PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF Online or (occasionally) in Olin103

Discussion for Lecture 7
Chapter 3.17 of F&W

Introduction to the calculus of variations

1. Mathematical construction
2. Practical use
3. Examples

Colloquium on Thursday --

WAKE FOREST UNIVERSITY

Department of Physics

Colloquium

Thursday, Sept. 10, 2020
4 PM

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"Metal Halide Hybrid Perovskite Semiconductors for Opto-Electronic Device"

Metal halide perovskites are emerging class of semiconducting materials that possess unique opto-electronic properties. On one hand, the photo-physical properties are drastically different than other conventional semiconductors originating from their hybrid structures. On the other hand, the electronic transport properties are tied closely to their local structure and dynamics which may show properties beyond the classical system. The complex system is thus a new interesting platform for exploring new physical properties used in opto-electronic devices.

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Wed, 8/26/2020	Chap. 1	Introduction	#1	8/31/2020
2	Fri, 8/28/2020	Chap. 1	Scattering theory	#2	9/02/2020
3	Mon, 8/31/2020	Chap. 1	Scattering theory	#3	9/04/2020
4	Wed, 9/02/2020	Chap. 1	Scattering theory		
5	Fri, 9/04/2020	Chap. 1	Scattering theory	#4	9/09/2020
6	Mon, 9/07/2020	Chap. 2	Non-inertial coordinate systems		
7	Wed, 9/09/2020	Chap. 3	Calculus of Variation	#5	9/11/2020
8	Fri, 9/11/2020	Chap. 3	Calculus of Variation	#6	9/14/2020

Your questions –
From Tim

1. When you say a well-defined function in slide 11, what does that mean? Also why does the first term in slide 12 go to zero when the second term does not? Aren't both terms in that equation equivalent?

From Gao

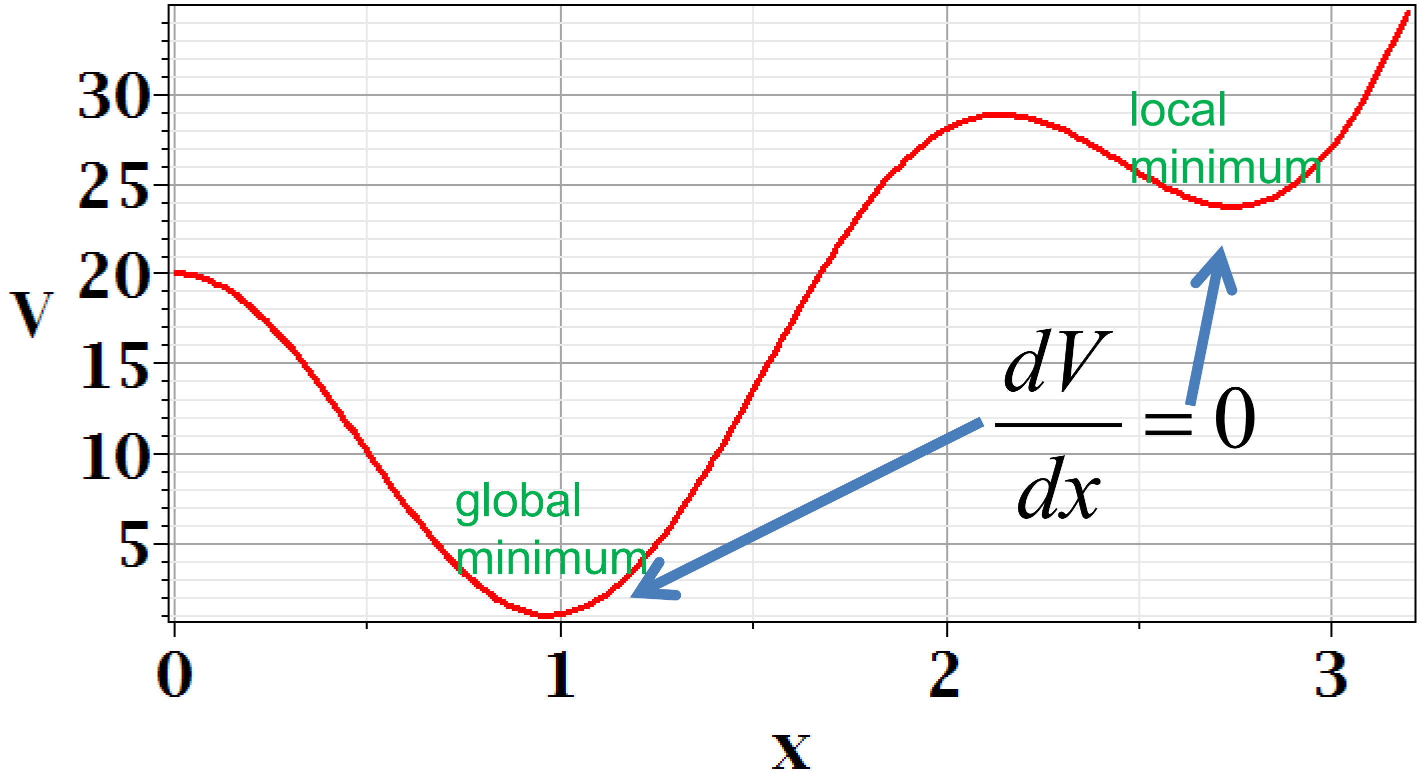
1. About lecture 7, Why use caculus of variations to find the function y(x)? I think it is abstract.

