Optimal Functions and Nanomechanics III

APP MTH 3022/7106

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Lecture 28

Last lecture

- Investigated extremals which were not continuous in the derivative for the whole domain.
- Derived the Weierstrauss-Erdman conditions for a "corner".
- Saw some examples of problems with broken extremals.
- Revisited Newton's aerodynamic problem and saw how the Weierstrass-Erdman conditions lead to the sort of corner we saw earlier.

Hamilton's formulation

We've seen the Hamiltonian H earlier on, but haven't explored its full power. Firstly, using H can often result in a simpler approach than solving the E-L equations, e.g., where f has no dependence on x, or where there is more than one dependent variable.

More importantly though, this formulation can lead to an understanding of how symmetries in the problem of interest lead to conservation laws.

Legendre transformation

- Contact transformation
  (as opposed to point transformation)
- transformation that depends on the derivatives of a variable
- simple one variable Legendre transform of $y : [x_0, x_1] \to \mathbb{R}$, by defining new variable p, by

$$p(x) = y'(x)$$

- provided $y''(x) \neq 0$ we can define x in terms of p, by introducing the Hamiltonian

$$H(p) = px - y(x)$$

Legendre transformation

Assume for convenience that y is convex, e.g. $y'' > 0$ for $x \in [x_0, x_1]$. Then

$$\begin{aligned}
\frac{dH}{dp} &= \frac{d}{dp}(xp) - \frac{dy}{dp} \\
&= p\frac{dx}{dp} + x - \frac{dy}{dp} \\
&= p\frac{dx}{dp} + x - \frac{dy}{dx}\frac{dx}{dp} \\
&= \left(p - \frac{dy}{dx}\right)\frac{dx}{dp} + x \\
&= x
\end{aligned}$$

and also note $px - H = y$, so from the pair (p, H) we can recover the original pair (x, y), by a Legendre transform.

Example Legendre transformation

Let $f(x) = x^4/4$, then

$$\begin{aligned} p &= \frac{df}{dx} &&= x^3 \\ H(p) &= px - \frac{1}{4}x^4 &&= \frac{3}{4}p^{4/3} \end{aligned}$$

Note that we can reverse with another Legendre transform

$$\begin{aligned} \frac{dH}{dp} &= p^{1/3} &&= x \\ px - H &= x^4 - \frac{3}{4}x^4 &&= f(x) \end{aligned}$$

Hamilton's formulation

Refer back to problems with more than one dependent variable, or where f has no dependence on x.

Define **generalized coordinates** $\boldsymbol{q} : [t_0, t_1] \to \mathbb{R}^n$.

- i.e. take a set of n functions $q_k(t)$, with two continuous derivatives with respect to t, and put them into a vector $\boldsymbol{q}(t)$
- dot notation:

$$\dot{q}_k = \frac{dq_k}{dt}, \quad \ddot{q}_k = \frac{d^2 q_k}{dt^2} \quad \text{and} \quad \dot{\boldsymbol{q}} = \left(\frac{dq_1}{dt}, \frac{dq_2}{dt}, \ldots, \frac{dq_n}{dt} \right)$$

- Lagrangian $L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})$

Hamilton's formulation

The extremals of the functional

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

satisfy the Euler-Lagrange equations

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

for all k.

Hamilton's formulation

Legendre transform introduces the **conjugate** variables

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

Suppose these equations can be solved to write $\dot{q}_i$ as a function of (t, q_i, p_i), then the **Hamiltonian** is

$$H(t, q_1, \ldots, q_n, p_1, \ldots, p_n) = \sum_{i=1}^{n} p_i \dot{q}_i - L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})$$

We've seen p_i and H before, for instance in transversality conditions.

