The first two questions are about **natural cubic splines**.

A cubic spline is a piecewise polynomial $S_3(x) \in C^2([a,b])$ such that

❶ $S_3(x_i) = f_i := f(x_i)$ for $i \in \{0, 1, \ldots, n\}$ and

❷ $S_3(x)$ is a cubic polynomial on $\Omega_i = [x_{i-1}, x_i]$ for $i \in 1, 2, \ldots, n$.

A *natural* cubic spline also satisfies the end conditions

$$S_3''(x_0) = 0 = S_3''(x_n).$$

Suppose we want to construct such a spline approximation with a uniformly spaced set of knots $K = \{x_i\}_{i=0}^n = \{a + ih\}_{i=0}^n$ on $\overline{\Omega} = [a,b]$ (so that $n = (b-a)/h$). The condition $S_3(x) \in C^2([a,b])$ requires that

$$S_3'(x_i)\big|_{\Omega_i} = S_3'(x_i)\big|_{\Omega_{i+1}} \qquad \text{and} \qquad S_3''(x_i)\big|_{\Omega_i} = S_3''(x_i)\big|_{\Omega_{i+1}}$$

for all *interior* data points x_i, $i = 1, \ldots, n-1$.

The simplest construction is to define $\sigma_i = S_3''(x_i)$, $i = 0, 1, \ldots, n$, and notice that $S_3''(x)$ is a linear function on Ω_i so that

$$S_3''(x) = \frac{x_i - x}{h}\sigma_{i-1} + \frac{x - x_{i-1}}{h}\sigma_i, \qquad x \in \Omega_i, \qquad i = 1, 2 \ldots, n.$$

Integrating twice gives two constants of integration, α_i and β_i, say, which are uniquely determined by the conditions $S_3(x_{i-1}) = f_{i-1}$, $S_3(x_i) = f_i$.

1. (a) Use the suggested method of construction to derive an explicit expression for $S_3(x)$ over the subinterval Ω_i.

   (b) Next, show that enforcing the continuity of $S_3'(x)$ at the *interior* knots $\{x_i\}_{i=1}^{n-1}$, leads to a tridiagonal system of linear equations,

   $$A\boldsymbol{\sigma} = \mathbf{b},$$

   for the unknowns $\sigma_i, i = 1, 2, \ldots, n-1$, where A has diagonal entries $A_{i,i} = \frac{2h}{3}$, off-diagonal entries $A_{i,i-1} = \frac{h}{6} = A_{i,i+1}$ and the right-hand side vector coefficients are given by $b_i = \frac{1}{h}(f_{i+1} - 2f_i + f_{i-1})$.

2. (a) Let $f(x) = x^3$ on $[0,1]$ and let $S_3(x)$ be the natural cubic spline interpolant of f constructed with uniformly spaced points (with $n \geq 2$). If we choose the natural conditions $\sigma_0 = 0 = \sigma_n$, show that the values $\sigma_i = f''(x_i)$ for $i = 1, \ldots, n-1$ do not satisfy the linear system $A\boldsymbol{\sigma} = \mathbf{b}$ derived in question 1(b). (This shows that the natural cubic spline interpolant S_3 is not equal to f, even though f is cubic).

   (b) Show that when we choose $\sigma_0 = f''(0)$ and $\sigma_n = f''(1)$ we have $\sigma_i = f''(x_i)$ for all $i = 1, \ldots, n-1$. Deduce then that the associated cubic spline interpolant $S_3(x)$ is identical to $f(x) = x^3$ on $[0,1]$.

The next two questions focus on **quadratic splines**.

3. (a) Consider a piecewise quadratic spline function $s(x)$, that interpolates a function $f(x)$ at a set of knots $K = \{x_i\}_{i=0}^n$ with $a = x_0$, $x_n = b$ and $h_i = x_i - x_{i-1}$. This interpolant $s(x)$ is characterised by three unknown coefficients in each subinterval $\Omega_i = [x_{i-1}, x_i]$. Show that if $s(x)$ is written in the form

$$s(x) = a_i + b_i(x - x_{i-1}) + c_i(x - x_{i-1})(x - x_i), \qquad x \in \Omega_i,$$

then the interpolation conditions $s(x_{i-1}) = f_{i-1}$, $s(x_i) = f_i$ uniquely determine the coefficients a_i and b_i.

