1. We want to solve the linear system $Ax = b$, where A is SPD. Consider the one-dimensional projection method

$$x_{k+1} = \arg \min_{x \in x_k + \mathrm{span}\{e_{i_k}\}} \|x - x_*\|_A, \tag{1}$$

where e_{i_k} is the i_k-th canonical basis and x_* is the true solution. If we choose $i_k = 1, \dots, n, 1, \dots, n, \dots$, then we obtain the Gauss-Seidel algorithm. Another better choice of i_k might be

$$i_k = \arg \max_{1 \le i \le n} |\langle x_k - x_*, e_i \rangle_A|, \tag{2}$$

i.e., we update the equation with the largest error.

(a) Construct an algorithm of (1)(2) such that the computational cost is $O(n)$ from x_k to x_{k+1}. The computation in your algorithm should be given explicitly.

(b) Prove that

$$\|x_* - x_{k+1}\|_A \le \left(1 - \frac{1}{n\gamma}\right)^{1/2} \|x_* - x_k\|_A,$$

where $\gamma = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$ is the 2-norm condition number of A.

(a) $$x_{k+1} = \arg\min_{x \in x_k + \mathrm{span}\{e_{i_k}\}} \|x - x_*\|_A$$

Since

$$\arg\min_{x \in x_k + \mathrm{span}\{e_{i_k}\}} \|x - x_*\|_A \iff \min_{t \in \mathbb{R}} \|x_k + te_{i_k} - x_*\|_A,$$

consider $$J(t) = \|x_k + te_{i_k} - x_*\|_A^2$$

$$= \|x_k - x_*\|_A^2 + 2t \langle e_{i_k}, x_k - x_* \rangle_A + t^2 \|e_{i_k}\|_A^2.$$

To get $\min_t J(t)$, we need $J'(t) = 0$,

which implies $$t = -\frac{\langle e_{i_k}, x_k - x_* \rangle_A}{\|e_{i_k}\|_A^2}.$$

Let $r_k = b - Ax_k$, then

$$\langle e_{i_k}, x_k - x_* \rangle_A = \langle e_{i_k}, A(x_k - x_*) \rangle$$

$$= -\langle e_{i_k}, r_k \rangle$$

$$= -r_k^{(i_k)}$$

$$\|e_{i_k}\|_A^2 = \langle e_{i_k}, Ae_{i_k} \rangle = a_{i_k, i_k}$$

Thus, we get $t_k = \dfrac{r_k^{(i_k)}}{a_{i_k, i_k}}$.

Hence, we get the algorithm,

> for $k = 1, 2, \cdots$
>
> $\quad r_k = b - Ax_k$
>
> $\quad i_k = \underset{1 \le i \le n}{\operatorname{argmax}} |r_k^{(i)}|$, $r_k^{(i)}$ is the i-th entry of r_k
>
> $\quad$ if $r_k = 0$, then x_k is the solution.
>
> $\qquad$ end.
>
> $\quad$ else
>
> $\qquad t_k = \dfrac{r_k^{(i_k)}}{a_{i_k, i_k}}$
>
> $\qquad x_{k+1} = x_k + t_k e_{i_k}$
>
> end.

We can verify that the computation cost is $O(n)$ from x_k to x_{k+1}.

(b) Since $x_{k+1} - x_* = x_k + t_k e_{i_k} - x_*$,

$$\|x_{k+1} - x_*\|_A^2 = \langle x_k - x_* + t_k e_{i_k}, x_k - x_* + t_k e_{i_k} \rangle_A$$

$$= \|x_k - x_*\|_A^2 + \langle t_k e_{i_k}, x_k - x_* \rangle_A$$

$$= \|x_k - x_*\|_A^2 - \langle r_k, t_k e_{i_k} \rangle$$

where $r_k = b - Ax_k$.

$$\langle r_k, t_k e_{i_k} \rangle = t_k r_k^{(i_k)}$$

$$= \frac{(r_k^{(i_k)})^2}{a_{i_k, i_k}}$$

$$= \frac{1}{a_{i_k, i_k}} |\langle b - Ax_k, e_{i_k} \rangle|^2$$

$$\ge \frac{1}{a_{i_k, i_k}} \frac{1}{n} \|b - Ax_k\|^2$$

due to $i_k = \arg\max_{1 \le i \le n} |r_k^{(i)}|$.

