Optimal Functions and Nanomechanics III

APP MTH 3022/7106

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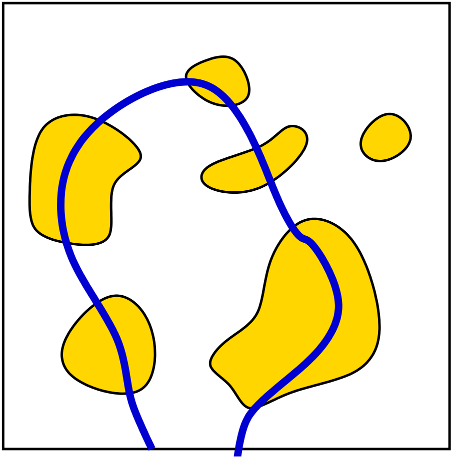
Lecture 1

Course outline

1. Introduction and background
2. The Euler-Lagrange equations
3. Specials cases: autonomous, y-independence
4. Extending to higher derivatives and several variables
5. Special functions and applications to nanomechanics
6. Numerical solutions of variational problems
7. Integral constraints and non-fixed endpoints
8. Formulations, conservation laws and classification

Gold digger

- Imagine a field containing patches of gold.
- Collect the most gold.
- We want to choose best path.
- But the path length is limited.



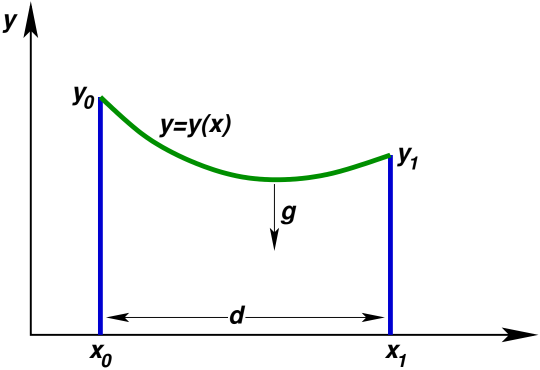
Gold digger

- The gold collected on the path is the integral of the gold at each point.
- The length of the path is fixed.
- We are maximizing an integral over a path for all possible paths.
- Maximizing a function of a function[1].

[1] We use the term *functional* for a function that takes other functions as arguments.

Catenary

Consider a thin, uniformly-heavy, flexible cable suspended from the top of two poles of height y_0 and y_1 spaced a distance d apart. What is the shape of the cable between the two poles?



What is the difference if the cable is coiled at the base of the poles and is free to move up and down via a pulley?

Brachistochrone

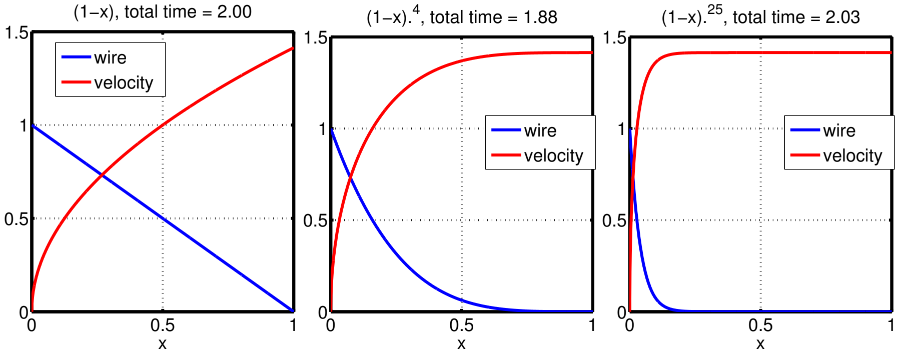
> *"Did Bernoulli sleep before he found the curves of quickest descent?" — Peter Parker, Spiderman II*

Find the shape of a wire along which a bead, initially at rest, slides from one end to the other as quickly as possible under the influence of gravity.

