Optimal Functions and Nanomechanics III

APP MTH 3022/7106

Barry Cox

Lecture 29

Last lecture

- Looked at the Legendre transformation.
- And the Hamilton's formulation of variational calculus.
- Solved the simple example of a harmonic oscillator.
- Derived the Hamilton-Jacobi equation.
- Looked at the pendulum using the Hamilton-Jacobi equation.

Hamilton's principle

We now have a group of equivalent methods

- Euler-Lagrange equations
- Hamilton's equations
- Hamilton-Jacobi equation

We saw earlier that these can give us other methods

- Hamilton's principle $\Rightarrow$ Newton's laws of motion
- When L is not explicitly dependent on t, then the Hamiltonian H is constant in time.
  - conservation of energy
  - this is an illustration of a symmetry in the problem appearing in the Hamiltonian

Conservation laws

Given the functional

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

if there is a function $\phi(x, y, y', \ldots, y^{(k)})$ such that

$$\frac{d}{dx}\phi(x, y, y', \ldots, y^{(k)}) = 0,$$

for all extremals of F, then this is called a **k^{th} order conservation law**

- use obvious extension for functionals of several dependent variables.

Conservation law example

Given the functional

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

where f is not explicitly dependent on x, we know that the Hamiltonian

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

is constant, and so

$$\frac{dH}{dx} = 0,$$

is a **first order conservation law** of the system.

Several independent variables

For functionals of several independent variables, e.g.

$$F\{z\} = \iint_{\Omega} z(x,y)\,dx\,dy,$$

the equivalent conservation law is

$$\nabla \cdot \phi = 0$$

For some function $\phi(x, y, z, z', \ldots, z^{(k)})$.

- Results here can be extended to these cases, but we won't look at them here.

Conservation laws

- physically interesting
  - tells you something about the system
- can simplify finding a solution
  - $\phi(x, y, y', \ldots, y^{(k)}) =$ const, is an order k DE, rather than Euler-Lagrange equations which are order $2k$
- $\phi(x, y, y', \ldots, y^{(k)}) =$ const, is often called the **first integral** of the Euler-Lagrange equations
  - RHS is a constant of integration (determined by boundary conditions)
- how do we find conservation laws?
  - Noether's theorem

Variational symmetries

The key to finding conservation laws lies in finding symmetries in the problem.

- "symmetries" are the result of transformations under which the functional is invariant
- e.g., time invariance symmetry results in constant H
- more generally, take a parameterised family of smooth transforms

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

  where

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

  i.e., we get the identity transform for $\epsilon = 0$
- examples are **translations** and **rotations**

Jacobian

The Jacobian is

$$J = \begin{vmatrix} \theta_x & \theta_y \\ \phi_x & \phi_y \end{vmatrix} = \theta_x \phi_y - \theta_y \phi_x$$

- **smooth:** if functions x and y have continuous partial derivatives.
- **non-singular:** if Jacobian is non-zero (and hence an inverse transform exists)

Now for $\epsilon = 0$, we require the identity transform, so $J = 1$. Also, we require a smooth transform, so J is a smooth function of ϵ, and so for sufficiently small $|\epsilon|$, the transform is non-singular.

Example transformations

- **translations** (ϵ is the translation distance)

$$\begin{array}{lrclcrcl} & X &=& x+\epsilon, & & Y &=& y, \\ \text{or} & X &=& x, & & Y &=& y+\epsilon. \end{array}$$

