Optimal Functions and Nanomechanics III

APP MTH 3022/7106

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Summary

Preliminary material

- Integral functionals, e.g.

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

- By assuming a certain functional form $y = g(x, \epsilon)$ we can convert to a function $F(\epsilon)$ and optimise, e.g. the "crude" brachistochrone.

$$F\{y\} = \int_{x_0}^{x_1} \sqrt{\frac{1 + y'^2}{y}}\, dx, \quad \text{with} \quad y(x, \epsilon) = (1 - x)^{\epsilon}.$$

- But what if $y(x, \epsilon)$ doesn't contain the true extremal?

Calculus of Variations

- First variation

$$\delta F = \lim_{\epsilon \to 0} \frac{F\{y + \epsilon\eta\} - F\{y\}}{\epsilon}$$

- Leads to the Euler-Lagrange equation

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} = 0$$

- For fixed end-point problems there is nothing else to worry about since δx and δy vanish at x_0 and x_1.

Special Cases

1. f depends only on y'
   - Solutions are straight lines.
2. f is x-absent (autonomous)
   - The Hamiltonian is conserved: i.e. $y'\frac{\partial f}{\partial y'} - f =$ const.
3. f is y-absent
   - Momentum is conserved: i.e. $\frac{\partial f}{\partial y'} =$ const.
4. $f = A(x,y)y' + B(x,y)$ (degenerate case)
   - Satisfy $\frac{\partial A}{\partial x} - \frac{\partial B}{\partial y} = 0$.
   - Functional is path independent (depends only on end-points).

Extension: Higher Order Derivatives

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

The Euler-Lagrange equation extend in a predictable way

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} + \frac{d^2}{dx^2}\frac{\partial f}{\partial y''} = 0$$

Sometimes called the Euler-Poisson equation. This is typically a fourth order ODE and requires four boundary conditions (say y and y' at both end-points).

Extension: Several dependent variables

Important in particle mechanics where we might have

$$F\{\boldsymbol{q}\} = \int_{t_0}^{t_1} L(x, \boldsymbol{q}, \dot{\boldsymbol{q}})\, dt.$$

We have many Euler-Lagrange equations

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} = 0$$

For all k up the the dimension of $\boldsymbol{q}$.

Nanostructures

- Looked at many graphene based structures
  - fullerenes (closed cages, typically spherical or spheroidal)
  - nanotubes (open or closed cylinders)
  - nanocones
- Continuum approach

$$E = \eta_1 \eta_2 \int_{\mathcal{S}_2} \int_{\mathcal{S}_1} \Phi(\rho)\, dA_1\, dA_2.$$

- Lennard-Jones potential

$$\Phi(\rho) = -A\rho^{-6} + B\rho^{-12}.$$

Special functions

- Gamma function: $\Gamma(z)$
- Beta function: $B(x, y)$
- Pochhammer symbol: $(a)_n$
- Hypergeometric function: $F(a, b; c; z)$
- Elliptic integrals: $F(\varphi, k)$ and $E(\varphi, k)$

Useful for evaluating the integrals arising from integrating up the Lennard-Jones potential.
Need to remember how to parameterise surfaces and derive scalar area elements.

Extension: Several independent variables

$$F\{z\} = \int_{y_0}^{y_1} \int_{x_0}^{x_1} f(x, y, z, z_x, z_y)\, dx\, dy.$$

Here the Euler-Lagrange equation generalises to

$$\frac{\partial f}{\partial z} - \frac{\partial}{\partial x}\frac{\partial f}{\partial z_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial z_y} = 0.$$

In general these are hard problems to solve.

Direct methods: Euler's finite difference

- Use an arbitrary set of mesh points, $\{x_0, x_1, \cdots x_n\}$.
- Approximate

$$y'(x_i) = \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$

- Rectangle rule

$$F\{y\} = \int_{x_0}^{x_n} f(x, y, y')\,dx \approx \sum_{i=0}^{n-1} f\left(x_i, y_i, \frac{\Delta y_i}{\Delta x_i}\right) \Delta x_1 = \bar{F}(\boldsymbol{y})$$

- $\bar{F}(\boldsymbol{y})$ is a function of the vector $\boldsymbol{y}$ which can be optimised in the usual way.

Direct methods: Ritz's

- Approximate $y(x)$ by

$$y(x) = \phi_0(x) + c_1\phi_1(x) + c_2\phi_2(x) + \cdots + c_n\phi_n(x).$$

- Choose ϕ_0 to satisfy the end-point conditions.
- Choose ϕ_1 ϕ_2, etc to vanish at the end-points.
- Substitute the approximation in the functional and integrate. This results in a function $F(\boldsymbol{c})$ depending on the constants c_1, c_2, etc.
- Now optimise $F(\boldsymbol{c})$ the usual way.

Direct methods: Kantorovich's

- For more than one independent variable
- Approximate $z(x,y)$ by

$$z(x,y) = \phi_0(x,y) + c_1(x)\phi_1(x,y) + \cdots + c_n(x)\phi_n(x,y).$$

- Substitute the approximation in the functional and integrate the y-variable. This results in a functional with one independent variable and n dependent variables.
- Now tackle this new functional with the Euler-Lagrange machinery.
- Works by approximately separating the two independent variables.

