## Homework 8

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## Problem 1

(a)

Since g is a natural cubic spline interpolant to the pairs  $(x_n, z_n)$  (n = 1, ..., N), where  $a < x_1 < ... < x_N < b$ , so g''(x) = 0 and g'''(x) = 0 for x in the two end intervals  $[a, x_1] \cup [x_N, b]$ , and that  $g'''(x) = g'''(x_n^+)$  for  $\forall x \in [x_n, x_{n+1}]$ 

Also, since  $\tilde{g}$  is any other twice differentiable function on [a,b] that interpolates the pairs  $(x_n,z_n)$  (n=1,...,N), so at the knots  $x_n$ 's we have:  $\tilde{g}(x_n)=g(x_n)=z_n$  (n=1,...,N), thus  $h(x_n)=g(x_n)-\tilde{g}(x_n)=0$  (n=1,...,N).

Therefore:

$$\int_{a}^{b} g''(x)h''(x)dx = \int_{a}^{b} g''(x)dh'(x) = g''(x)h'(x)|_{a}^{b} - \int_{a}^{b} h'(x)dg''(x) = g''(b)h'(b) - g''(a)h'(a) - \int_{a}^{b} g'''(x)h'(x)dx$$

$$= 0 - \int_{x_{1}}^{x_{N}} g'''(x)h'(x)dx = -\sum_{n=1}^{N-1} \int_{x_{n}}^{x_{n+1}} g'''(x)h'(x)dx = -\sum_{n=1}^{N-1} g'''(x_{n}^{+}) \int_{x_{n}}^{x_{n+1}} h'(x)dx = -\sum_{n=1}^{N-1} g'''(x_{n}^{+}) h(x)|_{x_{n}}^{x_{n+1}}$$

$$= -\sum_{n=1}^{N-1} g'''(x_{n}^{+}) [h(x_{n+1}) - h(x_{n})] = -\sum_{n=1}^{N-1} g'''(x_{n}^{+}) [0 - 0] = 0$$

(b)

In question (a), we have derived that:

$$\int_{a}^{b} g''(x)h''(x)dx = 0 \quad \Rightarrow \quad \int_{a}^{b} g''(x) \left[ g''(x) - \tilde{g}''(x) \right] dx = 0 \quad \Rightarrow \quad \int_{a}^{b} g''(x)^{2} dx = \int_{a}^{b} g''(x)\tilde{g}''(x) dx$$

Therefore, by Cauchy-Schwarz Inequality, we can obtain that:

$$\left(\int_{a}^{b} g''(x)^{2} dx\right)^{2} = \left(\int_{a}^{b} g''(x)\tilde{g}''(x)dx\right)^{2} \le \left(\int_{a}^{b} g''(x)^{2} dx\right) \left(\int_{a}^{b} \tilde{g}''(x)^{2} dx\right)$$

$$\Rightarrow \int_{a}^{b} g''(x)^{2} dx \le \int_{a}^{b} \tilde{g}''(x)^{2} dx$$

where the equality holds when there exists a nonzero constant C such that  $\tilde{g}''(x) = Cg''(x)$  for  $\forall x \in [a, b]$ .

Since g is a natural cubic spline interpolant to the pairs  $(x_n, z_n)$  (n = 1, ..., N), so when  $\tilde{g}''(x) = Cg''(x)$ , we have:  $\tilde{g}(x) = Cg(x) + A + Bx$  for  $\forall x \in [a, b]$ , where A and B are also constants. Because  $\tilde{g}(x_n) = g(x_n) = z_n$  at all the knots  $x_n$ 's (n = 1, ..., N), hence at the knots we have:  $(1 - C)g(x_n) = A + Bx_n$ . If  $C \neq 1, A \neq 0, B \neq 0$ , then g becomes a linear or constant function that can pass through all the  $(x_n, z_n)$  points, which contradicts the fact that g is a natural cubic spline. As a result, it must be that C = 1, A = B = 0. So we obtain that the equality holds only when  $\tilde{g}''(x) = g''(x)$  and  $\tilde{g}(x) = g(x)$  for  $\forall x \in [a, b]$ .

Therefore, the equality holds only when  $h(x) = g(x) - \tilde{g}(x) = 0$  for  $\forall x \in [a, b]$ .

(c)

Suppose  $\hat{f}$  is the minimizer of the penalized least squares problem, i.e.:

$$\min_{f \in F} \left[ \sum_{n=1}^{N} (Y_n - f(X_n))^2 + \lambda \int_a^b f''(x)^2 dx \right] = \sum_{n=1}^{N} \left( Y_n - \hat{f}(X_n) \right)^2 + \lambda \int_a^b \hat{f}''(x)^2 dx$$

Set  $\hat{f}(X_n) = Z_n$  (n = 1, ..., N), since  $\hat{f}$  is a function with continuous second derivatives on [a, b], so  $\hat{f}$  can be seen as a twice differentiable function on [a, b] that interpolates the pairs  $(X_n, Z_n)$  (n = 1, ..., N), which has all the properties that the function  $\tilde{g}$  has in question (a) and (b).

Next, we can generate a function g, which is a natural cubic spline interpolant to the pairs  $(X_n, Z_n)$  (n = 1, ..., N), so at the knots  $X_n$ 's we have:  $g(X_n) = \hat{f}(X_n) = Z_n$  (n = 1, ..., N), and that:  $\int_a^b \hat{f}''(x)^2 dx \ge \int_a^b g''(x)^2 dx$ , where the equality holds only when  $\hat{f}(x) = g(x)$  for  $\forall x \in [a, b]$ .

Since  $\lambda > 0$ , therefore:

$$\min_{f \in F} \left[ \sum_{n=1}^{N} \left( Y_n - f(X_n) \right)^2 + \lambda \int_a^b f''(x)^2 dx \right] = \sum_{n=1}^{N} \left( Y_n - \hat{f}(X_n) \right)^2 + \lambda \int_a^b \hat{f}''(x)^2 dx \ge \sum_{n=1}^{N} \left( Y_n - g(X_n) \right)^2 + \lambda \int_a^b g''(x)^2 dx$$

Since  $\hat{f}$  is the minimizer, thus the equality must holds here, otherwise function g will further minimize the penalized least squares problem which contradicts the fact that  $\hat{f}$  is the minimizer. And the equality holds only when  $\hat{f}(x) = g(x)$  for  $\forall x \in [a, b]$ .

Therefore, the minimizer of the penalized least squares problem must be a natural cubic spline with knots at the points  $X_n$  (n = 1, ..., N).