

Examination in School of Mathematical Sciences
Semester 2, 2017

107355 APP MTH 7106 Optimal Functions and Nanomechanics

Official Reading Time: 10 mins

Writing Time: 180 mins

Total Duration: 190 mins

NUMBER OF QUESTIONS: 8 TOTAL MARKS: 90

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 at the end.
- Only scientific calculators with basic capabilities are permitted. Graphics calculators are not permitted.

DO NOT COMMENCE WRITING UNTIL INSTRUCTED TO DO SO.

1. Find the extremals for the following functionals:

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

$$(b) \quad F\{y\} = \int_1^2 (xy'^2 + x^2y') dx, \quad y(1) = \frac{3}{4}, \quad y(2) = \log 4.$$

[14 marks]

2. Consider the functional

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

subject to the fixed end-points $y(0) = 0$, $y(\pi/2) = 1$ and the constraint

$$\int_0^{\pi/2} xy' dx = \frac{\pi}{4}.$$

- Write down a new functional based on $F\{y\}$ but one that incorporates the constraint by using a Lagrange multiplier.
- Derive the Euler–Lagrange equation for your functional from part (a).
- Solve the Euler–Lagrange equation from part (b) and therefore derive the general form for extremals of $F\{y\}$ that respects the constraint.
- Using the end-points values and the constraint, determine the values of the unknown constants in the general extremal found in part (c) to find the particular extremal to this problem.

Hint: Recall that

$$\int x \sin x dx = \sin x - x \cos x + \text{const}, \quad \int x \cos x dx = \cos x + x \sin x + \text{const}.$$

[12 marks]

3. (a) (i) From the series definition of the hypergeometric function write down the first four non-zero terms of the series expansion for

$$\log(1+x) = xF(1, 1; 2; -x).$$

- (ii) From the integral definitions show that

$$E(k) = \frac{\pi}{2} F\left(-\frac{1}{2}, \frac{1}{2}; 1; k^2\right).$$

- (b) A toroidal tube \mathcal{T} may be specified parametrically by its position vector

$$\mathbf{r}(\theta, \phi) = (R + r \cos \theta) \cos \phi \mathbf{i} + (R + r \cos \theta) \sin \phi \mathbf{j} + r \sin \theta \mathbf{k},$$

where r is the radius of the tube and R is the distance from the centre of the torus to the centre of the tube, and $-\pi < \theta \leq \pi$, $-\pi < \phi \leq \pi$.

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

[14 marks]

4. Consider the functional

$$F\{y\} = \int_0^1 (y'^2 - 8xy) dx,$$

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

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

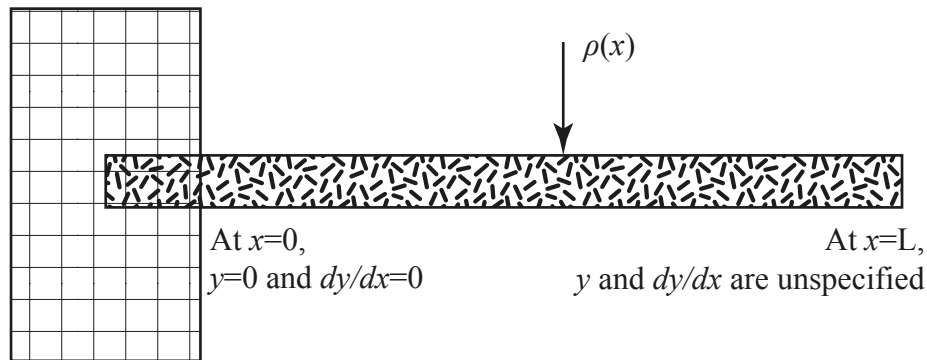
- (a) Write down the trial function y_1 (with one undetermined coefficient) by assuming

$$\phi_0(x) = x, \quad \text{and} \quad \phi_i(x) = x^i(1-x)^i.$$

- (b) Determine a function $F_1(c_1)$ which approximates the functional F for the y_1 from part (a).
(c) Determine the value of c_1 that leads to an extremal value for $F_1(c_1)$.
(d) Is this extremum a maximum or minimum? Justify your answer.

[10 marks]

5. Consider the cantilever of length L depicted in the following diagram



Assume that the elastic energy is modelled with a term

$$V_1 = \int_0^L \frac{\kappa y''^2}{2} dx,$$

where κ is the flexural rigidity, and the potential energy is represented by

$$V_2 = - \int_0^L \rho(x)y(x) dx,$$

where $\rho(x)$ is the load applied to the cantilever.

- Write down a functional $F\{y\}$ capturing the total elastic and potential energy of the cantilever.
- Assuming $\kappa = 1$ and $\rho(x) = 24$, derive a general solution of the Euler–Lagrange equation for this problem without applying boundary conditions.
- Using the fixed boundary conditions at $x = 0$ and the natural boundary conditions for $x = L$, find the particular solution to this problem.

Hint: The natural boundary conditions for a second order functional are

$$\left[\frac{\partial f}{\partial y''} \delta y' + \left(\frac{\partial f}{\partial y'} - \frac{d}{dx} \frac{\partial f}{\partial y''} \right) \delta y - H \delta x \right]_{x_0}^{x_1} = 0.$$

[10 marks]

6. (a) Prove that the functional

$$J\{y\} = \int_{x_0}^{x_1} (ay'^2 + byy' + cy^2) dx, \quad y(x_0) = y_0, \quad y(x_1) = y_1,$$

where $a \neq 0$ can have no broken extremals.

- (b) Find and sketch the extremals of

$$K\{y\} = \int_0^4 (y' - 1)^2 (y' + 1)^2 dx,$$

subject to the end-points $y(0) = 0$ and $y(4) = 2$, and allowing at most one corner.

[13 marks]

7. Find and sketch the curves that are extremals of the functional

$$L\{y\} = \int_0^{x_1} \frac{\sqrt{1 + y'^2}}{y} dx,$$

subject to $y(0) = 0$ and where the end-point (x_1, y_1) can vary along:

(a) $y = x - 5$.

(b) $(x - 9)^2 + y^2 = 9$.

[13 marks]

8. The *incomplete* beta function is defined by the integral

$$B_z(x, y) = \int_0^z t^{x-1} (1-t)^{y-1} dt,$$

where $\Re(x) > 0$, $\Re(y) > 0$, and $z \in [0, 1]$. Derive an expression for $B_z(x, y)$ in terms of one hypergeometric function and no other special functions.

[4 marks]

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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

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

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”.