Both have Jacobian

$$J = 1,$$

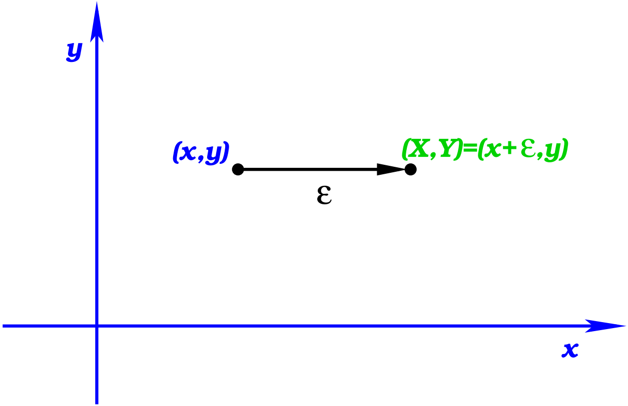
and inverse transformations

$$\begin{array}{lrclcrcl} & x &=& X-\epsilon, & & y &=& Y, \\ \text{or} & x &=& X, & & y &=& Y-\epsilon. \end{array}$$

Example transformations

- **translations** (ϵ is the translation distance)

$$X = x + \epsilon, \qquad Y = y.$$



Example transformations

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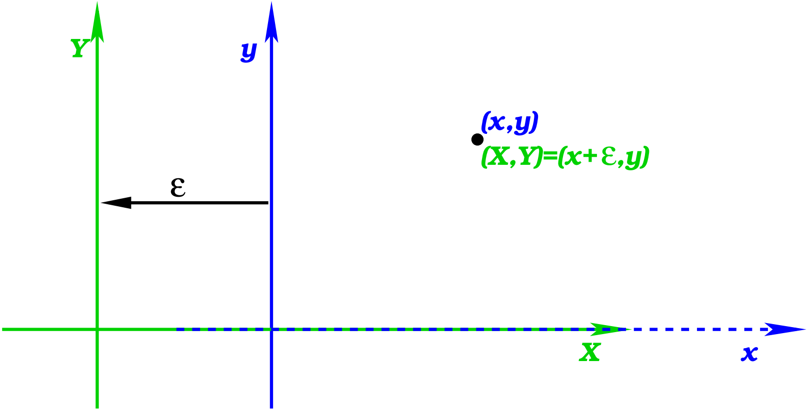


Example transformations

- **rotations** (ϵ is the rotation angle)

$$X = x\cos\epsilon - y\sin\epsilon, \quad Y = x\sin\epsilon + y\cos\epsilon,$$

has Jacobian

$$J = \cos^2\epsilon + \sin^2\epsilon = 1,$$

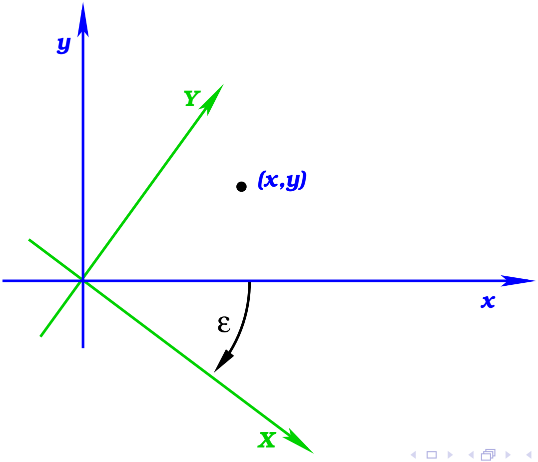
and inverse

$$x = X\cos\epsilon + Y\sin\epsilon, \quad y = -X\sin\epsilon + Y\cos\epsilon.$$

Example transformations

- **rotations** (ϵ is the rotation angle)

$$X = x\cos\epsilon - y\sin\epsilon, \quad Y = x\sin\epsilon + y\cos\epsilon.$$



Example transformations

- **rotations** (ϵ is the rotation angle)

$$X = x\cos\epsilon - y\sin\epsilon, \quad Y = x\sin\epsilon + y\cos\epsilon.$$

To derive this, change coordinates to polar coordinates

$$x = r\cos(\theta), \quad \text{and} \quad y = r\sin(\theta).$$

Under a rotation by ϵ, the new coordinates (X, Y) are

$$X = r\cos(\theta+\epsilon), \quad \text{and} \quad Y = r\sin(\theta+\epsilon).$$