From Nick

1. Can you explain what we mean by a well-defined function?
2. I'm getting lost in the notation starting around slide 9. Hopefully we can go over that tomorrow. In particular, I'm not sure I'm following the \delta notation.

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".

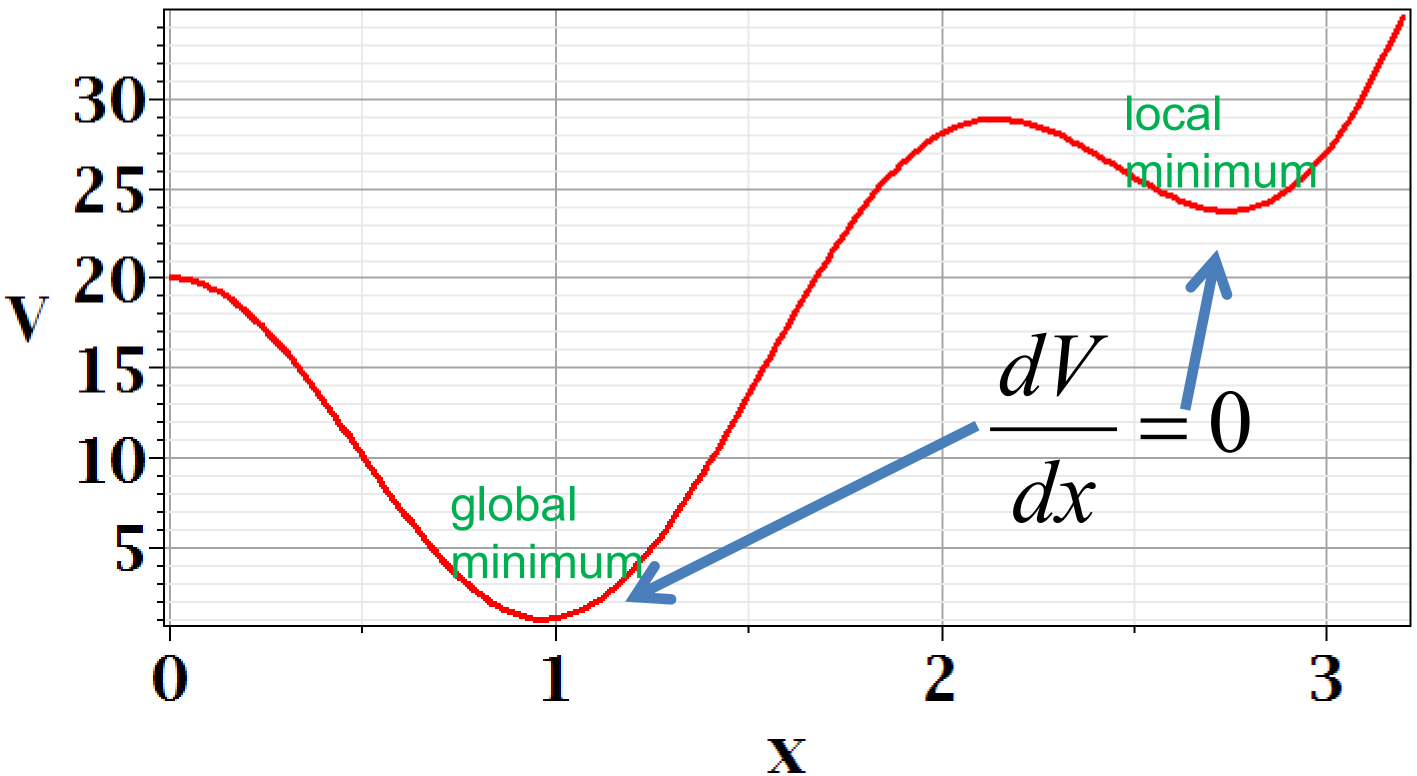
Minimization of a simple function



Minimization of a simple function

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

Necessary condition : $\dfrac{dV}{dx} = 0$



Functional minimization

Consider a family of functions $y(x)$, with fixed end points

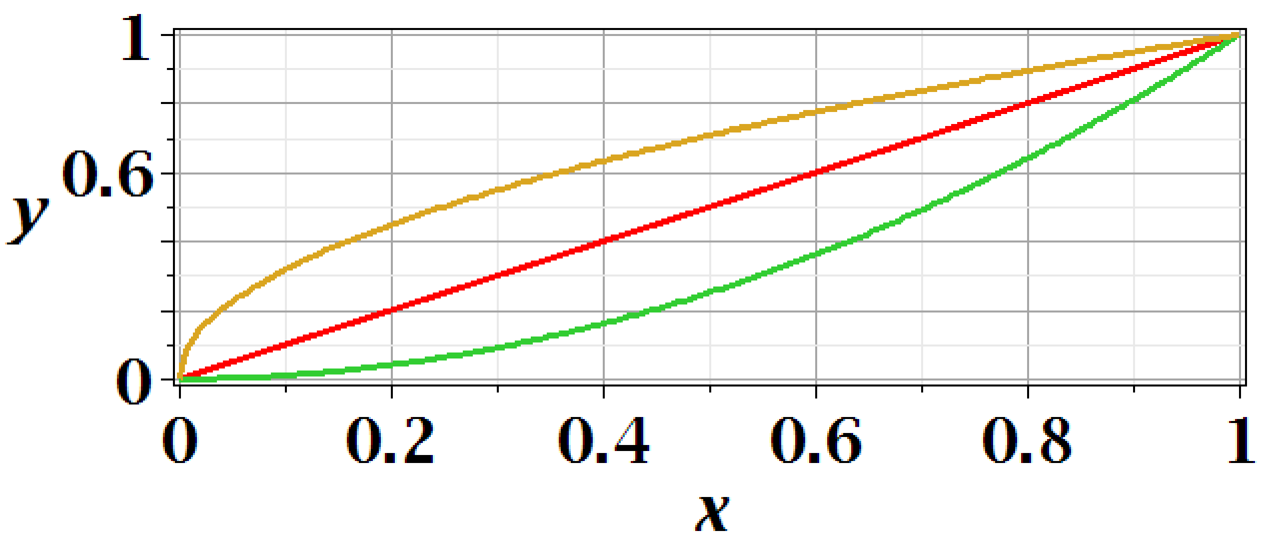
$y(x_i) = y_i$ and $y(x_f) = y_f$ and a function $L\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right)$.

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

Necessary condition: $\delta L = 0$

Example:

$$L = \int_{(0,0)}^{1,1} \sqrt{(dx)^2 + (dy)^2}$$



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

Minimization of a function

➔Know V(x) ➔Find x_0 such that $V(x_0)$ is a minimum.

Calculus of variation

For $x_i \leq x \leq x_f$ 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 $y(x)$.

Functional minimization

Consider a family of functions $y(x)$, with fixed end points

$y(x_i) = y_i$ and $y(x_f) = y_f$ and a function $L\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right)$.