- the p_i are called **generalised momenta**

Hamilton's formulation

$$H(t, q_1, \ldots, q_n, p_1, \ldots, p_n) = \sum_{i=1}^{n} p_i \dot{q}_i - L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})$$

So

$$\begin{aligned} \frac{\partial H}{\partial p_i} &= \dot{q}_i \\ \frac{\partial H}{\partial q_i} &= -\frac{\partial L}{\partial q_i} \end{aligned}$$

Given the E-L equations, the second equation gives

$$\frac{\partial H}{\partial q_i} = -\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = -\frac{dp_i}{dt}$$

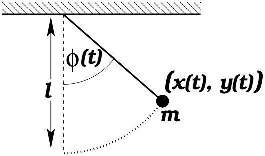
Canonical Euler-Lagrange equations

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

- called **Hamilton's equations**, or
  Canonical Euler-Lagrange equations
- The n E-L DEs converted into $2n$ first-order DEs
- derivatives are now uncoupled
  - therefore maybe easier to solve

Harmonic oscillator example

Simple pendulum



$$F\{\phi\} = \int_{t_0}^{t_1} \left(\frac{1}{2} m\ell^2 \dot{\phi}^2 - mg\ell(1-\cos\phi) \right) \, dt$$

E-L equations

$$\begin{aligned} \frac{d}{dt}\frac{\partial L}{\partial \dot{\phi}} - \frac{\partial L}{\partial \phi} &= 0 \\ \frac{d}{dt} m\ell^2 \dot{\phi} + mg\ell \sin\phi &= 0 \\ \ddot{\phi} + \frac{g}{\ell} \sin\phi &= 0 \end{aligned}$$

standard pendulum equations, solve for small ϕ

Harmonic oscillator example

Generalized momentum (in this case angular momentum)

$$p = \frac{\partial L}{\partial \dot\phi} = m\ell^2 \dot\phi \quad \Rightarrow \quad \dot\phi = \frac{p}{m\ell^2}$$

Hamiltonian is

$$H(\phi, p) = p\dot\phi - L = \frac{p^2}{2m\ell^2} + mg\ell(1 - \cos\phi)$$

Hamilton's equations are

$$\begin{array}{rclcrcl} \dfrac{\partial H}{\partial p} & = & \dfrac{d\phi}{dt} & \Rightarrow & \dot\phi & = & \dfrac{p}{m\ell^2} \\ \dfrac{\partial H}{\partial \phi} & = & -\dfrac{dp}{dt} & \Rightarrow & \dot p & = & -mg\ell \sin\phi \end{array}$$

Harmonic oscillator example

Hamilton's equations (2 first order DEs)

$$\begin{aligned}\dot{\phi} &= \frac{p}{m\ell^2}\\ \dot{p} &= -mg\ell\sin\phi\end{aligned}$$

Differentiate the first equation and we get

$$\ddot{\phi} = \frac{\dot{p}}{m\ell^2}$$

Substitute the value of $\dot{p}$ from the second of Hamilton's equations and we get

$$\ddot{\phi} + \frac{g}{\ell}\sin\phi = 0$$

the Euler-Lagrange equation.

Canonical Euler-Lagrange equations

We can get the same Canonical E-L equations from finding extremals of the functional of $2n$ variables

$$\tilde{F}\{q_1, \ldots, q_n, p_1, \ldots, p_n\} = \int_a^b \left[\sum_{i=1}^{n} p_i \dot{q}_i - H \right] dx$$

E.G.

$$\begin{aligned} \left(\frac{\partial}{\partial q_i} - \frac{d}{dt} \frac{\partial}{\partial \dot{q}_i} \right) \left[\sum_{i=1}^{n} p_i \dot{q}_i - H \right] &= 0 \\ \left(\frac{\partial}{\partial p_i} - \frac{d}{dt} \frac{\partial}{\partial \dot{p}_i} \right) \left[\sum_{i=1}^{n} p_i \dot{q}_i - H \right] &= 0 \end{aligned}$$

Hamilton's formulation

- F and $\tilde{F}$ are equivalent under the Legendre transformation
  - make q and p independent, whereas before it was a bit of a trick to pretend q and $\dot{q}$ were independent
- If L does not depend on t, then it should be clear from the Legendre transformation that H won't depend on t.
  - the system will be **conservative**
  - i.e. H is a conserved (constant) quantity

Hamilton-Jacobi equation

Find stationary points of

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

given particular fixed end points (x_0, y_0) and (x_1, y_1).

