PHY 711 Classical Mechanics and Mathematical Methods 10-10:50 AM MWF in Olin103

Lecture notes for Lecture 2 Chapter 3.17 of F&W

Introduction to the calculus of variations

- **1. Mathematical construction**
- **2. Practical use**
- **3. Examples**

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

PHY 711 -- Assignment #2

Assigned: 8/28/2024 Due: 9/2/2024

Start reading Chapter 3, especially Section 17, in Fetter & Walecka.

• Using calculus of variations, find the equation, $y(x)$, of the shortest length "curve" which passes through the points ($x=0$, $y=0$) and ($x=2$, $y=4$). What is the length of this "curve"?

PHYSICS COLLOQUIUM

AUGUST 29, 2024

Olin 101 Refreshments at 3:30 PM Olin Lobby

Exploring Alternative Origins of Life with Genes and Proteins Designed De Novo

All life on Earth arose from common ancestry. And all living systems contain similar genes, proteins, and metabolisms. Do these commonalities among living systems exist because they diverged from shared ancestry? Alternatively, if living systems arose from different ancestry (or no ancestry), would they contain different genes, proteins, and metabolisms? There are two ways to address this question: (i) Find life on another planet (different ancestry); or (ii) Create novel biomolecules and metabolisms in the laboratory (no ancestry). Our lab does not have the budget for the first option; we'll leave that to NASA. Instead, the Hecht Lab creates vast collections of synthetic genes to encode novel (non-natural) proteins. Many of these novel proteins fold into stable 3-dimensional structures. Moreover, many of them bind biologically relevant metals, metabolites, and cofactors. Most

The "calculus of variation" as a mathematical construction.

According wikipedia – **Joseph-Louis Lagrange** (born **Giuseppe Luigi Lagrangia** or **Giuseppe Ludovico De la Grange Tournier**; 25 January 1736 – 10 April 1813), also reported as **Giuseppe Luigi Lagrange** or **Lagrangia**, was an Italian mathematician and astronomer, later naturalized French. He made significant contributions to the fields of analysis, number theory, and both classical and celestial mechanics.

According to Wikipedia –

Leonard Euler (April 7, 1707-September 18, 1783) Swiss mathematician, physicist, astronomer, geographer, logician and engineer who founded the studies of graph theory and topology and made pioneering and influential discoveries in many other branches of mathematics such as analytic number theory, complex analysis, and infinitesimal calculus. He introduced much of modern mathematical terminology and notation, including the notion of a mathematical function. He is also known for his work in mechanics, fluid dynamics, optics, astronomy and music theory.

In Chapter 3, the notion of Lagrangian dynamics is developed; reformulating Newton's laws in terms of minimization of related functions. In preparation, we need to develop a mathematical tool known as "the calculus of variation".

Minimization of a simple function

Minimization of a simple function for which $V(x)$ is minimized (or maximized). Given a function $V(x)$, find the value(s) of x

Necessary condition : $\frac{dv}{dx} = 0$ *dx dV*

Functional minimization of an integral relationship Consider a family of functions $y(x)$, with fixed end points

 $(x_i) = y_i$ and $y(x_f) = y_f$ and an integral form $L \left(\frac{1}{2} y(x), \frac{dy}{dx} \right)$, x |. $y(x_i) = y_i$ and $y(x_f) = y_f$ and an integral form $L\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right)$ $= y_i$ and $y(x_f) = y_f$ and an integral form $L\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right)$

Find the function $y(x)$ which extremizes $L | \{ y(x), \frac{dy}{dx} \}, x|.$ $y(x)$ which extremizes $L\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right)$

Necessary condition: $\delta L = 0$

Difference between minimization of a function *V(x)* and the minimization in the calculus of variation.

Minimization of a function – *V(x)* \rightarrow Know *V(x)* \rightarrow Find *x₀* such that *V(x₀)* is a minimum.

Calculus of variation

For $x_i \le x \le x_f$ want to find a function $y(x)$

that minimizes an integral that depends on $y(x)$.

The analysis involves deriving and solving a differential equation for the function $y(x)$.

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Calculus of variation example for a pure integral function

Find the function $y(x)$ which extremizes $L \left(\left\{ y(x), \frac{dy}{dx} \right\}, x \right)$ $\overline{}$ \int $\left\{\left\{y(x), \frac{dy}{dx}\right\}, x\right\}$ $\overline{}$ \setminus $\bigg($ \int $\left\{ \right.$ \vert $\overline{\mathcal{L}}$ $\left\{ \right.$ \int *x dx* $y(x)$ which extremizes $L\left(\frac{1}{2}y(x), \frac{dy}{dx}\right)$

where
$$
L\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right) \equiv \int_{x_i}^{x_f} f\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right) dx
$$
.