(b) In addition, show that requiring $s(x) \in C^1([a, b])$ means that

$$c_{i+1} = -\frac{1}{h_{i+1}} \left\{ c_i h_i + \left(\frac{f_i - f_{i-1}}{h_i} \right) - \left(\frac{f_{i+1} - f_i}{h_{i+1}} \right) \right\},$$

for $i = 1, \ldots, n-1$, so that the spline function $s(x)$ on $[a, b]$ is uniquely specified by setting the value of c_1.

4. (a) Suppose that the quadratic spline interpolant $s(x)$ is applied to two data sets differing only in the first value, f_0 and f_0^* say, and assume that the data is equally spaced so that $h = h_i, i = 1, 2, \ldots, n$. Denote the two resulting interpolants by $s(x)$ and $s^*(x)$ and suppose that the same initial value $c_1 = c_1^*$ is specified for each. Use proof by induction to show that

$$c_i^* = c_i + \frac{(-1)^i}{h^2}(f_0^* - f_0), \quad i = 2, \ldots, n.$$

(b) Deduce then that

$$s^*(x) = s(x) + \frac{(-1)^i}{h^2}(f_0^* - f_0)(x - x_{i-1})(x - x_i), \qquad x \in \Omega_i,$$

for $i = 1, \ldots, n$. (This means that a small change in the first data point will be propagated undamped throughout the domain of interpolation. This is why quadratic splines are rarely used in practice).

The focus of the final two questions is **least-squares data fitting**, otherwise known as 'best $L^2(\Omega)$ approximation'.

5. Let $\Omega = (0, 1)$. Instead of being required to interpolate a function f at a chosen set of knots $K = \{x_i\}_{i=0}^n$, suppose a linear spline approximation $S_1(x)$ is constructed to minimise $||f - S_1||_{L^2(\Omega)}$. By writing $S_1(x)$ as a linear combination of linear 'hat' functions

$$S_1(x) = \sum_{i=0}^{n} \alpha_i \phi_i(x),$$

use calculus to show that the coefficients $\{\alpha_i\}_{i=0}^n$ can be computed by solving a linear system of $n+1$ linear equations

$$Q\boldsymbol{\alpha} = \boldsymbol{b}, \qquad (\star)$$

where Q has entries given by

$$Q_{i,\,j} = \int_0^1 \phi_i(x)\phi_j(x)\,dx$$

for $i, j = 0, 1, \ldots, n$ and the entries of $\boldsymbol{b}$ are

$$b_i = \int_0^1 f(x)\phi_i(x)\,dx,$$

for $i = 0, 1, \ldots, n$. [Note that here the counter i starts at zero so the (1,1) entry of Q is $Q_{0,0}$ and the first entry of of $\mathbf{b}$ is b_0].

6. (a) Suppose that the knots in the previous question are equally spaced. Use properties of the hat functions $\phi_i(x)$ to show that Q is a symmetric and tridiagonal matrix with diagonal entries

$$Q_{0,\,0} = \frac{h}{3}, \quad Q_{i,\,i} = \frac{2h}{3}, \quad i = 1, \ldots, n-1, \quad Q_{n,\,n} = \frac{h}{3}$$

and off-diagonal entries $Q_{i,\,i-1} = \frac{h}{6} = Q_{i,\,i+1}$.

[Hint: the easiest way to integrate a quadratic or cubic function $f(x)$ over an interval (a, b) is to use Simpson's quadrature rule:

$$\int_a^b f(x)dx = S := \frac{h}{6}(f_a + 4f_m + f_b),$$

where m is the midpoint of the interval and $h = b - a$.]

(b) Consider $f(x) = x$. Verify that the ith equation in the system $(\star)$ is satisfied with $\alpha_i = ih$ for $i = 0, 1, 2, \ldots, n$. Deduce then that $S_1(x) = f(x)$ on $[0, 1]$.