Constraints

- Integral constraints of the form

$$\int_{x_0}^{x_1} g(x, y, y')\, dx = \text{const.}$$

- Are used to create a new functional

$$H\{y\} = F\{y\} + \lambda G\{y\} = \int_{x_0}^{1} \left[f(x, y, y') + \lambda g(x, y, y')\right] dx.$$

- the problem is then tackled using the calculus of variations, Euler-Lagrange equations, etc.

Free endpoints

- We find the first variation may be written

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

- So wherever x or y can vary at an endpoint then H or p must vanish at that endpoint.
- These are modular in the sense that you only apply them when x and/or y are allowed to vary at the endpoint.

Line curvature

The line curvature κ is given by

$$\kappa = \frac{y''}{(1 + y'^2)^{3/2}}.$$

Euler's elastica is a class of curve which originates from the variational problem of minimising the square of line curvature, that is

$$F\{y\} = \int_{x_0}^{x_1} \kappa^2 \, ds = \int_{x_0}^{x_1} \frac{y''^2}{(1 + y'^2)^{5/2}} \, dx$$

Traversals

Given that an endpoint is constrained to lie on some curve

$$\Gamma : (x, y) = (x_\Gamma . y_\Gamma)$$

then the traversality condition says that

$$p\frac{dy_\Gamma}{d\xi} - H\frac{dx_\Gamma}{d\xi} = 0$$

Special case: If the functional is of the form

$$F\{y\} = \int_{x_0}^{x_1} K(x, y)\sqrt{1 + y'^2}\, dx,$$

then the traversality connection degenerates to simple orthogonality.

Broken extremals

- Solve the Euler-Lagrange equations
- Look for solutions for each end condition
- Match up solutions at a corner $x^\star$ so that
  - Total solution is continuous

$$y(x^{\star -}) = y(x^{\star +})$$

  - Weierstrass–Erdmann corner conditions are satisfied

$$p|_{x^{\star -}} = p|_{x^{\star +}}, \quad \text{and} \quad H|_{x^{\star -}} = H|_{x^{\star +}}.$$

  - Solution is only piecewise continuous in the derivative

Hamilton's formulation

For a problem of the form

$$F\{\boldsymbol{q}\} = \int_{t_0}^{t_1} L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})\, dt$$

- We introduce the conjugate variable $p_i = \dfrac{\partial L}{\partial \dot{q}_i}$.
- Hamiltonian is $H(t, \boldsymbol{q}, \boldsymbol{p}) = \displaystyle\sum_{i=1}^{n} p_i \dot{q}_i - L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})$
- Then Hamilton's equations are

$$\frac{\partial H}{\partial p_i} = \frac{dq_i}{dt}, \quad \frac{\partial H}{\partial q_i} = -\frac{dp_i}{dt}$$

Hamilton-Jacobi equation

$$\frac{\partial S}{\partial x} + H\left(x, y, \frac{\partial S}{\partial y}\right) = 0.$$

- First order partial differential equation
- Solutions are like $S(x, y, \alpha)$ where α is an arbitrary constant.
- The extrema lie along the curves

$$\frac{\partial S}{\partial \alpha} = \text{const.}$$

Smooth transformations

Consider a parameterised family of smooth transformations

$$X = \theta(x, y; \epsilon), \quad Y = \phi(x, y; \epsilon),$$

where $\epsilon = 0$ denotes the identity transform

$$x = \theta(x, y; 0), \quad y = \phi(x, y; 0),$$

Using Taylor's theorem we can write

$$X = \theta(x, y; 0) + \epsilon \left.\frac{\partial \theta}{\partial \epsilon}\right|_{(x,y;0)} + \mathcal{O}(\epsilon^2)$$

$$Y = \phi(x, y; 0) + \epsilon \left.\frac{\partial \phi}{\partial \epsilon}\right|_{(x,y;0)} + \mathcal{O}(\epsilon^2)$$

Noether's theorem

So

$$X \approx x + \epsilon\xi, \quad Y \approx y + \epsilon\eta.$$

where ξ and η are called the infinitesimal generators.

Now suppose that $f(x, y, y')$ is variational invariant on $[x_0, x_1]$ under a transform with infinitesimal generations ξ and η then

$$\eta p - \xi H = \text{constant},$$

along any extremal of

$$F\{y\} = \int_{x_0}^{x_1} f(x, y, t')\, dx.$$

Exam - Rubric

THE UNIVERSITY of ADELAIDE

Examination in School of Mathematical Sciences
Semester 2, 2018

107352 APP MTH 3022 Optimal Functions and Nanomechanics III

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 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.

Page 1 of 6

- Writing time 120 mins
- Questions
  - Number of Questions: 5
  - Total Marks: 60
- Materials
  - Formulae sheets are provided
  - Only scientific calculators with basic capabilities are permitted. Graphics calculators are not permitted.

Exam - Formula Sheets

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	$\Phi(\rho) = -\frac{A}{\rho^6} + \frac{B}{\rho^{12}}.$

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Formula Sheet, Variational

Theorem 2.2.1: Let $F : C^2[x_0,x_1] \to \mathbb{R}$ 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 $x \in [x_0,x_1]$

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

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

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

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

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

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

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

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".