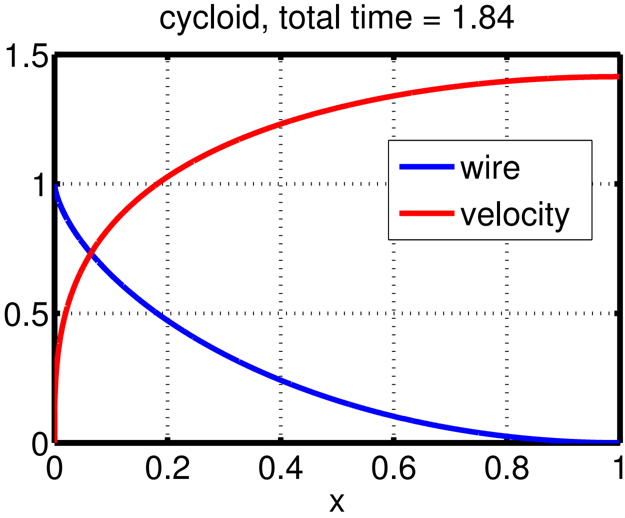
- endpoints are fixed
- motion is frictionless

Can think of it as the "optimal" slippery dip.

Brachistochrone



Brachistochrone

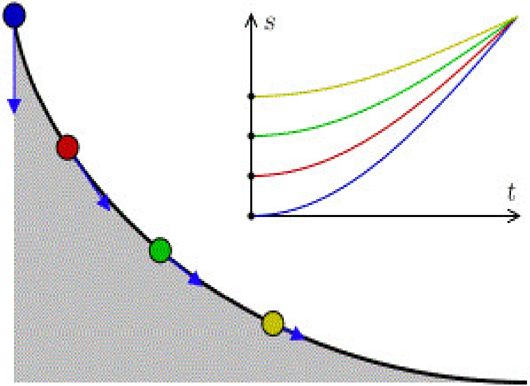


Brachistochrone: a history

- problem posed by Johann Bernoulli (1696)
- Newton, Liebnitz, Huygens, various Bernoullis
- Euler developed method to solve it that was generalizable
- Jacob first to solve?
- Johann, "Ah, I recognize the paws of a lion"
- Christiaan Huygens discovered cycloid property

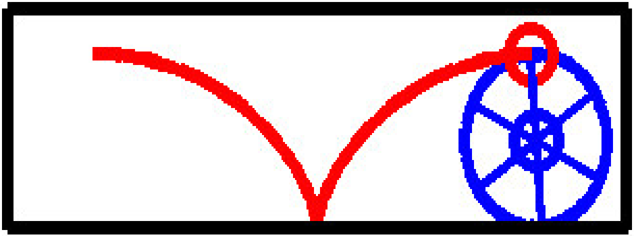
  A bead sliding down a cycloid generated by a circle of radius ρ under gravity g reaches the bottom after $\pi\sqrt{\rho/g}$ regardless of where the bead starts.

Huygens' tautochrone/isochrone



Animation by Claudio Rocchini, 2009

Generating a cycloid



Geodesics

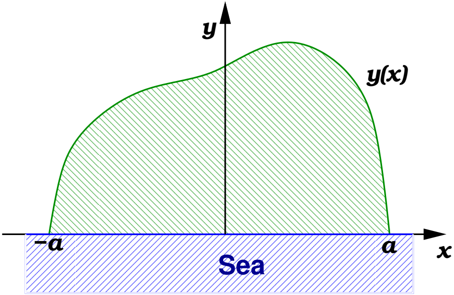
- shortest path between two points on a plane
- shortest path between two points on a sphere

- shortest path on an arbitrary manifold on $\mathbb{R}^n$

Dido's problem

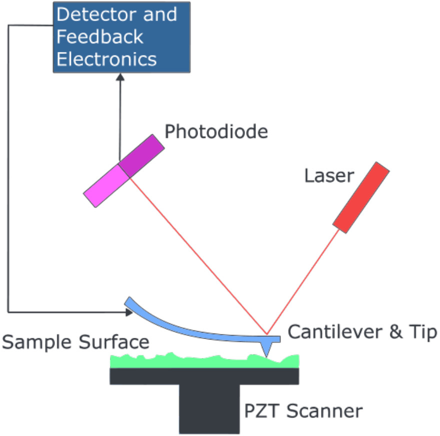
Isoperimetric problem: what shaped curve encompasses the largest area given a fixed perimeter.