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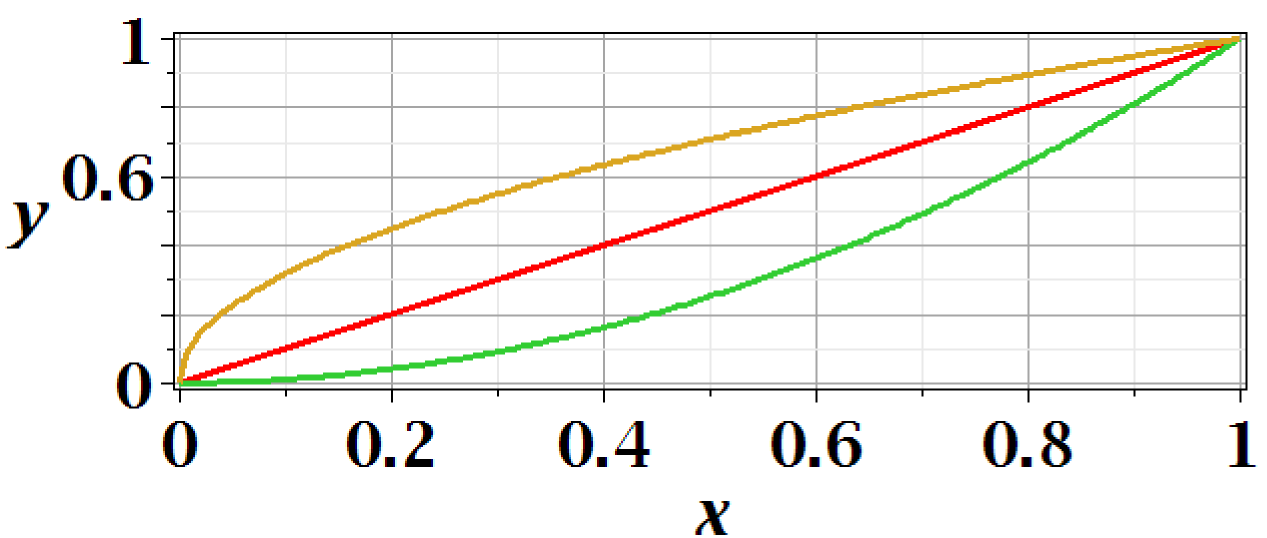
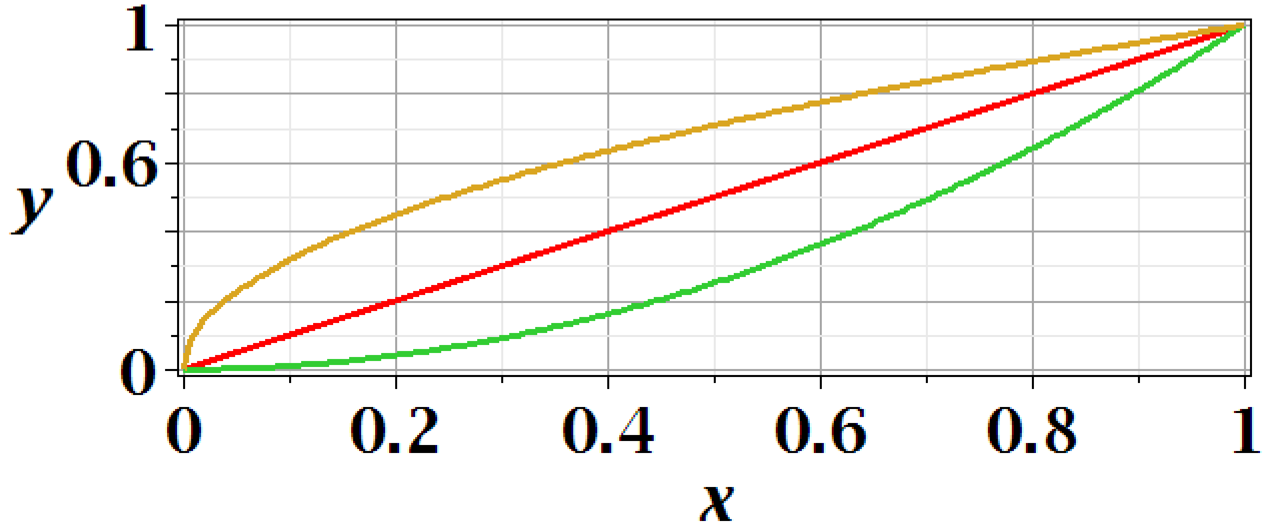


Example:

$$L = \int_{(0,0)}^{(1,1)} \sqrt{(dx)^2 + (dy)^2}$$

$$= \int_0^1 \sqrt{1 + \left(\frac{dy}{dx}\right)^2}\, dx$$



Sample functions :