Necessary condition : $\delta L = 0$

At any x, let
$$
y(x) \to y(x) + \delta y(x)
$$

\n
$$
\frac{dy(x)}{dx} \to \frac{dy(x)}{dx} + \delta \frac{dy(x)}{dx}
$$

Formally:

$$
\delta L = \int_{x_i}^{x_f} \left[\left(\frac{\partial f}{\partial y} \right)_{x, \frac{dy}{dx}} \delta y + \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta \left(\frac{dy}{dx} \right) \right] \right] dx.
$$

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Comment on partial derivatives -- function $f(a,b)$

Comment about notation concerning functional dependence and partial derivatives

Suppose x, y, z represent independent variables that determine a function f : We write $f(x, y, z)$. A partial derivative with respect to x implies that we hold *y*, *z* fixed and infinitessimally change *x*

$$
\left(\frac{\partial f}{\partial x}\right)_{y,z} = \lim_{\Delta x \to 0} \left(\frac{f(x + \Delta x, y, z) - f(x, y, z)}{\Delta x}\right)_{y,z}
$$

After some derivations, we find
\n
$$
\delta L = \int_{x_i}^{x_f} \left[\left(\frac{\partial f}{\partial y} \right)_{x, \frac{dy}{dx}} \delta y + \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta \left(\frac{dy}{dx} \right) \right] \right] dx
$$
\n
$$
= \int_{x_i}^{x_f} \left[\left(\frac{\partial f}{\partial y} \right)_{x, \frac{dy}{dx}} - \frac{d}{dx} \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \right] \right] dy dx = 0 \text{ for all } x_i \le x \le x_f
$$
\n
$$
\Rightarrow \left(\frac{\partial f}{\partial y} \right)_{x, \frac{dy}{dx}} - \frac{d}{dx} \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \right] = 0 \text{ for all } x_i \le x \le x_f
$$
\nNote that this is a "total" derivative

"Some" derivations -- Consider the term

$$
\int\limits_{x_{i}}^{x_{f}}\Biggl[\Biggl(\frac{\partial f}{\partial\bigl(d y\,/\,d x\bigr)}\Biggr)_{x,y}\delta\biggl(\frac{d y}{d x}\biggr)\Biggr]dx:
$$

If $y(x)$ is a well-defined function, then $y(x)$ is a well-defined function, then $\delta \left(\frac{dy}{dx} \right) = \frac{d}{dx} \delta y$

$$
\delta \left(\frac{dy}{dx} \right) = \frac{d}{dx} \delta y
$$

$$
\int_{x_i}^{x_f} \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta \left(\frac{dy}{dx} \right) \right] dx = \int_{x_i}^{x_f} \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \frac{d}{dx} \delta y \right] dx
$$

$$
= \int_{x_i}^{x_f} \left[\frac{d}{dx} \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] - \frac{d}{dx} \left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] dx
$$

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Note that the δy notation is meant to imply a general infinitessimal variation of the function $y(x)$

Clarification -- what is the meaning of the following statement:

$$
\delta \left(\frac{dy}{dx} \right) = \frac{d}{dx} \delta y
$$

Up to now, the operator δ is not well defined and meant to represent

a general infinitessimal difference. Suppose that $\delta y = \frac{dy}{dx}$, where $y \equiv \frac{dy}{da}$, where *a* $\delta y \equiv$

appears in the functional form somehow. For most functional forms

that one can think of,
$$
\frac{d^2 y(x, a)}{dxda} = \frac{d^2 y(x, a)}{dxdx}.
$$
 One can show this to be
the case even for $y(x, a) = x^a$ where
$$
\frac{d^2 y(x, a)}{dxda} = \frac{d^2 y(x, a)}{dxdx} = x^{a-1} (1 + a \ln(x)).
$$

(Note that here we are being imprecise wrt partial and total derivatives.)

"Some" derivations (continued)--

$$
\int_{x_i}^{x_f} \left[\frac{d}{dx} \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] - \frac{d}{dx} \left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] dx
$$
\n
$$
= \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right]_{x_i}^{x_f} - \int_{x_i}^{x_f} \left[\frac{d}{dx} \left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] dx
$$
\n
$$
= 0 \qquad - \int_{x_i}^{x_f} \left[\frac{d}{dx} \left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] dx
$$

Euler-Lagrange equation:
\n
$$
\Rightarrow \left(\frac{\partial f}{\partial y}\right)_{x,\frac{dy}{dx}} - \frac{d}{dx}\left[\left(\frac{\partial f}{\partial (dy/dx)}\right)_{x,y}\right] = 0 \text{ for all } x_i \le x \le x_f
$$

Clarfication – Why does this term go to zero?

$$
\int_{x_i}^{x_f} \left[\frac{d}{dx} \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] - \frac{d}{dx} \left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] dx
$$
\n
$$
= \left[\left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right]_{x_i}^{x_f} - \int_{x_i}^{x_f} \left[\frac{d}{dx} \left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] dx
$$
\n
$$
= 0 \qquad - \int_{x_i}^{x_f} \left[\frac{d}{dx} \left(\frac{\partial f}{\partial (dy/dx)} \right)_{x,y} \delta y \right] dx
$$

