

Examination in School of Mathematical Sciences
Semester 2, 2016

107352 APP MTH 3022 Optimal Functions and Nanomechanics III
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Official Reading Time: 10 mins
Writing Time: 120 mins
Total Duration: 130 mins

NUMBER OF QUESTIONS: 5 TOTAL MARKS: 60

Instructions

- Attempt all questions.
- Begin each answer on a new page.
- Examination materials must not be removed from the examination room.

Materials

- 1 Blue book is provided.
- Formulae sheets are provided.
- Only scientific calculators with basic capabilities are permitted. Graphics calculators are not permitted.

DO NOT COMMENCE WRITING UNTIL INSTRUCTED TO DO SO.

1. Consider the functional

$$F\{y\} = \int_0^1 xy^2y'^3 dx.$$

- (a) If we constrain our investigation of possible functions for y to $y(x) = x^\epsilon$, what is the value of $\epsilon > 1/5$ which leads to an extremum of F .
- (b) What value does the functional take for this value of ϵ .
- (c) Is this a maximum or a minimum? Justify your answer.

[8 marks]

2. Find the extremals for the following functionals:

(a) $F\{y\} = \int_0^1 (y^2 - y'^2 - 2y \sin x) dx, \quad y(0) = 0, \quad y(1) = 1.$

(b) $F\{y\} = \int_0^1 \left(\frac{1}{2}y'^2 + yy' + y' + y \right) dx, \quad y(0) = 0, \quad y(1) = \frac{3}{2}.$

(c) $F\{y\} = \int_0^1 (y''^2 - 360x^2y) dx, \quad y(0) = 0, \quad y'(0) = 1, \quad y(1) = 1, \quad y'(1) = 5/2.$

[18 marks]

3. (a) From the integral definitions given on the formula sheet show that

$$K(k) = \frac{\pi}{2} F(1/2, 1/2; 1; k^2).$$

- (b) A spheroidal surface \mathcal{P} is given parametrically by the position vector $\mathbf{x}(\theta, \phi)$ as

$$\mathbf{x}(\theta, \phi) = (b \cos \theta \sin \phi, b \sin \theta \sin \phi, c \cos \phi),$$

where $-\pi < \theta \leq \pi$, and $0 \leq \phi \leq \pi$ and the constant b is the minor semi-axis length and c is the major semi-axis length.

- (i) Derive an expression for the scalar surface element dA for \mathcal{P} .
- (ii) Integrate your answer from part (i) to find the surface area of \mathcal{P} as a function of b and c .

Hint: it is easiest to express this in terms of a hypergeometric function.

[13 marks]

4. Consider the functional

$$F\{y\} = \int_0^1 \left(\frac{1}{2}y' + \frac{1}{2}y^2 - y \right) dx,$$

subject to the end-point constraints $y(0) = 0$, $y(1) = 0$. Moreover consider a Ritz trial function of the form

$$y_n = \phi_0 + \sum_{i=1}^n c_i \phi_i.$$

- Write down the approximate solution (with one undetermined coefficient) y_1 , by assuming $\phi_0 = 0$ and $\phi_i = x^i(1-x)^i$.
- Determine a function $F(c_1)$ which approximates the functional for the y_1 from part (a).
- Determine the value of c_1 that leads to an extremal value for $F(c_1)$.
- Is this extremum a maximum or minimum? Justify your answer.

[6 marks]

5. Consider the problem of finding extremals curves for

$$F\{y\} = \int_0^1 (y'^2 + x^2) dx,$$

subject to $y(0) = y(1) = 0$, and the integral constraint

$$G\{y\} = \int_0^1 y^2 dx = 2.$$

- Using the method of Lagrange multipliers, form a new functional $H\{y\}$ which incorporates the original functional $F\{y\}$ and the integral constraint.
- Derive the Euler-Lagrange equation for $H\{y\}$.
- Show that the only non-trivial solutions to the Euler-Lagrange equation and boundary conditions involve trigonometric functions and a discrete spectrum of Lagrange multipliers.
- Thus find the curve or curves y that is both an extremal of $F\{y\}$ and satisfies the constraint $G\{y\} = 2$. Calculate the value of $F\{y\}$ for this extremal.