$y_1(x) = \sqrt{x}$ $\qquad L = \int_0^1 \sqrt{1 + \frac{1}{4x}}\, dx = 1.4789$

$y_2(x) = x$ $\qquad L = \int_0^1 \sqrt{1+1}\, dx = \sqrt{2} = 1.4142$

$y_2(x) = x^2$ $\qquad L = \int_0^1 \sqrt{1+4x^2}\, dx = 1.4789$

Calculus of variation example for a pure integral functions

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

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 $y(x) \rightarrow y(x) + \delta y(x)$

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

Formally:

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

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

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

After some derivations, we find

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

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

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

Note that this is a
"total" derivative

“Some” derivations --

Consider the term

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

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

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

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

*Your question -- 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 be general.

Now let us suppose that it implies an infinitessimal difference to its function.

As an example, suppose that $y(x,\eta)$ where x and η are independent such as

$y(x,\eta) = x^\eta$ For $\eta > 0$, and $0 \le x \le 1$

assume $\eta > 0$

$$\frac{d}{d\eta}\frac{d}{dx}y(x,\eta) = \frac{d}{dx}\frac{d}{d\eta}y(x,\eta) = \left(1+\eta\ln(x)\right)x^{\eta-1}$$

Note that the construction of this system is that

$y(x_i,\eta)$ has the same value for all η and

$y(x_f,\eta)$ has the same value for all η.

Example $y(x,\eta) = x^\eta$ for $x_i = 0$ and $x_f = 1$

$y_i = y(0,\eta) = 0$ and $y_f = y(1,\eta) = 1$

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

“Some” derivations (continued)--

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

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

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

Euler-Lagrange equation:

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

Your question – Why does this term go to zero?

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

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

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

Answer --

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

Recap --

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

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

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

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 -- $y(0)=0; y(1)=1$

$$L=\int_0^1 \sqrt{1+\left(\frac{dy}{dx}\right)^2}\,dx \qquad \Rightarrow f\left(\left\{y(x),\frac{dy}{dx}\right\},x\right)=\sqrt{1+\left(\frac{dy}{dx}\right)^2}$$

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

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

Solution:

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

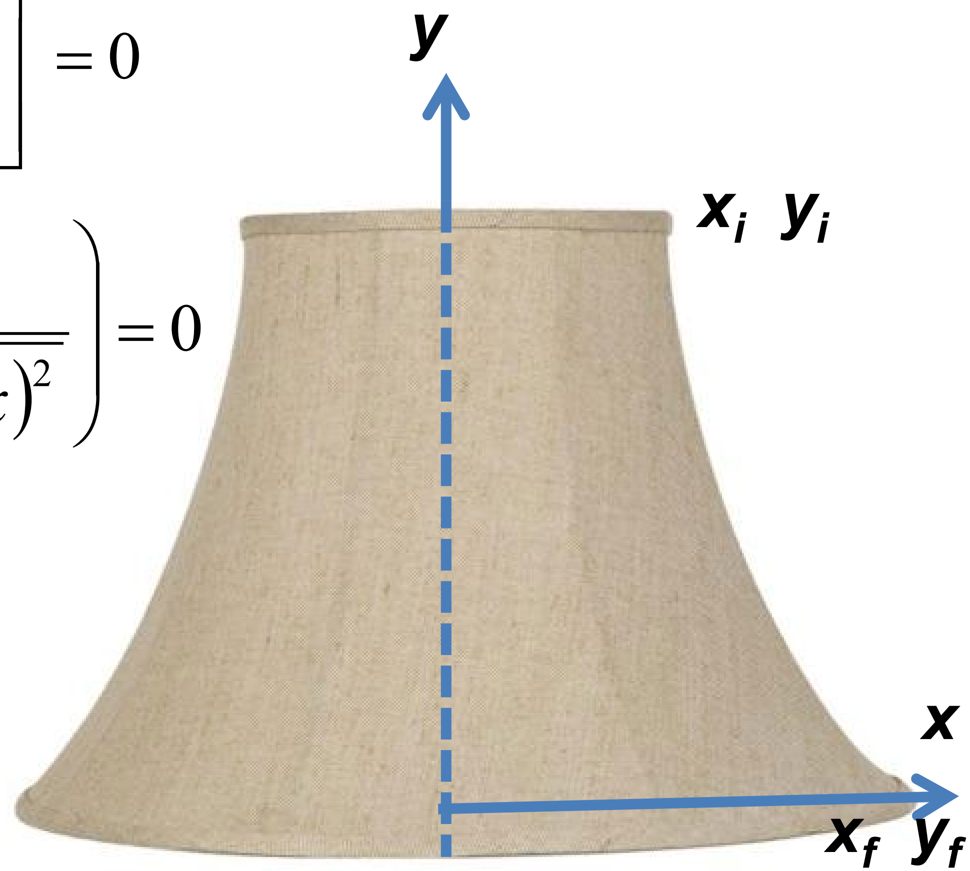
$$\Rightarrow y(x)=K'x+C \qquad y(x)=x$$

