Symmetric factorizations

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The LDL* factorization

Let $A \in \mathbb{C}^{n \times n}$ and suppose that its first $n-1$ leading principal minors are nonzero. Then A has a *unique* LU factorization $A = LU$, and moreover $u_{11}, \dots, u_{n-1,\, n-1}$ are nonzero (being the pivots in the LU factorization). As a result, A has a *unique* **LDU factorization** $A = LD\hat{U}$, where $L \in \mathbb{C}^{n \times n}$ is *unit* lower triangular, $D \in \mathbb{C}^{n \times n}$ is diagonal, and $\hat{U} \in \mathbb{C}^{n \times n}$ is *unit* upper triangular; given by the unique factorization of U as $U = D\hat{U}$. When A is also *self-adjoint*, we must have $\hat{U} = L^*$, in which case this factorization is called the **LDL* factorization** (or **LDL$^\mathsf{T}$ factorization** if A is real).

Given a self-adjoint $A \in \mathbb{C}^{n \times n}$, we can also derive the LDL* factorization directly: if

$$A = \begin{bmatrix} \alpha & c^* \\ c & B \end{bmatrix}$$

for some $\alpha \in \mathbb{C}$ (in fact, $\alpha \in \mathbb{R}$ since A is self-adjoint), $c \in \mathbb{C}^{n-1}$, and $B \in \mathbb{C}^{(n-1)\times(n-1)}$, then

$$A = \begin{bmatrix} 1 & \\ \frac{c}{\alpha} & I \end{bmatrix} \begin{bmatrix} \alpha & \\ & B - \frac{cc^*}{\alpha} \end{bmatrix} \begin{bmatrix} 1 & \frac{c^*}{\alpha} \\ & I \end{bmatrix},$$

and if $L'D'(L')^*$ is the LDL* factorization of the Schur complement $A' = B - \frac{cc^*}{\alpha}$, then

$$A = \underbrace{\begin{bmatrix} 1 & \\ \frac{c}{\alpha} & L' \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} \alpha & \\ & D' \end{bmatrix}}_{D} \underbrace{\begin{bmatrix} 1 & \frac{c^*}{\alpha} \\ & (L')^* \end{bmatrix}}_{L^*}$$

is the LDL* factorization of A.

Diagonal pivoting methods

Let $A \in \mathbb{C}^{n \times n}$ be self-adjoint. Just as an LU factorization may fail to exist because of a zero pivot, an LDL* factorization may fail to exist as well. To obtain a nonzero pivot while preserving the symmetry of A, we can interchange two rows of A along with the corresponding columns (illustrated below), which amounts to replacing A with $P_1 A P_1^*$ for some permutation matrix P_1.

$$\begin{bmatrix} & 1 & \\ 1 & & \\ & & 1 \end{bmatrix} \begin{bmatrix} 0 & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} & 1 & \\ 1 & & \\ & & 1 \end{bmatrix} = \begin{bmatrix} a_{22} & a_{21} & a_{23} \\ a_{12} & 0 & a_{13} \\ a_{32} & a_{31} & a_{33} \end{bmatrix}$$

However, using a symmetric interchange as such, pivots can only be selected from the diagonal entries of A, which could all be zero despite the matrix itself being nonzero. To remedy this, we can use a permutation to move a nonzero off-diagonal entry at position (i, j) to position $(2, 1)$ (illustrated below), which allows us to then perform a 2×2 block elimination step.

$$\begin{bmatrix} & 1 & \\ & & 1 \\ 1 & & \end{bmatrix} \begin{bmatrix} 0 & a_{12} & a_{13} \\ a_{21} & 0 & a_{23} \\ a_{31} & a_{32} & 0 \end{bmatrix} \begin{bmatrix} & & 1 \\ 1 & & \\ & 1 & \end{bmatrix} = \begin{bmatrix} 0 & a_{23} & a_{21} \\ a_{32} & 0 & a_{31} \\ a_{12} & a_{13} & 0 \end{bmatrix}$$

In general, if A is nonzero, there exists a permutation matrix P_1 such that

$$P_1 A P_1^* = \begin{bmatrix} E & C^* \\ C & B \end{bmatrix},$$

where the pivot $E \in \mathbb{C}^{s \times s}$ is invertible and $s \in \{1, 2\}$, $C \in \mathbb{C}^{(n-s) \times s}$, and $B \in \mathbb{C}^{(n-s) \times (n-s)}$. We then have

$$P_1 A P_1^* = \begin{bmatrix} I & \\ CE^{-1} & I \end{bmatrix} \begin{bmatrix} E & \\ & B - CE^{-1}C^* \end{bmatrix} \begin{bmatrix} I & E^{-1}C^* \\ & I \end{bmatrix}.$$

Continuing symmetric elimination with the Schur complement $A' = B - CE^{-1}C^*$, we ultimately produce a factorization of the form $PAP^* = LDL^*$, where P is a permutation matrix, L is unit lower triangular, and D is self-adjoint quasi-diagonal (block diagonal with 1×1 or 2×2 blocks).