Hint: You may find the following results useful

$$\int_0^1 \cos^2(n\pi x) dx = \int_0^1 \sin^2(n\pi x) dx = \frac{1}{2}, \quad \text{for } n = 1, 2, 3, \dots$$

[15 marks]

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Please turn over for page 5

Formula Sheet, Special Functions

Gamma function, definition	$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt, \quad \text{for } \Re(z) > 0.$
Gamma function, duplication	$\Gamma(2z) = 2^{2z-1} \pi^{-1/2} \Gamma(z) \Gamma(z + 1/2).$
Beta function, definition	$B(x, y) = \int_0^1 t^{x-1} (1-t)^{y-1} dt, \quad \text{for } \Re(x), \Re(y) > 0.$
Beta function, gamma relation	$B(x, y) = \frac{\Gamma(x) \Gamma(y)}{\Gamma(x+y)}.$
Pochhammer symbol, definition	$(a)_n = a(a+1)(a+2) \cdots (a+n-1) = \frac{\Gamma(a+n)}{\Gamma(a)}.$
Hypergeometric function, series	$F(a, b; c; z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n n!} z^n.$
Hypergeometric function, integral	$F(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(b) \Gamma(c-b)} \times \int_0^1 t^{b-1} (1-t)^{c-b-1} (1-tz)^{-a} dt.$
Hypergeometric function, derivative	$\frac{d^n}{dz^n} F(a, b; c; z) = \frac{(a)_n (b)_n}{(c)_n} F(a+n, b+n; c+n; z).$
Elliptic integral, first kind	$F(\varphi, k) = \int_0^\varphi \frac{d\vartheta}{\sqrt{1 - k^2 \sin^2 \vartheta}}.$
Elliptic integral, second kind	$E(\varphi, k) = \int_0^\varphi \sqrt{1 - k^2 \sin^2 \vartheta} d\vartheta.$
Complete elliptic integrals	$K(k) = F\left(\frac{\pi}{2}, k\right), \quad E(k) = E\left(\frac{\pi}{2}, k\right).$
Lennard-Jones potential	$\Phi(\rho) = -\frac{A}{\rho^6} + \frac{B}{\rho^{12}}.$

Formula Sheet, Variational

Theorem 2.2.1: Let $F : C^2[x_0, x_1] \rightarrow \mathbb{R}$ be a functional of the form

$$F\{y\} = \int_{x_0}^{x_1} f(x, y, y') dx,$$

where f has continuous partial derivatives of second order with respect to x , y , and y' , and $x_0 < x_1$. Let

$$S = \{y \in C^2[x_0, x_1] \mid y(x_0) = y_0, y(x_1) = y_1\},$$

where y_0 and y_1 are real numbers. If $y \in S$ is an extremal for F , then for all $x \in [x_0, x_1]$

$$\boxed{\frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) - \frac{\partial f}{\partial y} = 0} \quad \text{The Euler-Lagrange equation}$$

Theorem 2.3.1: Let J be a functional of the form

$$J\{y\} = \int_{x_1}^{x_2} f(y, y') dx$$

and define the function H by

$$H(y, y') = y' \frac{\partial f}{\partial y'} - f(y, y')$$

Then H is constant along any extremal of y .

Generalisation: Let $F : C^2[x_0, x_1] \rightarrow \mathbb{R}$ be a functional of the form

$$F\{y\} = \int_{x_0}^{x_1} f(x, y, y', \dots, y^{(n)}) dx,$$

where f has continuous partial derivatives of second order with respect to $x, y, y', \dots, y^{(n)}$, and $x_0 < x_1$, and the values of $y, y', \dots, y^{(n-1)}$ are fixed at the end-points, then the extremals satisfy the condition

$$\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} + \frac{d^2}{dx^2} \frac{\partial f}{\partial y''} + \dots + (-1)^n \frac{d^n}{dx^n} \frac{\partial f}{\partial y^{(n)}} = 0$$

Natural boundary condition: When we extend the theory to allow a free x and y , we find the additional constraint

$$\left[p \delta y - H \delta x \right]_{x_0}^{x_1} = 0,$$

where $p = f_{y'}$ and $H = y' f_{y'} - f$.

Weierstrass-Erdman corner conditions: For a broken extremal

$$p \Big|_{x^{*-}} = p \Big|_{x^{*+}}, \quad H \Big|_{x^{*-}} = H \Big|_{x^{*+}},$$

must hold at any “corner”.