Example: Lamp shade shape *y(x)*

$$A = 2\pi \int_{x_i}^{x_f} x\sqrt{1+\left(\frac{dy}{dx}\right)^2}\,dx \qquad \Rightarrow f\left(\left\{y(x),\frac{dy}{dx}\right\},x\right) = x\sqrt{1+\left(\frac{dy}{dx}\right)^2}$$

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

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



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

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

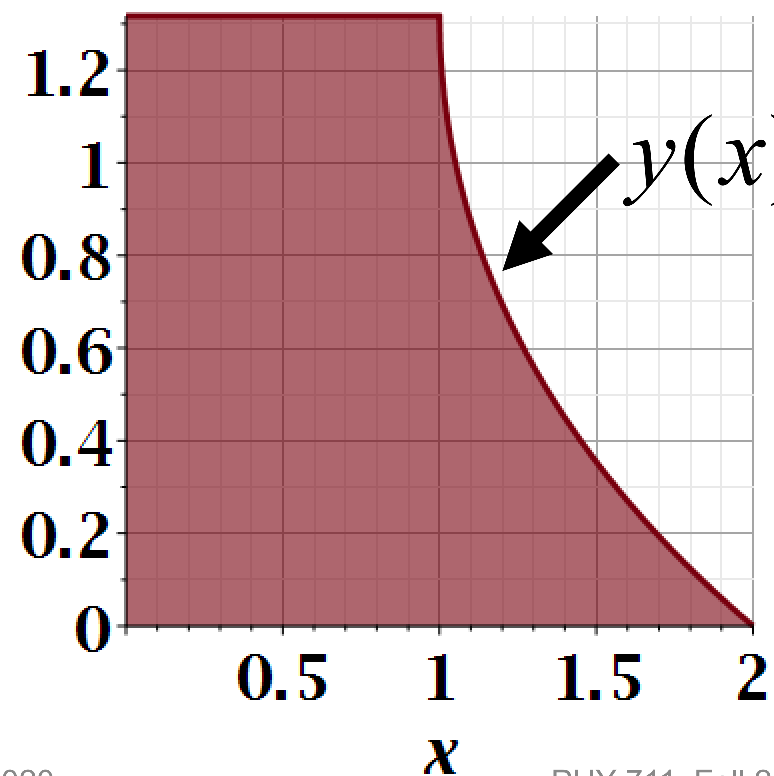
$$\frac{dy}{dx}=-\frac{1}{\sqrt{\left(\frac{x}{K_1}\right)^2-1}}$$