The Bunch–Parlett factorization

Let $\mu_0 := \max_{i,j} |a_{ij}| = \|A\|_{1,\infty}$ and $\mu_1 := \max_i |a_{ii}|$. The **Bunch–Parlett factorization** is a diagonal pivoting method that uses a 1×1 pivot with $|e_{11}| = \mu_1$ whenever $\mu_1 \geq \alpha\mu_0$ and a 2×2 pivot with $|e_{21}| = \mu_0$ otherwise, where $\alpha \in (0, 1)$ is a constant chosen to minimize an upper bound for $\mu_0' := \max_{i,j} |a_{ij}'| = \|A'\|_{1,\infty}$.

Namely, for a 1×1 pivot, we have

$$\begin{aligned} \mu_0' &\leq \|B\|_{1,\infty} + \|C\|_{1,\infty} \|E^{-1}\|_{\infty,1} \|C^*\|_{1,\infty} \\ &\leq \mu_0 + \mu_0 \cdot \frac{1}{\mu_1} \cdot \mu_0 \\ &\leq \left(1 + \frac{1}{\alpha}\right)\mu_0, \end{aligned}$$

and for a 2×2 pivot, we have

$$\begin{aligned} \mu_0' &\leq \|B\|_{1,\infty} + \|C\|_{1,\infty} \|E^{-1}\|_{\infty,1} \|C^*\|_{1,\infty} \\ &\leq \mu_0 + \mu_0 \cdot \frac{2(\mu_0 + \mu_1)}{|\det(E)|} \cdot \mu_0 \\ &\leq \mu_0 + \mu_0 \cdot \frac{2(\mu_0 + \mu_1)}{\mu_0^2 - \mu_1^2} \cdot \mu_0 \\ &< \left(1 + \frac{2}{1 - \alpha}\right)\mu_0. \end{aligned}$$

To choose α, we equate the growth factor $(1 + \frac{1}{\alpha})^2$ for two 1×1 pivots to the growth factor $1 + \frac{2}{1-\alpha}$ for one 2×2 pivot, which yields $\alpha = \frac{1+\sqrt{17}}{8} \approx 0.640$.

The Cholesky factorization

Let $A \in \mathbb{C}^{n \times n}$ be (self-adjoint) *positive definite*. Then A has a *unique* LDL* factorization $A = LDL^*$ since its principal submatrices are also positive definite, and moreover $D = (L^{-1})A(L^{-1})^*$ is positive definite. As a result, A has a *unique* **Cholesky factorization** $A = \tilde{L}\tilde{L}^*$, where $\tilde{L} \in \mathbb{C}^{n \times n}$ is lower triangular with *positive* diagonal entries, given by $\tilde{L} = L\sqrt{D}$.

Given a positive definite $A \in \mathbb{C}^{n \times n}$, we can also derive the Cholesky factorization directly: if

$$A = \begin{bmatrix} \alpha & c^* \\ c & B \end{bmatrix}$$

for some $\alpha \in \mathbb{C}$ (in fact, $\alpha \in \mathbb{R}_{>0}$ since A is positive definite), $c \in \mathbb{C}^{n-1}$, and $B \in \mathbb{C}^{(n-1)\times(n-1)}$, then

$$A = \begin{bmatrix} \sqrt{\alpha} & \\ \frac{c}{\sqrt{\alpha}} & I \end{bmatrix} \begin{bmatrix} 1 & \\ & B - \frac{cc^*}{\alpha} \end{bmatrix} \begin{bmatrix} \sqrt{\alpha} & \frac{c^*}{\sqrt{\alpha}} \\ & I \end{bmatrix},$$

and if $\tilde{L}'(\tilde{L}')^*$ is the Cholesky factorization of the Schur complement $A' = B - \frac{cc^*}{\alpha}$, then

$$A = \underbrace{\begin{bmatrix} \sqrt{\alpha} & \\ \frac{c}{\sqrt{\alpha}} & \tilde{L}' \end{bmatrix}}_{\tilde{L}} \underbrace{\begin{bmatrix} \sqrt{\alpha} & \frac{c^*}{\sqrt{\alpha}} \\ & (\tilde{L}')^* \end{bmatrix}}_{\tilde{L}^*}$$

is the Cholesky factorization of A.