Problem 1

Since A is symmetric and has k distinct eigenvalues, the minimal polynomial of A has order k, then $\forall r_0 \in \mathbb{R}^n, m \geq k+1$, the Krylov subspace $\mathcal{K}(A, r_0, m) = \mathcal{K}(A, r_0, k+1)$. Then after k iterates of CG, x_{k+1} minimize $||x - x_*||_A$ in $\mathcal{K}(A, r_0, k+1) = \mathcal{K}(A, r_0, n) = \mathbb{R}^n$, hence converges.

Problem 2

Suppose we are going to use PCG on $Ax = b$, and the preconditioner (also symmetric and positive define) is M. Let C be the square root of M.
Let

$$
\begin{aligned}
\tilde{A} &= C^{-1} A C^{-1}, \\
\tilde{x} &= Cx, \\
\tilde{b} &= C^{-1} b,
\end{aligned}
$$

and we write the scheme of CG on $\tilde{A}\tilde{x} = \tilde{b}$:

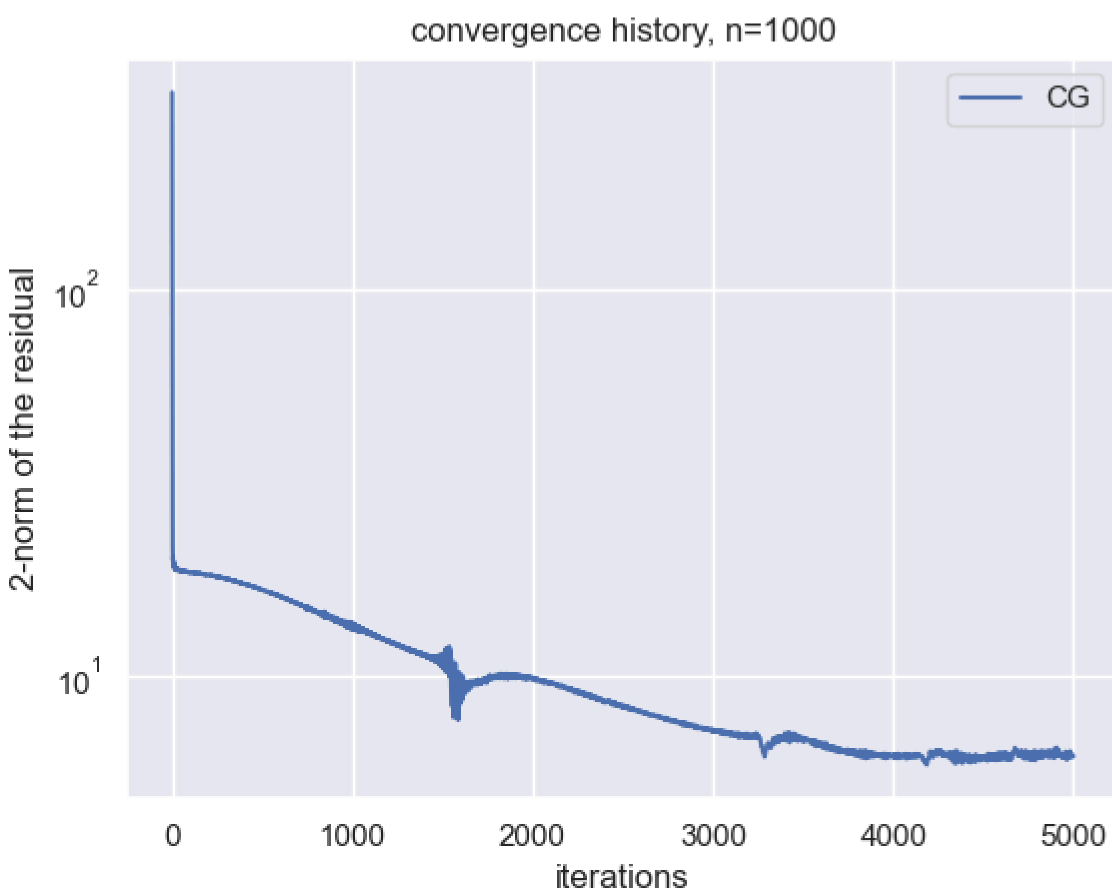
$$
\begin{aligned}
\tilde{r}_0 &= \tilde{b} - \tilde{A}\tilde{x}, \\
\tilde{p}_0 &= \tilde{r}_0, \\
\alpha_k &= \frac{\tilde{r}_k^T \tilde{r}_k}{\tilde{p}_k^T \tilde{A} \tilde{p}_k}, \\
\tilde{x}_{k+1} &= \tilde{x}_k + \alpha_k \tilde{x}_k, \\
\tilde{r}_{k+1} &= \tilde{r}_k - \alpha_k \tilde{A} \tilde{p}_k, \\
\beta_k &= \frac{\tilde{r}_{k+1}^T \tilde{r}_{k+1}}{\tilde{r}_k^T \tilde{r}_k}, \\
\tilde{p}_{k+1} &= \tilde{r}_{k+1} + \beta_k \tilde{p}_k.
\end{aligned}
$$

