What happens with

$$C = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad X_0 = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}.$$

The problem of determining when square roots of matrices exist and procedures for finding them are thoroughly investigated in Higham [91] (Chapter 6).

Problem 41.4. (1) Show that Newton's method applied to the function

$$f(x) = \alpha - \frac{1}{x}$$

with $\alpha \neq 0$ and $x \in \mathbb{R} - \{0\}$ yields the sequence (x_k) with

$$x_{k+1} = x_k(2 - \alpha x_k), \quad k \geq 0.$$

(2) If we let $r_k = 1 - \alpha x_k$, prove that $r_{k+1} = r_k^2$ for all $k \geq 0$. Deduce that Newton's method converges to $1/\alpha$ if $0 < \alpha x_0 < 2$.

Problem 41.5. (1) Show that Newton's method applied to the matrix function

$$f(X) = A - X^{-1},$$

with A and X invertible $n \times n$ matrices and started with any $n \times n$ matrix X_0 yields the sequence (X_k) with

$$X_{k+1} = X_k(2I - AX_k), \quad k \geq 0.$$

(2) If we let $R_k = I - AX_k$, prove that

$$R_{k+1} = I - (I - R_k)(I + R_k) = R_k^2$$

for all $k \geq 0$. Deduce that Newton's method converges to A^{-1} iff the spectral radius of $I - AX_0$ is strictly smaller than 1, that is, $\rho(I - AX_0) < 1$.

(3) Assume that A is symmetric positive definite and let $X_0 = \mu I$. Prove that the condition $\rho(I - AX_0) < 1$ is equivalent to

$$0 < \mu < \frac{2}{\rho(A)}.$$

(4) Write a `Matlab` program implementing Newton's method specified in (1). Test your program with the $n \times n$ matrix

$$A_n = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ldots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix},$$

and with $X_0 = \mu I_n$, for various values of n, including $n = 8, 10, 20$, and various values of μ such that $0 < \mu \leq 1/2$. Find some $\mu > 1/2$ causing divergence.