b_{33}	b_{33} $-c_{33}$	a_{34} b_{34}	0 0	a_{35} b_{35}	a_{36} b_{36}	a_{37} b_{37}
m	a_{41} 0	b_{14} 0	a_{42} 0	b_{24} 0	a_{43} 0	b_{34} 0	a_{44} b_{44}	b_{44} $-c_{44}$	a_{45} b_{45}	a_{46} b_{46}	a_{47} b_{47}
$m+1$	a_{51} a_{61}	b_{15} b_{16}	a_{52} a_{62}	b_{25} b_{26}	a_{53} a_{63}	b_{35} b_{36}	a_{54} a_{64}	b_{45} b_{46}	a_{55} a_{65}	a_{56} a_{66}	a_{57} a_{67}
n	a_{71}	b_{17}	a_{72}	b_{27}	a_{73}	b_{37}	a_{74}	b_{47}	a_{75}	a_{76}	a_{77}

and uses it to construct a preconditioner \hat{Y} ① of Crout-type: $\hat{Y} = \hat{L} \text{diag}^{-1}(\hat{L}) \hat{L}^T$;

Concept 1: New factorization [9] uses this micro-block structure.

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	a_{31} 0	b_{13} 0	a_{32} 0	b_{23} 0	a_{33} b_{33}	b_{33} $-c_{33}$	a_{34} b_{34}	0 0	a_{35} b_{35}	a_{36} b_{36}	a_{37} b_{37}
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and uses it to construct a preconditioner $\hat{\mathbf{Y}}$

- 1 of Crout-type: $\hat{\mathbf{Y}} = \hat{\mathcal{L}} \text{diag}^{-1}(\hat{\mathcal{L}}) \hat{\mathcal{L}}^T$;
- 2 which satisfies $\text{diag}(\hat{\mathbf{Y}}) = \text{diag}(\mathbf{Y})$.

Concept 1: New factorization [9] uses this micro-block structure.

Schilders' II: The macro-block factorization $\mathbf{X} = \mathcal{L}\mathcal{D}\mathcal{L}^T$

In addition [12] shows that for $\mathbf{C} = \mathbf{0}$:

- ① macro-block factorizations $\mathbf{X} = \mathcal{L}\mathcal{D}\mathcal{L}^T$ exist where

$$\mathcal{L} = \begin{bmatrix} \mathbf{B}_1^T & \mathbf{0} & \mathbf{L}_1 \\ \mathbf{B}_2^T & \mathbf{I}_{n-m} + \mathbf{L}_2 & \mathbf{M} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix}, \quad \mathcal{D} = \begin{bmatrix} \mathbf{D}_1 & \mathbf{0} & \mathbf{I} \\ \mathbf{0} & \mathbf{D}_2 & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \end{bmatrix};$$

- ② $x \mapsto \mathcal{L}^{-1}\mathbf{x}$ and $x \mapsto \mathcal{D}^{-1}\mathbf{x}$ can be calculated efficiently;
- ③ This factorization is not unique;
- ④ A full micro-block factorization leads to a different factorization unless $\text{diag}(\mathbf{B}) = \mathbf{I}$.

Concept 2: New factorization [9] shows micro-block factorization existence using a different macro-block factorization.

The new factorization for $C \neq 0$, structure of X

The current work [9] focuses on

$$X = \begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & -\mathbf{C} \end{bmatrix} = \begin{bmatrix} \square & | & \triangle \\ \hline \text{---} & | & \text{---} \\ \triangle & | & \diagdown \end{bmatrix}$$

- 1 \mathbf{A} n by n symmetric positive definite;

Results do extend to maximal rank \mathbf{B} and symmetric positive semi-definite \mathbf{C} .

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- 3 \mathbf{C} , m by m positive semi-definite diagonal matrix.

Results do extend to maximal rank \mathbf{B} and symmetric positive semi-definite \mathbf{C} .

The factorizations $\mathbf{X} = \mathbf{L}_X \mathbf{D}_X^{-1} \mathbf{L}_X^T$, $\mathbf{X} = \mathcal{L}_X \mathbf{D}_X \mathcal{L}_X^T$

For $\mathbf{C} \neq \mathbf{0}$ [9] introduces an *exact micro-block factorization*:

- 1 efficient, since updates are only on the \mathbf{A} -block part of \mathbf{X} ;
- 2 induces factorization ($\mathbf{D}_X = \text{diag}(\mathbf{L}_X)$): $\mathbf{X} = \mathbf{L}_X \mathbf{D}_X^{-1} \mathbf{L}_X^T$ where

$$\mathbf{L}_X = \begin{bmatrix} \mathbf{L}_1 & \mathbf{0} & \mathbf{B}_1^T \\ \mathbf{M} & \mathbf{L}_2 & \mathbf{B}_2^T \\ d\mathbf{B}_1 & \mathbf{0} & -\mathbf{C} \end{bmatrix}, \quad \mathbf{D}_X^{-1} = \begin{bmatrix} \mathbf{FC} & \mathbf{0} & \mathbf{FdB}_1 \\ \mathbf{0} & \mathbf{D}_2^{-1} & \mathbf{0} \\ \mathbf{FdB}_1 & \mathbf{0} & -\mathbf{FD}_1 \end{bmatrix};$$

- 3 alternative formulation $\mathbf{X} = \mathcal{L}_X \mathbf{D}_X \mathcal{L}_X^T$ where

$$\begin{bmatrix} \mathbf{B}_1^T \mathbf{FdB}_1 + \mathbf{L}_1 \mathbf{FC} & \mathbf{0} & -\mathbf{B}_1^T \mathbf{FD}_1 + \mathbf{L}_1 \mathbf{FdB}_1 \\ \mathbf{B}_2^T \mathbf{FdB}_1 + \mathbf{MFC} & \mathbf{L}_2 \mathbf{D}_2^{-1} & -\mathbf{B}_2^T \mathbf{FD}_1 + \mathbf{MFdB}_1 \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix};$$

- 4 factorizations are unique (m-diag. blocks are 1x1 or 2x2 identity).