Now vary the second end-point. We can consider that the value of $F\{y\}$ along the extremal is now a function of (x_1, y_1), e.g.

$$F\{y\} = S(x_1, y_1)$$

Hamilton-Jacobi equation

Make a small variation in the end-point $(\delta x, \delta y)$. We know that the first variation will consist of an E-L component, plus a (free end-point) term like

$$p\,\delta y - H\,\delta x$$

but we are only considering extremal curves here, so the E-L component must be zero. Hence, we can write

$$\delta S = S(x + \delta x, y + \delta y) - S(x, y) = p\,\delta y - H\,\delta x$$

Keep x fixed, and vary only y, and we get

$$\frac{\delta S}{\delta y} = p$$

where the LHS is $\partial S/\partial y$ in the limit as $\delta y \to 0$

Hamilton-Jacobi equation

Similarly keeping y fixed and varying x we get an expression for $\partial S/\partial x$, which together with the previous expressions give

$$\begin{aligned} \frac{\partial S}{\partial y} &= p \\ \frac{\partial S}{\partial x} &= -H(x, y, p) \end{aligned}$$

Substitute the former equation into the latter, and we get

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

This is the **Hamilton-Jacobi** equation

Hamilton-Jacobi equation

Given a solution $S(x, y, \alpha)$ to the Hamilton-Jacobi equations (where α is a constant of integration), the extrema lie along the curves

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

Proof: see

- Arthurs, Thm 8.1, p. 32
- van Brunt, Thm 8.4.1, p. 177

Simple example

Find extrema of

$$F\{y\} = \int_a^b y'^2 \, dx$$

The conjugate variable and Hamiltonian are given by

$$\begin{aligned} p &= \frac{\partial f}{\partial y'} \\ &= 2y' \\ H(x, y, p) &= y' \frac{\partial f}{\partial y'} - f \\ &= y'^2 \\ &= \frac{1}{4} p^2 \end{aligned}$$

Simple example

So the Hamilton-Jacobi equation is

$$\begin{aligned}\frac{\partial S}{\partial x} + H\left(x, y, \frac{\partial S}{\partial y}\right) &= 0\\ \frac{\partial S}{\partial x} + \frac{1}{4}\left(\frac{\partial S}{\partial y}\right)^2 &= 0\end{aligned}$$

To solve we take $S(x, y) = u(x) + v(y)$ which gives

$$\frac{du}{dx} + \frac{1}{4}\left(\frac{dv}{dy}\right)^2 = 0$$

As u doesn't depend on y, and v doesn't depend on x, the above equation implies that du/dx is a constant, hence we can write

$$u(x) = -\alpha^2 x + \gamma$$

Simple example

Then, the Hamilton-Jacobi equation becomes

$$-\alpha^2 + \frac{1}{4}\left(\frac{dv}{dy}\right)^2 = 0$$

Or

$$\frac{dv}{dy} = 2\alpha$$

So

$$v(x) = 2\alpha y + \beta$$

So we now have

$$S(x, y) = -\alpha^2 x + 2\alpha y + \gamma + \beta$$

Simple example

Taking the derivative of S WRT to β and γ just gives an identity, and so nothing new.

Taking the derivative of S WRT to α gives

$$2y - 2\alpha x = \text{const},$$

which is the equation of a straight line.

Simple example

The functional is

$$F\{y\} = \int_a^b y'^2 \, dx$$

The E-L equation is

$$\frac{d}{dt}\frac{\partial f}{\partial y'} = \frac{d}{dt} 2y' = y'' = 0$$

which obviously has straight lines as solutions. So the Hamilton-Jacobi equations gave us the same result (in the end).

Pendulum example

$$
\begin{aligned}
\frac{\partial S}{\partial \phi} &= p = m\ell^2\dot{\phi} \\
\frac{\partial S}{\partial t} &= -H(t,\phi,p) = -\frac{p^2}{2m\ell^2} - mg\ell(1-\cos\phi)
\end{aligned}
$$

So the Hamilton-Jacobi equation is

$$
\frac{\partial S}{\partial t} + \frac{1}{2m\ell^2}\left(\frac{\partial S}{\partial \phi}\right)^2 + mg\ell(1-\cos\phi) = 0
$$

Hamilton-Jacobi equation

Where there are multiple dependent variables, we write the Hamilton-Jacobi equation as

$$\frac{\partial S}{\partial t} + H\left(t, q_1, \ldots, q_n, \frac{\partial S}{\partial q_1}, \ldots, \frac{\partial S}{\partial q_n}\right) = 0$$

- Note this is a first order **partial** DE
- May be easier to solve in some cases, but often partial DEs are harder
- Helps if we can separate the variables.