- 200 B.C. proof by Zendorus (but flawed)
- Steiner proved that "if it exists" it's a circle
- Weierstraß proved using the Calculus of Variations



Other problems

- Design of vehicle profile that minimizes drag
- Finding shapes of soap bubbles, shapes of least curvature, etc
- Joining surfaces for carbon nanostructures
- Finding the shape of a buckling cantilever in an Atomic Force Microscope (AFM)



Atomic force microscope block diagram

Revision

Calculus of variations is concerned with maximisation (minimisation).

We are going to maximise (minimise) functionals, not functions.

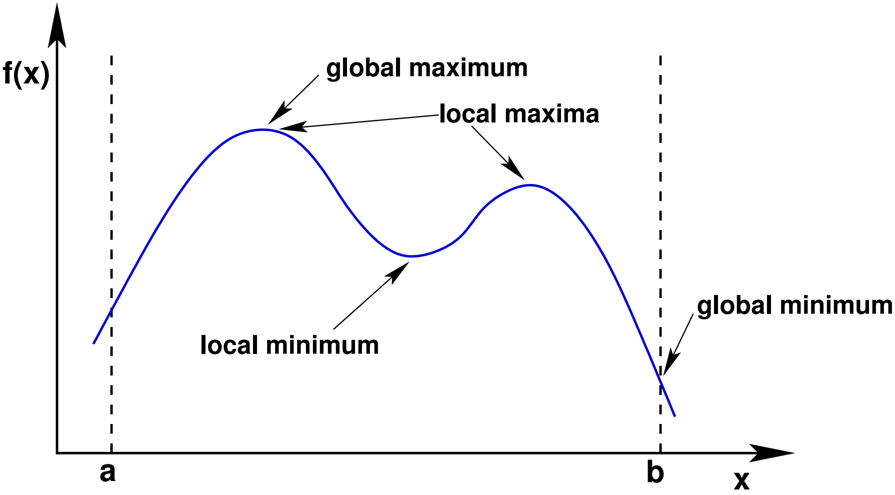
Let us first revise maximisation (minimisation) of function.

Global and local minima and maxima

For functions of one variable:

- Let $x \in [a, b]$ and $f(x) : [a, b] \to \mathbb{R}$
- If there is a point $x_{\min}$ such that $f(x_{\min}) \leqslant f(x)$ for all $x \in [a, b]$, then $x_{\min}$ is called a **global minimum** of $f(x)$ in $[a, b]$.
- The set of points x such that $f(x) = f(x_{\min})$ is called the **minimal set**.
- If there is an interior point $x \in (a, b)$ such that there exists a $\delta > 0$ with $f(x) \leqslant f(\hat{x})$ for all $\hat{x} \in (x - \delta, x + \delta)$, then x is called a **local minimum** of $f(x)$.
- similar definitions apply for maxima, note that the maxima of $f(x)$ are the minima of $-f(x)$