The structure of micro-block factor $Q^T \mathcal{L}_X Q$

$Q^T \mathcal{L}_X Q$ only differs from the lower triangular micro-block part of Y at entries a_{ij} :

1	$\begin{pmatrix} *_{11} & b_{11} \\ b_{11} & -c_{11} \end{pmatrix}$	2			m	$m+1$			n
	$\begin{pmatrix} *_{21} & b_{12} \\ 0 & 0 \end{pmatrix}$	$\begin{pmatrix} *_{22} & b_{22} \\ b_{22} & -c_{22} \end{pmatrix}$							
	$\begin{pmatrix} *_{31} & b_{13} \\ 0 & 0 \end{pmatrix}$	$\begin{pmatrix} *_{32} & b_{23} \\ 0 & 0 \end{pmatrix}$	$\begin{pmatrix} *_{33} & b_{33} \\ b_{33} & -c_{33} \end{pmatrix}$						
m	$\begin{pmatrix} *_{41} & b_{14} \\ 0 & 0 \end{pmatrix}$	$\begin{pmatrix} *_{42} & b_{24} \\ 0 & 0 \end{pmatrix}$	$\begin{pmatrix} *_{43} & b_{34} \\ 0 & 0 \end{pmatrix}$	$\begin{pmatrix} *_{44} & b_{44} \\ b_{44} & -c_{44} \end{pmatrix}$					
$m+1$	$\begin{pmatrix} *_{51} & b_{15} \\ *_{61} & b_{16} \end{pmatrix}$	$\begin{pmatrix} *_{52} & b_{25} \\ *_{62} & b_{26} \end{pmatrix}$	$\begin{pmatrix} *_{53} & b_{35} \\ *_{63} & b_{36} \end{pmatrix}$	$\begin{pmatrix} *_{54} & b_{45} \\ *_{64} & b_{46} \end{pmatrix}$	$\begin{pmatrix} *_{55} \\ *_{65} \end{pmatrix}$			$\begin{pmatrix} *_{66} \end{pmatrix}$	
n	$\begin{pmatrix} *_{71} & b_{17} \end{pmatrix}$	$\begin{pmatrix} *_{72} & b_{27} \end{pmatrix}$	$\begin{pmatrix} *_{73} & b_{37} \end{pmatrix}$	$\begin{pmatrix} *_{74} & b_{47} \end{pmatrix}$	$\begin{pmatrix} *_{75} \\ *_{76} \end{pmatrix}$	$\begin{pmatrix} *_{77} \end{pmatrix}$			

Similarities between macro-factorizations in [12] and [9]

For $\mathbf{C} = \mathbf{0}$:

- 1 Old and new factorizations are identical for $\text{diag}(\mathbf{B}_1) = \mathbf{I}_m$.

For $\mathbf{C} \geq \mathbf{0}$:

- 1 Blocks of Schilders' \mathcal{L} and new factorization $\mathcal{L}_\mathbf{X}$ have identical shapes – zero, diagonal, (strictly) triangular, rectangular;
- 2 $\mathbf{D}_\mathbf{X}$ has one extra non-zero block more than \mathcal{D} .

The new factorization conceptually generalizes Schilders' factorization.

Existence of factorizations $\mathbf{X} = \mathbf{L}_\mathbf{X} \mathbf{D}_\mathbf{X}^{-1} \mathbf{L}_\mathbf{X}^\mathbf{T}$, $\mathbf{X} = \mathcal{L}_\mathbf{X} \mathbf{D}_\mathbf{X} \mathcal{L}_\mathbf{X}^\mathbf{T}$

Shown is existence for \mathbf{A} spd., \mathbf{B} upper trngl. of max. row rank

- ① $\mathbf{C} = \mathbf{0}$, uses Lemma 4.1 in Schilders [12] – but differs, uses $\mathbf{B} = [\mathbf{I}_m, \mathbf{0}_{m,n-m}]$ plus transformation;
- ② $\mathbf{C} > \mathbf{0}$, uses existence of Schur-complement $\mathbf{A} + \mathbf{B}^\mathbf{T} \mathbf{C}^{-1} \mathbf{B}$;
- ③ $\mathbf{C} = \text{diag}(0, \dots, 0, c_{d+1,d+1}, \dots, c_{mm})$ with d zeros at start.

Extensions are likely and under investigation:

- ① $\mathbf{C} \geq \mathbf{0}$, no order in zero and positive coefficients;
- ② k by k micro-block approach (calculation of $\mathbf{D}_\mathbf{X}^{-1}$ is similar);
- ③ construction of preconditioners: Incomplete, etc.

General positive (semi-)definite \mathbf{C} and full-rank \mathbf{B}

For the general case existence can be shown as follows:

- 1 Factor $\mathbf{C} = \mathbf{L}_\mathbf{C}\mathbf{D}_\mathbf{C}\mathbf{L}_\mathbf{C}^T$ – use Cholesky form;
- 2 Apply a QR -based transformation to make $\hat{\mathbf{B}} = \mathbf{B}(\mathbf{L}_\mathbf{C}\sqrt{\mathbf{D}_\mathbf{C}})^{-1}$ upper triangular;
- 3 Apply the micro-block factorization;
- 4 Read off the macro-block factors.

The extra work is the factorization of \mathbf{C} .

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