Use trig. identities $\cos(u+v) = \cos u\cos v - \sin u\sin v$ and $\sin(u+v) = \sin u\cos v + \cos u\sin v$, to get

$$\begin{aligned} X &= r\cos(\theta)\cos(\epsilon) - r\sin(\theta)\sin(\epsilon) = x\cos(\epsilon) - y\sin(\epsilon), \\ Y &= r\sin(\theta)\cos(\epsilon) + r\cos(\theta)\sin(\epsilon) = y\cos(\epsilon) + x\sin(\epsilon). \end{aligned}$$

Transformation of a function

Given a function $y(x)$, we can rewrite $Y(X)$ using the inverse transformation, e.g.

$$\phi^{-1}(X, Y(X); \epsilon) = y(x) = y(\theta^{-1}(X, Y; \epsilon))$$

For example, taking the curve $y = x$ under rotations

$$-X \sin \epsilon + Y \cos \epsilon = X \cos \epsilon + Y \sin \epsilon$$

which we rearrange to get

$$Y(X) = \frac{\cos \epsilon + \sin \epsilon}{\cos \epsilon - \sin \epsilon} X$$

Similarly we can derive $Y'(X)$

Transform invariance

Now if

$$\int_{x_0}^{x_1} f(x, y, y'(x))\, dx = \int_{X_0}^{X_1} f(X, Y, Y'(X))\, dX,$$

for all smooth functions $y(x)$ on $[x_0, x_1]$, then we say that the functional in invariant under the transformation.

- also called **variational invariance**
- The transform is called a **variational symmetry**
- Related to conservation laws

Also note that the Euler-Lagrange equations are invariant under the same transform, i.e., they produce the same extremal curves.

Infinitesimal generators

For small ϵ we can use Taylor's theorem to write

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

We define the **infinitesimal generators**

$$\xi(x,y) = \left.\frac{\partial\theta}{\partial\epsilon}\right|_{(x,y;0)}, \quad \eta(x,y) = \left.\frac{\partial\phi}{\partial\epsilon}\right|_{(x,y;0)},$$

and then for small ϵ

$$\begin{aligned} X &\simeq x + \epsilon\xi, \\ Y &\simeq y + \epsilon\eta. \end{aligned}$$

Examples

- **translations:**

$$
\begin{array}{rrcllcl}
 & (X,Y) & = & (x+\epsilon, y), & \Rightarrow & (\xi,\eta) & = & (1,0), \\
\text{or} & (X,Y) & = & (x, y+\epsilon), & \Rightarrow & (\xi,\eta) & = & (0,1).
\end{array}
$$

- **rotations:**

$$
(X,Y) = (x\cos\epsilon - y\sin\epsilon, x\sin\epsilon + y\cos\epsilon),
$$

So

$$
\begin{aligned}
\xi &= \left.\frac{\partial\theta}{\partial\epsilon}\right|_{\epsilon=0} &= \left[-x\sin\epsilon - y\cos\epsilon\right]_{\epsilon=0} &= -y \\
\eta &= \left.\frac{\partial\phi}{\partial\epsilon}\right|_{\epsilon=0} &= \left[x\cos\epsilon - y\sin\epsilon\right]_{\epsilon=0} &= x
\end{aligned}
$$

Emmy Noether

- Amalie Emmy Noether, 23 March 1882 – 14 April 1935
- Described by Einstein and many others as the most important woman in the history of mathematics.
- Most of her work was in algebra
- Worked at the Mathematical Institute of Erlangen without pay for seven years
- Invited by David Hilbert and Felix Klein to join the mathematics department at the University of Göttingen, a world-renowned center of mathematical research. The philosophical faculty objected, however, and she spent four years lecturing under Hilbert's name.