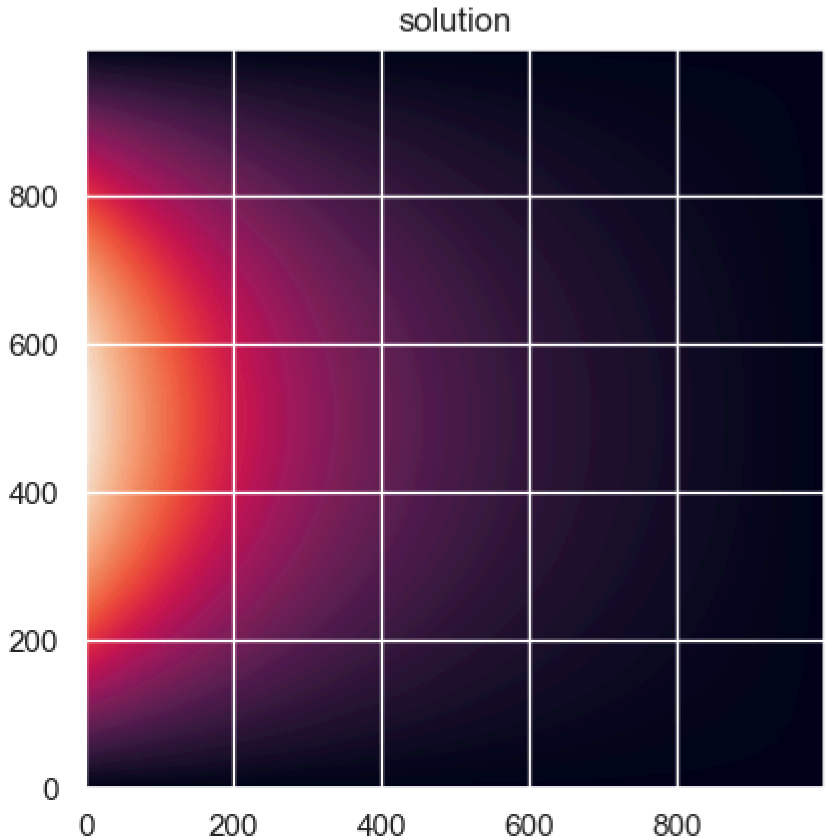
Substitute by $\tilde{x}_k = Cx_k, \tilde{r}_k = C^{-1} r_k, \tilde{p}_k = Cp_k$, we have

$$
\begin{aligned}
r_0 &= b - Ax_0, \\
p_0 &= M^{-1} r_0, \\
\alpha_k &= \frac{r_k^T M^{-1} r_k}{p_k^T A p_k}, \\
x_{k+1} &= x_k + \alpha_k p_k, \\
r_{k+1} &= r_k - \alpha_k A p_k, \\
\beta_k &= \frac{r_{k+1}^T M^{-1} r_{k+1}}{r_k^T M^{-1} r_k}, \\
p_{k+1} &= M^{-1} r_{k+1} + \beta_k p_k.
\end{aligned}
$$

Problem 3

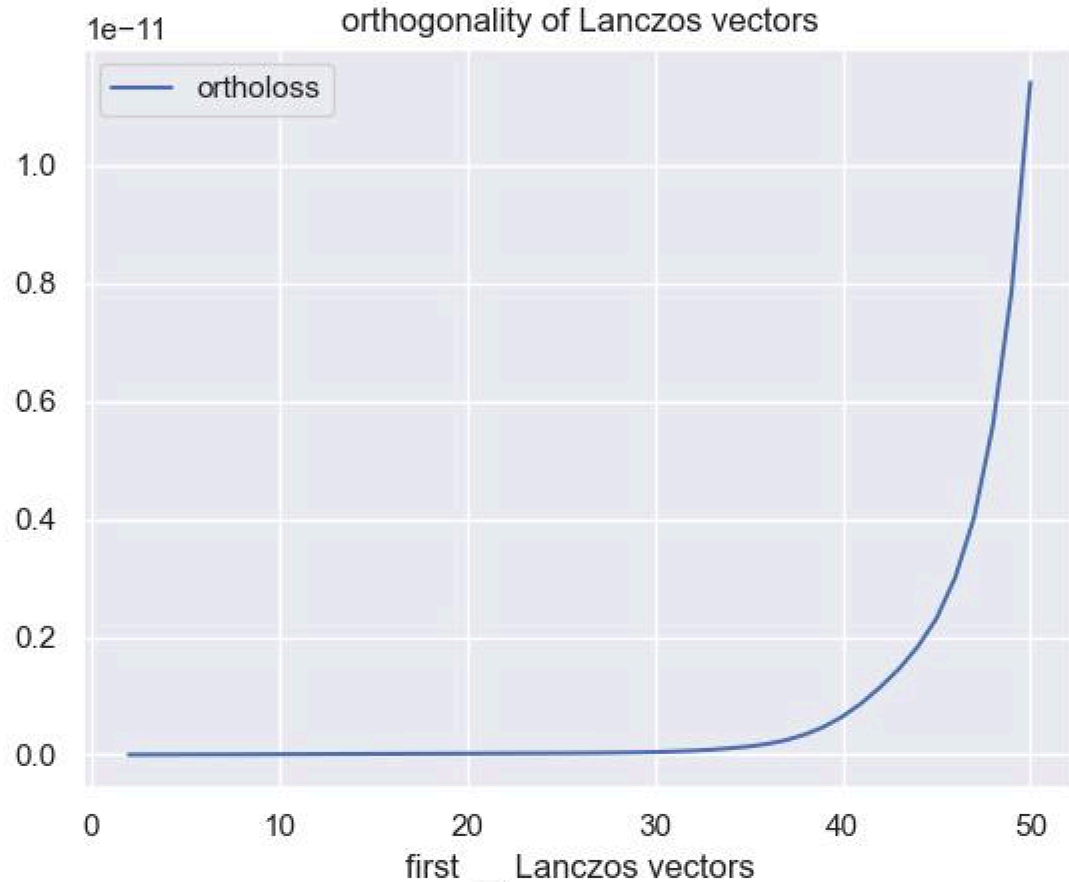
see `prob03.py`.