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

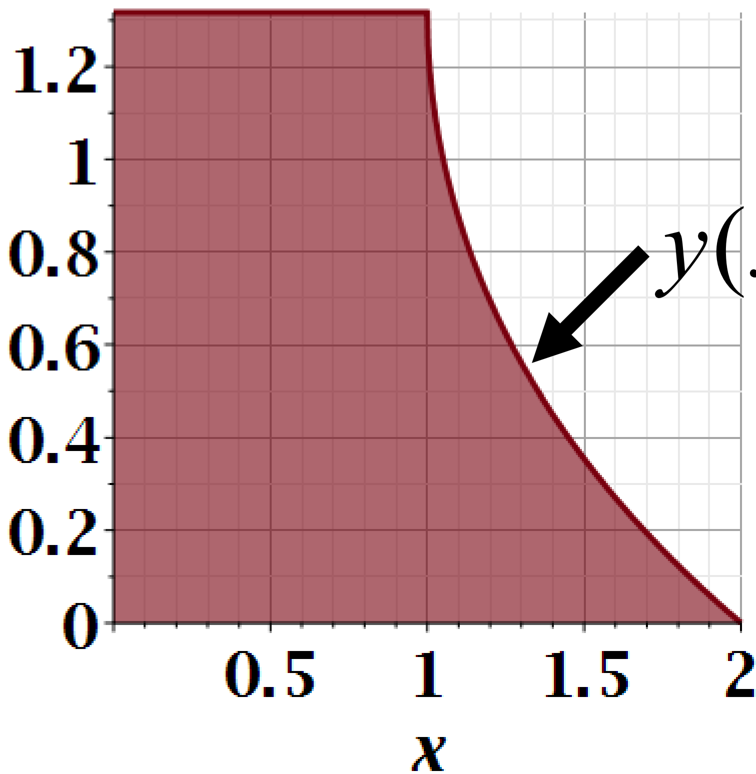
General form of solution --

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

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



$$y(x) = \ln\left(\frac{2+\sqrt{3}}{x + \sqrt{x^2 - 1}} \right)$$



$$y(x) = \ln\left(\frac{2+\sqrt{3}}{x+\sqrt{x^2-1}}\right)$$

$$A = 2\pi\int_1^2 x\sqrt{1+\left(\frac{dy}{dx}\right)^2}\,dx = 15.02014144$$

(according to Maple)

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:

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

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

Review: for $f\left(\left\{y(x),\frac{dy}{dx}\right\},x\right),$

a necessary condition to extremize $\int_{x_i}^{x_f} f\left(\left\{y(x),\frac{dy}{dx}\right\},x\right)dx$:

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

⇦ Euler-Lagrange equation

Note that for $f\left(\left\{y(x),\frac{dy}{dx}\right\},x\right),$

$$\frac{df}{dx} = \left(\frac{\partial f}{\partial y}\right)\frac{dy}{dx} + \left(\frac{\partial f}{\partial(dy/dx)}\right)\frac{d}{dx}\frac{dy}{dx} + \left(\frac{\partial f}{\partial x}\right)$$

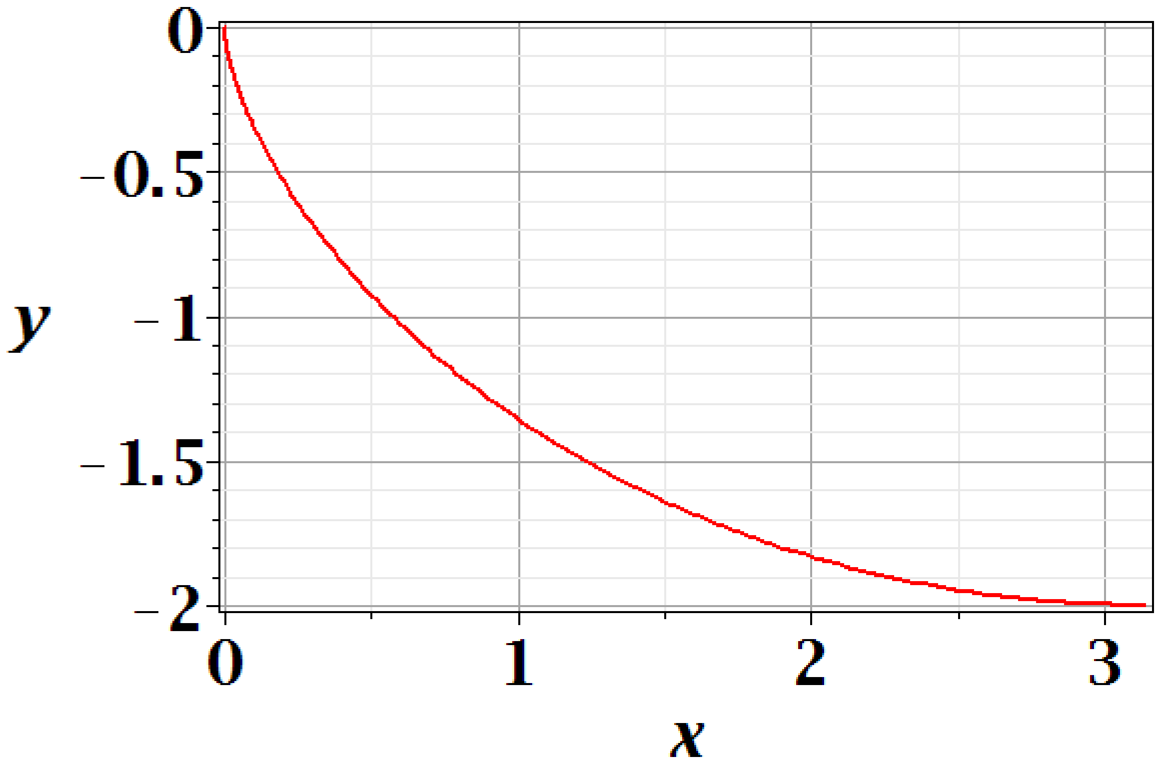
$$= \left(\frac{d}{dx}\left(\frac{\partial f}{\partial(dy/dx)}\right)\right)\frac{dy}{dx} + \left(\frac{\partial f}{\partial(dy/dx)}\right)\frac{d}{dx}\frac{dy}{dx} + \left(\frac{\partial f}{\partial x}\right)$$