Answer --

By construction $\delta y(x_i) = \delta y(x_f) = 0$

$$
\begin{split}\n\text{Recap} &= \int_{x_i}^{x_f} \left[\left(\frac{\partial f}{\partial y} \right)_{x, \frac{dy}{dx}} \delta y + \left[\left(\frac{\partial f}{\partial (dy / dx)} \right)_{x, y} \delta \left(\frac{dy}{dx} \right) \right] \right] dx \\
&= \int_{x_i}^{x_f} \left[\left(\frac{\partial f}{\partial y} \right)_{x, \frac{dy}{dx}} - \frac{d}{dx} \left[\left(\frac{\partial f}{\partial (dy / dx)} \right)_{x, y} \right] \right] \delta y dx = 0 \quad \text{for all } x_i \le x \le x_f \\
& \Rightarrow \left(\frac{\partial f}{\partial y} \right)_{x, \frac{dy}{dx}} - \frac{d}{dx} \left[\left(\frac{\partial f}{\partial (dy / dx)} \right)_{x, y} \right] = 0 \quad \text{for all } x_i \le x \le x_f\n\end{split}
$$

Here we conclude that the integrand has to vanish at every argument in order for the integral to be zero

- a. Necessary?
- b. Overkill?

Example: End points $-y(0) = 0; y(1) = 1$

$$
L = \int_{0}^{1} \sqrt{1 + \left(\frac{dy}{dx}\right)^{2}} dx \implies f\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right) = \sqrt{1 + \left(\frac{dy}{dx}\right)^{2}}
$$

$$
\left(\frac{\partial f}{\partial y}\right)_{x, \frac{dy}{dx}} - \frac{d}{dx} \left[\left(\frac{\partial f}{\partial (dy/dx)}\right)_{x,y}\right] = 0
$$

$$
\implies -\frac{d}{dx} \left(\frac{dy/dx}{\sqrt{1 + (dy/dx)^{2}}}\right) = 0
$$

Solution:

$$
\left(\frac{dy/dx}{\sqrt{1 + (dy/dx)^2}}\right) = K \qquad \frac{dy}{dx} = K' = \frac{K}{\sqrt{1 - K^2}}
$$

\n
$$
\Rightarrow y(x) = K'x + C \qquad y(x) = x
$$

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$$
-\frac{d}{dx}\left(\frac{xdy/dx}{\sqrt{1+(dy/dx)^2}}\right) = 0
$$

$$
\frac{xdy/dx}{\sqrt{1+(dy/dx)^2}} = K_1
$$

$$
\frac{dy}{dx} = -\frac{1}{\sqrt{\left(\frac{x}{K_1}\right)^2 - 1}}
$$

$$
\Rightarrow y(x) = K_2 - K_1 \ln\left(\frac{x}{K_1} + \sqrt{\frac{x^2}{K_1^2} - 1}\right)
$$

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General form of solution --

$$
y(x) = K_2 - K_1 \ln\left(\frac{x}{K_1} + \sqrt{\frac{x^2}{K_1^2} - 1}\right)
$$

Suppose $K_1 = 1$ and $K_2 = 2 + \sqrt{3}$

$$
A = 2\pi \int_{1}^{2} x \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx = 15.02014144
$$

(according to Maple)

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Another example:

(Courtesy of F. B. Hildebrand, Methods of Applied Mathematics)

Consider all curves $y(x)$ with $y(0) = 0$ and $y(1) = 1$ that minimize the integral:

$$
I = \int_0^1 \left(\left(\frac{dy}{dx} \right)^2 - ay^2 \right) dx \quad \text{for constant } a > 0
$$

Euler-Lagrange equation :

$$
\frac{d^2y}{dx^2} + ay = 0
$$

\n
$$
\Rightarrow y(x) = \frac{\sin(\sqrt{ax})}{\sin(\sqrt{a})}
$$

Review: for
$$
f\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right)
$$
,
\na necessary condition to extremize $\int_{x_1}^{x_1} f\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right) dx$:
\n $\left(\frac{\partial f}{\partial y}\right)_{x, \frac{dy}{dx}} - \frac{d}{dx} \left[\left(\frac{\partial f}{\partial (dy/dx)}\right)_{x,y}\right] = 0$
\nNote that for $f\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right)$,
\n
$$
\frac{df}{dx} = \left(\frac{\partial f}{\partial y}\right) \frac{dy}{dx} + \left(\frac{\partial f}{\partial (dy/dx)}\right) \frac{d}{dx} \frac{dy}{dx} + \left(\frac{\partial f}{\partial x}\right)
$$
\n
$$
= \left(\frac{d}{dx} \left(\frac{\partial f}{\partial (dy/dx)}\right) \frac{dy}{dx} + \left(\frac{\partial f}{\partial (dy/dx)}\right) \frac{d}{dx} \frac{dy}{dx} + \left(\frac{\partial f}{\partial x}\right)
$$
\n
$$
\Rightarrow \frac{d}{dx} \left(f - \frac{\partial f}{\partial (dy/dx)} \frac{dy}{dx}\right) = \left(\frac{\partial f}{\partial x}\right) \text{Alternative}.
$$
\nAlternative: The equation