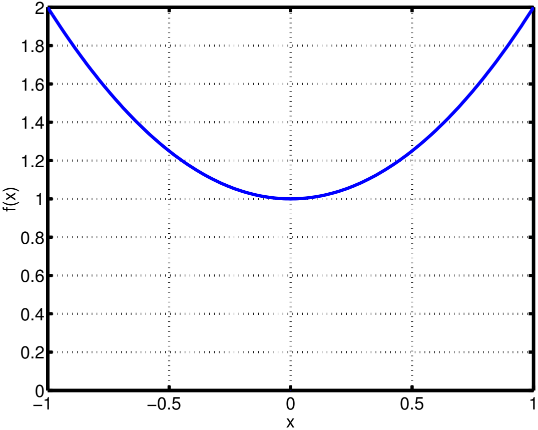
Minima and maxima: Example 1



Minima and maxima: Example 2

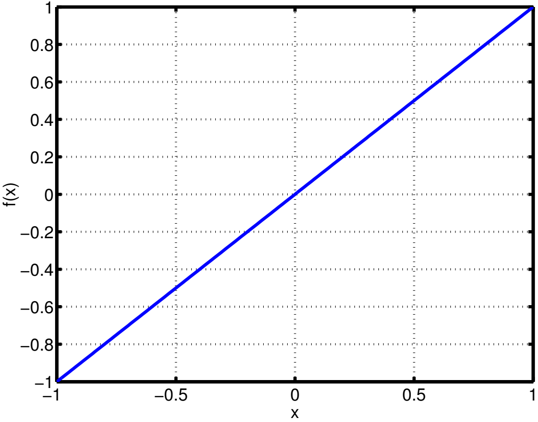
$$f(x) = 1 + x^2 \text{ on } [-1, 1]$$

- global minimum at $x = 0$
- local minimum at $x = 0$
- maximal set $\{-1, 1\}$



Minima and maxima: Example 3

$$f(x) = x \text{ on } [-1, 1]$$

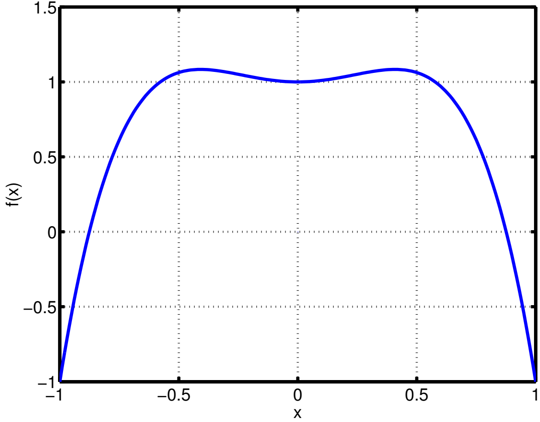


- global minimum at $x = -1$
- not a local min. because not an interior point
- global maximum at $x = 1$

Minima and maxima: Example 4

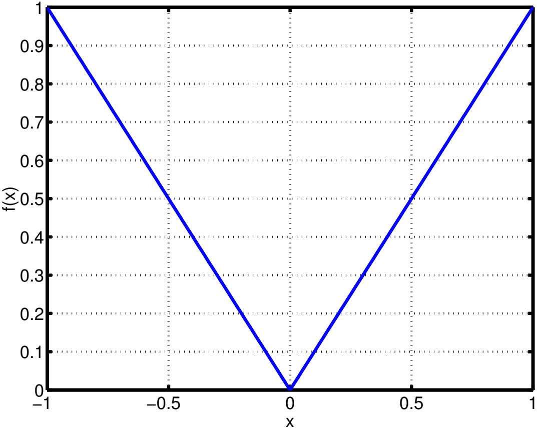
$$f(x) = 1 + x^2 - 3x^4 \text{ on } [-1, 1]$$

- global minima at $x = -1$ and $x = 1$
- local minimum at $x = 0$.
- global maxima at $x = \sqrt{6}/6$ and $x = -\sqrt{6}/6$.