$$\Rightarrow \frac{d}{dx}\left(f - \frac{\partial f}{\partial(dy/dx)}\frac{dy}{dx}\right) = \left(\frac{\partial f}{\partial x}\right)$$

⇦ Alternate Euler-Lagrange equation

Brachistochrone problem: (solved by Newton in 1696)

http://mathworld.wolfram.com/BrachistochroneProblem.html



A particle of weight *mg* travels frictionlessly down a path of shape *y(x).* What is the shape of the path *y(x)* that minimizes the travel time from $y(0)=0$ to $y(\pi)=-2$?

$$T = \int_{x_i y_i}^{x_f y_f} \frac{ds}{v} = \int_{x_i}^{x_f} \frac{\sqrt{1+\left(\frac{dy}{dx}\right)^2}}{\sqrt{-2gy}}\, dx \quad \text{because} \quad \tfrac{1}{2}mv^2 = -mgy$$

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

$$\frac{d}{dx}\left(f - \frac{\partial f}{\partial(dy/dx)}\frac{dy}{dx}\right) = 0$$

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

Note that for the original form of Euler-Lagrange equation:

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

differential equation is more complicated:

$$-\frac{1}{2}\sqrt{\frac{1+\left(\frac{dy}{dx}\right)^2}{-y^3}} - \frac{d}{dx}\left(\frac{\frac{dy}{dx}}{\sqrt{-y\left(1+\left(\frac{dy}{dx}\right)^2\right)}}\right) = 0$$

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

$$\frac{d}{dx}\left(f - \frac{\partial f}{\partial(dy/dx)}\frac{dy}{dx}\right) = \left(\frac{\partial f}{\partial x}\right)$$

$$\Rightarrow \frac{d}{dx}\left(\frac{1}{\sqrt{-y\left(1+\left(\frac{dy}{dx}\right)^2\right)}}\right) = 0 \qquad -y\left(1+\left(\frac{dy}{dx}\right)^2\right) = K \equiv 2a$$

$$-y\left(1+\left(\frac{dy}{dx}\right)^2\right)=K\equiv 2a \qquad \text{Let} \quad y=-2a\sin^2\tfrac{\theta}{2}=a(\cos\theta-1)$$

$$\frac{dy}{dx}=-\sqrt{\frac{2a}{-y}-1}$$

$$-\frac{dy}{\sqrt{\frac{2a}{-y}-1}}=\frac{2a\sin\frac{\theta}{2}\cos\frac{\theta}{2}\,d\theta}{\sqrt{\frac{2a}{2a\sin^2\frac{\theta}{2}}-1}}=dx$$

$$-\frac{dy}{\sqrt{\frac{2a}{-y}-1}}=dx$$

$$x=\int_0^\theta a(1-\cos\theta')\,d\theta'=a(\theta-\sin\theta)$$

Parametric equations for Brachistochrone:

$$x=a(\theta-\sin\theta)$$

$$y=a(\cos\theta-1)$$

Parametric plot --

plot([theta-sin(theta), cos(theta)-1, theta = 0 .. Pi])