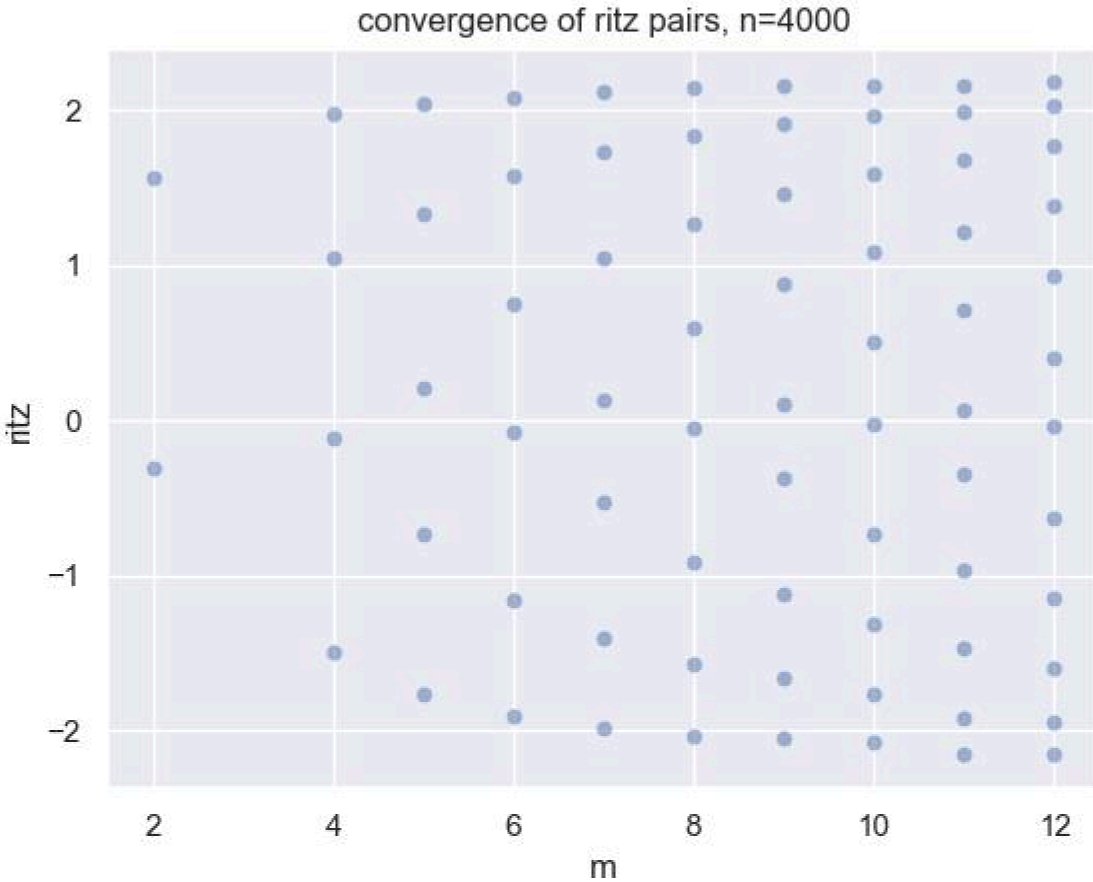




Problem 4

see `prob04.py`.


orthogonality of Lanczos vectors
1e−11
ortholoss
1.0
0.8
0.6
0.4
0.2
0.0
0
10
20
30
40
50
first __ Lanczos vectors



Problem 5

Since $f(A)$ is also symmetric,

$$(v-u)^T f(A)(v-u) = v^T f(A)v + u^T f(A)u - 2u^T f(A)v,$$
$$(v+u)^T f(A)(v+u) = v^T f(A)v + u^T f(A)u + 2u^T f(A)v,$$

then we can compute $u^T f(A)v$ by

$$u^T f(A)v = \frac{1}{4}((v+u)^T f(A)(v+u) - (v-u)^T f(A)(v-u)).$$