Minima and maxima: Example 5

$$f(x) = |x| \text{ on } [-1, 1]$$



- global minimum at $x = 0$
- local minimum at $x = 0$
- maximal set $\{-1, 1\}$

How to find maxima and minima

Theorem 1: Let $f(x) : [a, b] \to \mathbb{R}$ be differentiable in (a, b). If $f(x)$ has a local extrema at x then

$$\frac{df}{dx} = f'(x) = 0$$

Proof: The derivative is given by

$$f'(x) = \lim_{\hat{x} \to x} \frac{f(\hat{x}) - f(x)}{\hat{x} - x}$$

Suppose x is a local minima, then $\exists \delta > 0$ such that $\hat{x} \in (x - \delta, x + \delta) \Rightarrow f(\hat{x}) > f(x)$, hence the numerator > 0. The denominator changes sign at $\hat{x} = x$. Differentiability implies the left and right hand limits exist and are equal, and hence $f'(x) = 0$.

Sufficient conditions

Theorem 2: Let $f(x) : [a, b] \to \mathbb{R}$ be twice differentiable in (a, b). Sufficient conditions for a local minimum at x are

$$f'(x) = 0 \quad \text{and} \quad f''(x) > 0$$

Proof: see following.

Some useful theorems

- **Mean value theorem:** Let $x_0 < x_1$, and $f(x)$ be a continuous function in $[x_0, x_1]$, and differentiable in (x_0, x_1), then $\exists \xi \in (x_0, x_1)$ such that

$$f(x_1) = f(x_0) + (x_1 - x_0) f'(\xi)$$

- **Taylor's theorem:** Let $f(x)$ be a function whose first n derivatives exist and are continuous in the interval $[x_0, x_1]$, and $f^{(n+1)}(x)$ exists for all $x \in (x_0, x_1)$, then $\exists \xi \in (x_0, x_1)$

$$\begin{aligned} f(x_1) = f(x_0) + (x_1 - x_0) f'(x_0) + \frac{(x_1 - x_0)^2}{2} f''(x_0) + \cdots \\ + \frac{(x_1 - x_0)^n}{n!} f^{(n)}(x_0) + \frac{(x_1 - x_0)^{n+1}}{(n+1)!} f^{(n+1)}(\xi) \end{aligned}$$

Necessary and sufficient condition

Theorem 3: Let $f(x) : [a, b] \to \mathbb{R}$ have derivatives of all orders, then a necessary and sufficient condition for a local minima is that for some n

$$f'(x) = f''(x) = \cdots = f^{(2n-1)}(x) = 0 \quad \text{and} \quad f^{(2n)}(x) > 0$$

Proof: Taylor's theorem, where $\hat{x} - x = \epsilon$

$$f(\hat{x}) = f(x) + \epsilon f'(x) + \cdots + \frac{\epsilon^{2n-1}}{(2n-1)!} f^{(2n-1)}(x) + \frac{\epsilon^{2n}}{(2n)!} f^{(2n)}(x) + O(\epsilon^{2n+1})$$

Then

$$\begin{aligned} f(\hat{x}) - f(x) &= \frac{\epsilon^{2n}}{(2n)!} f^{(2n)}(x) + O(\epsilon^{2n+1}) \\ &> 0 \quad \text{for small enough } \epsilon \end{aligned}$$

Classifying extrema

Assume that $f'(x) = 0$

- local maxima $f''(x) < 0$
- local minima $f''(x) > 0$
- turning point $f''(x) = 0$, and $f^{(3)}(x) \neq 0$
- $+$ a lot of higher order conditions

Call all points with $f'(x) = 0$ the set of **stationary** points

Notation

- $[a, b]$ is the closed interval, i.e. the set $\{x \in \mathbb{R} | a \leqslant x \leqslant b\}$
- (a, b) is the open interval, i.e. the set $\{x \in \mathbb{R} | a < x < b\}$
- $(a, b]$ is the set $\{x \in \mathbb{R} | a < x \leqslant b\}$
- $f(x) : [a, b] \to \mathbb{R}$ denotes a function that maps the set $[a, b]$ to a real number.
- $\dfrac{d^n f}{dx^n} = f^{(n)}(x)$ denotes the nth derivative of $f(x)$.

