Problem 1

We have seen the application of the conjugate gradient algorithm on the solution of symmetric, positive definite systems. Now assume that in the system \( Ax = b \), the \( n \times n \) matrix \( A \) is symmetric positive semi-definite with a nullspace of dimension \( p < n \). This problem illustrates that one can use a modified version of conjugate gradients to solve this system as well.

1. Prove that we can write \( A \) as
   \[
   A = M\tilde{A}M^T
   \]
   where \( M \) is an \( n \times (n-p) \) matrix with orthonormal columns that form a basis for the column space of \( A \), while \( \tilde{A} \) is an \( (n-p) \times (n-p) \) symmetric positive definite matrix (no nullspace) [Hint: Use the diagonal form of \( A = Q\Lambda Q^T \)]

2. Let the \( n \times n \) matrix \( P \) be defined as \( P = MM^T \). Explain (no formal proof required) why this is a projection matrix and onto what space it projects. How can we compute \( P \) without knowledge of the eigenvalues-eigenvectors of \( A \)?

3. Show that, in order to have a solution to \( Ax = b \), we must be able to write
   \[
   b = M\tilde{b}
   \]
   for an appropriate vector \( \tilde{b} \in \mathbb{R}^{n-p} \)

4. Let \( \tilde{x} \) be the solution to the system \( \tilde{A}\tilde{x} = \tilde{b} \) and explain why \( \tilde{x} \) is unique. Show that any solution to the original system \( Ax = b \) can be written as \( x = M\tilde{x} + x_0 \) where \( x_0 \) is in the nullspace of \( A \).

5. Consider the conjugate gradients algorithm for solving \( \tilde{A}\tilde{x} = \tilde{b} \)
   \[
   \begin{align*}
   \tilde{x}_0 & = \text{initial guess} \\
   \tilde{s}_0 & = \tilde{r}_0 = \tilde{b} - \tilde{A}\tilde{x}_0 \\
   \text{for } k = 0, 1, \ldots, 2 \\
   \tilde{\alpha}_k & = \frac{\tilde{r}_k^T\tilde{r}_k}{\tilde{s}_k^T\tilde{A}\tilde{s}_k} \\
   \tilde{x}_{k+1} & = \tilde{x}_k + \tilde{\alpha}_k\tilde{s}_k \\
   \tilde{r}_{k+1} & = \tilde{r}_k - \tilde{\alpha}_k\tilde{A}\tilde{s}_k \\
   \tilde{s}_{k+1} & = \tilde{r}_{k+1} + \frac{\tilde{r}_{k+1}^T\tilde{r}_{k+1}}{\tilde{r}_k^T\tilde{r}_k}\tilde{s}_k
   \end{align*}
   \]
   end
Show that we can compute a solution to the original system $Ax = b$ by using the following modification of the algorithm

$$
x_0 = \text{initial guess}
$$

$$
s_0 = r_0 = P(b - Ax_0)
$$

for $k = 0, 1, \ldots, 2$

$$
\alpha_k = \frac{r_k^T r_k}{s_k^T A s_k}
$$

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

$$
r_{k+1} = r_k - \alpha_k P A s_k
$$

$$
s_{k+1} = r_{k+1} + \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k} s_k
$$

end

[Hint: Show that $x_k = M \tilde{x}_k$, $r_k = M \tilde{r}_k$, $s_k = M \tilde{s}_k$, $\tilde{\alpha}_k = \alpha_k$]

**Problem 2**

Consider a real function $f(x)$ that is differentiable on an interval $[a, b]$.

1. Find a quadratic polynomial $g(x)$ that approximates $f(x)$ on $[a, b]$ such that $f'(a) = g'(a)$, $f'(b) = g'(b)$ and $f \left( \frac{a+b}{2} \right) = g \left( \frac{a+b}{2} \right)$ [Hint: Consider expressing $g(x)$ as a quadratic polynomial of $\left( x - \frac{a+b}{2} \right)$].

2. Define a numerical quadrature rule for $\int_a^b f(x) \, dx$ by integrating the interpolant $g(x)$ on $[a, b]$.

3. Prove that this integration scheme has degree of accuracy equal to 3.

4. Define the corresponding composite quadrature rule for $\int_a^b f(x) \, dx$ we obtain by subdividing $[a, b]$ into the $n$ sub-intervals $[a + k \frac{b-a}{n}, a + (k+1) \frac{b-a}{n}]$.

**Problem 3**

The first order divided difference is given by

$$
f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}.
$$

When $x_0$ is close to $x_1$ we have the approximation

$$
f[x_0, x_1] \approx f' \left( \frac{x_0 + x_1}{2} \right)
$$

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Now let $z = (x_0 + x_1)/2$, $h = (x_1 - x_0)/2$ then the error is given as

$$E = f[x_0, x_1] - f' \left( \frac{x_0 + x_1}{2} \right) = \frac{f(z + h) - f(z - h)}{2h} - f'(z)$$

Prove that the error is

$$E = \frac{h^2}{6} f'''(z) + O(h^3)$$