Moreover, A is SPD,

$$a_{i_k, i_k} \|x_k - x_*\|_A^2$$

$$\le \lambda_{max} \|x_k - x_*\|_A^2$$

$$= \gamma \lambda_{min} \|x_k - x_*\|_A^2$$

$$= \gamma \lambda_{min} \langle A(x_k - x_*), x_k - x_* \rangle$$

$$\le \gamma \langle A(x_k - x_*), A(x_k - x_*) \rangle$$

$$= \gamma \|Ax_k - b\|^2$$

we can get

$$\langle r_k, t_k e_{i_k} \rangle \ge \frac{1}{a_{i_k, i_k}} \frac{1}{n} \|b - Ax_k\|^2$$

$$\ge \frac{1}{\gamma n} \|x_k - x_*\|_A^2 .$$

Thus $\|x_{k+1} - x_*\|_A \le (1 - \frac{1}{\gamma n})^{1/2} \|x_k - x_*\|_A$

2. On the Chebychev polynomial C_k of degree k.

(a) Find k distinct real roots of C_k on $(-1, 1)$.

(b) Prove that $\frac{1}{2^{k-1}} C_k$ solves $\min_{p \in \mathbb{P}_k^{(1)}} \max_{t \in [-1,1]} |p(t)|$, where $p \in \mathbb{P}_k^{(1)}$ means p is a polynomial of degree at most k and the coefficient before the term t^k in $p(t)$ is 1.

(c) Prove the weighted orthogonality

$$\int_{-1}^{1} \frac{C_k(t) C_l(t)}{\sqrt{1-t^2}} dt = \begin{cases} \pi, & k = l = 0, \\ \pi/2, & k = l \neq 0, \\ 0, & k \neq l. \end{cases}$$

Chebychev polynomial: $C_n(x) = \cos(n \arccos x) \quad |x| \le 1$

(a) $\arccos x \in [0, \pi]$

$n \arccos x \in [0, n\pi]$

$C_n(x) = \cos(n \arccos x) = 0$ indicates

$n \arccos x_k = k\pi - \frac{\pi}{2} \quad k = 1, 2, \cdots, n$

i.e. $\arccos x_k = \frac{2k\pi - \pi}{2n}$

$x_k = \cos \frac{2k-1}{2n} \pi$

Thus the roots of $C_n(x)$ are $x_k = \cos \frac{2k-1}{2n}\pi$, $k=1,2,\cdots,n$

(b) ① We first prove $C_n(t) = 2t\, C_{n-1}(t) - C_{n-2}(t)$ with $C_0(t) = 1$, $C_1(t) = t$.

Let $t = \cos\theta$, $C_n(\cos\theta) = \cos(n\theta)$.

Note that $\cos(n\theta) = 2\cos\theta \cdot \cos(n-1)\theta - \cos(n-2)\theta$,

i.e. $C_n(t) = 2t\, C_{n-1}(t) - C_{n-2}(t)$.

② Then we prove that the coefficient before the term t^n in $C_n(t)$ is 2^{n-1}.

By induction,

1) $k=1$, $C_1(t) = 1$, satisfying the assumption.

2) $C_{n+1}(t) = 2t\,C_n(t) - C_{n-1}(t)$, indicating the coefficient before term t^{n+1} in $C_{n+1}(t)$ is 2^n.

Thus the coefficient before the highest order term $\frac{1}{2^{n-1}} C_n(t)$ is 1.

③ Let $q(t) \in \arg\min\limits_{p \in \mathbb{P}_k^{(1)}} \max\limits_{t\in[-1,1]} |p(t)|$. (Since $\mathbb{P}_k^{(1)}$ is a space with finite dimension, $\arg\min\limits_{p\in\mathbb{P}_k^{(1)}} \max\limits_{t\in[-1,1]} |p(t)| \neq \phi$)

By the above definition, we have

$$\max_{t\in[-1,1]} |q(t)| \leq \max_{t\in[-1,1]} \frac{1}{2^{k-1}} |C_k(t)| = \frac{1}{2^{k-1}}.$$

Assume $\max\limits_{t\in[-1,1]} |q(t)| < \frac{1}{2^{k-1}}$.

For $C_k(t) = \cos(k \arccos t)$,

$$\frac{1}{2^{k-1}} C_k\left(\cos\frac{2j\pi}{k}\right) = \frac{1}{2^{k-1}}$$

$$\frac{1}{2^{k-1}} C_k\left(\cos\frac{(2j+1)\pi}{k}\right) = -\frac{1}{2^{k-1}}$$

for any $0 \leq 2j,\ 2j+1 \leq k$.