Synonyms

- the global minimum is sometimes called a strong minimum
- a local minimum is sometimes called a weak minimum
- the local extrema are the collection of local minima and maxima
  We sometimes abuse notation to include stationary points in the set of extrema.

Continuity

- a function $f(x)$ is **continuous** at x_0 iff the left and right limits at x_0 exist and are equal, i.e.,

$$\lim_{x \to x_0^-} f(x) = \lim_{x \to x_0^+} f(x)$$

otherwise it is said to have a **discontinuity**.

- We say a function is continuous on an interval if it is continuous at every point inside the interval and the limits exist at the boundaries.
- A function is **piecewise continuous** on an interval if it has at most finite number of discontinuities.

Differentiability

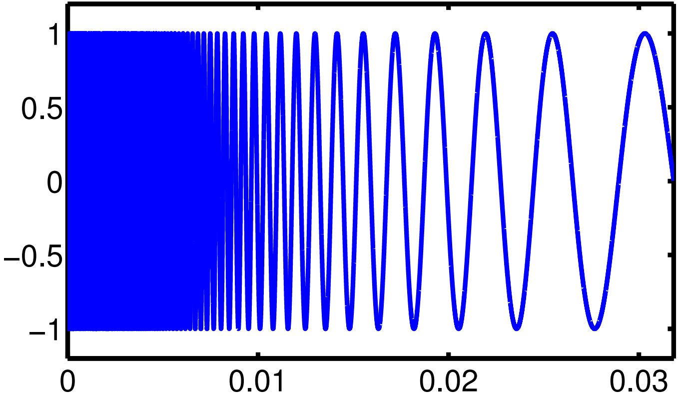
- A function is **differentiable** at x_0 if its derivative exists, and is continuous at x_0, i.e., the following limit exists and is the same from both directions

$$\lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

- We say a function is differentiable on an interval if it is differentiable at every point inside the interval and the limits exist at the boundaries.
- A function is **piecewise differentiable** if the derivative has at most a finite number of discontinuities.
- A function is **twice differentiable** if its second derivative exists and is continuous.

Exception

- We also eliminate from consideration functions whose derivative changes sign an infinite number of times in a finite interval.
  - e.g. $\sin(1/x)$



Notation: Vector derivatives

We define the **del** or **grad** operator (in Cartesian coordinates) by

$$\boldsymbol{\nabla} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$$

So, given a scalar function $\phi(x, y, z)$, then $\boldsymbol{\nabla}\phi$ is a vector function

$$\boldsymbol{\nabla}\phi = \left(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}, \frac{\partial \phi}{\partial z} \right)$$

Given a vector function $\boldsymbol{f}(x, y, z) = (f_1, f_2, f_3)$ then we define the **div** operator $\mathrm{div}\, \boldsymbol{f} = \boldsymbol{\nabla} \cdot \boldsymbol{f}$, e.g.

$$\boldsymbol{\nabla} \cdot \boldsymbol{f} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \cdot (f_1, f_2, f_3) = \frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} + \frac{\partial f_3}{\partial z}$$

Notation: Curl and Laplacian

We can also use del to define the **curl** operator using a cross-product $\mathrm{curl} = \mathrm{del}\ \times$, e.g.

$$\begin{aligned}\mathrm{curl}\ \boldsymbol{f} &= \boldsymbol{\nabla} \times \boldsymbol{f} \\ &= \left(\frac{\partial f_3}{\partial y} - \frac{\partial f_2}{\partial z}, \frac{\partial f_1}{\partial z} - \frac{\partial f_3}{\partial x}, \frac{\partial f_2}{\partial x} - \frac{\partial f_1}{\partial y} \right)\end{aligned}$$

The **Laplacian operator**, or del-squared operator of a scalar function $\phi(x, y, z)$ is defined by

$$\nabla^2 \phi = \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \phi) = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2}$$