Noether's theorem

Suppose the $f(x, y, y')$ is variationally invariant on $[x_0, x_1]$ under a transform with infinitesimal generators ξ and η, then

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

along any extremal of

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

Example (i)

Invariance of translations in x, i.e.

$$\begin{aligned}(X, Y) &= (x+\epsilon, y), \\ (\xi, \eta) &= (1, 0).\end{aligned}$$

So, a system with such invariance has

$$H = \text{const},$$

which is what we showed earlier regarding functionals with no explicit dependence on x (Beltrami identity).

Example (ii)

Invariance in translations in y, i.e.

$$\begin{aligned} (X, Y) &= (x, y+\epsilon), \\ (\xi, \eta) &= (0, 1). \end{aligned}$$

So, a system with such invariance has

$$p = \text{const},$$

which is what we showed earlier regarding functionals with no explicit dependence on y.

More than one dependent variable

Transforms with more than one dependent variable

$$\begin{aligned} T &= \theta(t, \boldsymbol{q}; \epsilon), \\ Q_k &= \phi_k(t, \boldsymbol{q}; \epsilon), \end{aligned}$$

and the infinitesimal generators are

$$\begin{aligned} \xi &= \left.\frac{\partial \theta}{\partial \epsilon}\right|_{\epsilon=0}, \\ \eta_k &= \left.\frac{\partial \phi_k}{\partial \epsilon}\right|_{\epsilon=0}. \end{aligned}$$

More than one dependent variable

Noether's theorem: Suppose $L(t, \boldsymbol{q}, \dot{\boldsymbol{q}})$ is variationally invariant on $[t_0, t_1]$ under a transform with infinitesimal generators ξ and η_k. Given

$$p_k = \frac{\partial L}{\partial \dot{q}_k}, \quad H = \sum_{k=1}^{n} p_k \dot{q}_k - L.$$

Then

$$\sum_{k=1}^{n} p_k \eta_k - H\xi = \text{const},$$

along any extremal of

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

Example: rotations

Invariance in rotations, i.e.

$$
\begin{aligned}
(T, Q_1, Q_2) &= (t, q_1 \cos\epsilon - q_2 \sin\epsilon, q_2 \cos\epsilon + q_1 \sin\epsilon), \\
(t, q_1, q_2) &= (T, Q_1 \cos\epsilon + Q_2 \sin\epsilon, Q_2 \cos\epsilon - Q_1 \sin\epsilon).
\end{aligned}
$$

The infinitesimal generators are

$$
\begin{aligned}
\xi &= 0 \\
\eta_1 &= -q_1 \sin\epsilon - q_2 \cos\epsilon\big|_{\epsilon=0} &= -q_2 \\
\eta_2 &= -q_2 \sin\epsilon + q_1 \cos\epsilon\big|_{\epsilon=0} &= q_1
\end{aligned}
$$

So, a system with such invariance has

$$
\sum_{i=1}^{2} p_i \eta_i - H\xi = -p_1 q_2 + p_2 q_1 = \text{const},
$$

So **angular momentum** in conserved.

Common symmetries

Given a system in 3D with Kinetic Energy $T(\dot{\boldsymbol{q}}) = \frac{1}{2}m\dot{\boldsymbol{q}}\cdot\dot{\boldsymbol{q}}$, and Potential Energy $V(t, \boldsymbol{q})$.

- invariance of L under time translations corresponds to conservation of Energy
- invariance of L under spatial translations corresponds to conservation of momentum
- invariance of L under rotations corresponds to conservation of angular momentum

Finding symmetries

- Testing for non-trivial symmetries can be tricky.
- Useful result is the *Rund-Trautman identity*:
- It leads also to a simple proof of Noether's theorem

More advanced cases

- Laplace-Runge-Lenz vector in planetary motion corresponds to rotations of 3D sphere in 4D
- symmetries in general relativity
- symmetries in quantum mechanics
- symmetries in fields