Let $f(t) = \frac{1}{2^{k-1}} C_k(t) - q(t) \in \mathbb{P}_{k-1}$

then $f(t) > 0$ when $t = \cos \frac{2j\pi}{k}$

and $f(t) < 0$ when $t = \cos \frac{(2j+1)\pi}{k}$.

Since $f(t)$ is continuous, from the intermediate value theorem, $f(t)$ has at least k roots.

However, it is impossible, as $f(t) \in \mathbb{P}_{k-1}$ and the fundamental theorem of algebra implies it has at most $k-1$ roots.

Thus $\max_{t\in[-1,1]} |q(t)| = \frac{1}{2^{k-1}} = \max_{t\in[-1,1]} \frac{1}{2^{k-1}} |C_k(t)|$ and

$$\frac{1}{2^{k-1}} C_k(t) \in \arg\min_{p \in \mathbb{P}_k^{(1)}} \max_{t\in[-1,1]} |p(t)| .$$

(C) $C_k(t) = \cos(k \arccos t)$

Let $t = \cos\theta$.

$$\int_{-1}^{1} \frac{C_k(t)\, C_l(t)}{\sqrt{1-t^2}}\, dt$$

$$= \int_0^{\pi} \cos k\theta \cdot \cos l\theta \, d\theta$$

$$= \int_0^{\pi} \frac{1}{2} \left[\cos (k+l)\theta + \cos(k-l)\theta\right] d\theta$$

$$= \begin{cases} \pi, & k = l = 0 \\ \frac{\pi}{2}, & k = l \neq 0 \\ 0, & k \neq l \end{cases}$$

3. The CG algorithm can also be applied to general non-symmetric linear systems. Let $A \in \mathbb{R}^{n\times n}$ be a general non-singular matrix. To solve $Ax = b$, we have two possible approaches to apply CG.

   (a) We apply CG to $A^TAx = A^Tb$, which is equivalent to $Ax = b$ and the coefficient matrix A^TA is SPD. Write out the algorithm, where the matrix-vector products Az and A^Tz with an input z are allowed to use for only once respectively in each iteration. This algorithm is called *Conjugate Gradient Normal Equation Residual* (CGNR) method.

   (b) We apply CG to $AA^Ty = b$ and $x = A^Ty$. This is again equivalent to $Ax = b$ and AA^T is SPD. Write out the algorithm, where the matrix-vector products Az and A^Tz with an input z are allowed to use for only once respectively in each iteration. This algorithm is called *Conjugate Gradient Normal Equation Error* (CGNE) method.

Note that in both CGNR and CGNE, the condition number of the coefficient matrix is $\kappa^2(A)$, where $\kappa(A)$ the condition number of A. Therefore, both of their convergence factor is $\frac{\kappa-1}{\kappa+1}$ instead of $\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$ when A is SPD with standard CG. Nevertheless, CGNR and CGNE can have a fast convergence if singular values of A (i.e., square root of eigenvalues of A^TA and AA^T) have a good clustering.

(a) We apply CG to $A^TAx = A^Tb$.

Set $d_0 = 0$

For $k = 1, 2, \cdots$

$$r_k = A^Tb - A^TAx_k$$

$$\beta_k = -\frac{\langle r_k, A^TAd_{k-1}\rangle}{\langle d_{k-1}, A^TAd_{k-1}\rangle}$$

$$d_k = r_k + \beta_k d_{k-1}$$

$$\alpha_k = \frac{\langle d_k, r_k\rangle}{\langle A^TAd_k, d_k\rangle}$$

$$x_{k+1} = x_k + \alpha_k d_k$$

end.

(b) We apply CG to $AA^Ty = b$ and $x = A^Ty$.

Set $d_0 = 0$

For $k = 1, 2, \cdots$

$$r_k = b - AA^Ty_k$$

$$\beta_k = -\frac{\langle r_k, AA^Td_{k-1}\rangle}{\langle d_{k-1}, AA^Td_{k-1}\rangle}$$

$$d_k = r_k + \beta_k d_{k-1}$$

$$\alpha_k = \frac{\langle d_k, r_k\rangle}{\langle AA^Td_k, d_k\rangle}$$

$$y_{k+1} = y_k + \alpha_k d_k$$

end.