Optimal Functions and Nanomechanics III

APP MTH 3022/7106

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Lecture 17

Last lecture

- Examined the dynamics of scaled oscillators with
  - Newtonian mechanics
  - Variational approach
- Saw that nanoscaled oscillators are capable of generating frequencies in the gigahertz range
- Briefly considered other sorts of nanomechanical oscillators

Extension 3: Several independent variables

When there are several independent variables, e.g., (x, y) and the extremal we wish to find represents, for instance, a surface $z(x, y)$, and f is a function $f(x, y, z(x, y), z_x, z_y)$, then the E-L equation generalizes to give

$$\frac{\partial f}{\partial z} - \frac{\partial}{\partial x}\frac{\partial f}{\partial z_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial z_y} = 0$$

Several independent variables

Consider a surface minimization problem. We have a surface in 3D that is a function of (x, y), e.g. $z = z(x, y)$ then x and y are both independent variables.

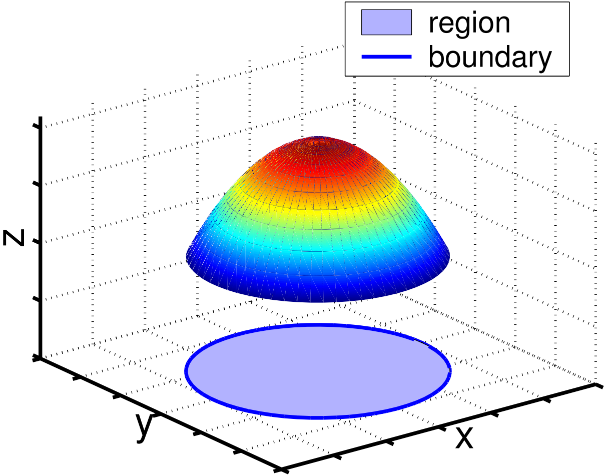
Examples:

- minimal area surfaces
  - soap films and bubbles
  - for construction
- problems of the form, minimize

$$F\{z\} = \iint_{\Omega} (z_x^2 + z_y^2)\, dx\, dy$$

Notation

$$
\begin{aligned}
\text{region} &= \Omega \\
\text{boundary} &= \delta\Omega \\
\text{surface} &= z(x,y)
\end{aligned}
$$



Formalisms

Ω is a simply connected, bounded region of $\mathbb{R}^2$

$\delta\Omega$ is the boundary of Ω

$\bar{\Omega} = \Omega \cup \delta\Omega$ is the closure of Ω

$C^2(\bar{\Omega}) = \{z : \bar{\Omega} \to \mathbb{R} \mid z$ has 2 continuous derivatives$\}$

$C^2(\delta\Omega) = \{z_0 : \delta\Omega \to \mathbb{R} \mid z_0$ has 2 continuous derivatives$\}$

$\iint_\Omega f(x,y)\,dx\,dy$ is an area integral of f over the region Ω

$\oint_{\delta\Omega} f(x,y)\,dx$ is a contour integral around the boundary $\delta\Omega$.

The problem

Find extremals for the functional

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

Analogy of fixed end points is a fixed boundary, e.g.

$$z(x, y) = z_0(x, y) \text{ for all } (x, y) \in \delta\Omega$$

for some specified function $z_0 \in C^2(\delta\Omega)$.

Solution

As before we consider perturbations, though in this case they are perturbations to a surface, with fixed edge, e.g.

$$\hat{z}(x,y) = z(x,y) + \epsilon\eta(x,y)$$

where $\eta(x,y) = 0$ for all $(x,y) \in \delta\Omega$.

Taylor's theorem gives

$$\begin{aligned} & f(x, y, z + \epsilon\eta, z_x + \epsilon\eta_x, z_y + \epsilon\eta_y) \\ = \quad & f(x, y, z, z_x, z_y) + \epsilon\left[\eta\frac{\partial f}{\partial z} + \eta_x\frac{\partial f}{\partial z_x} + \eta_y\frac{\partial f}{\partial z_y}\right] + O(\epsilon^2) \end{aligned}$$

The First Variation

As before we demand that at an extremal, the First Variation $\delta F(\eta, z) = 0$ for all possible η, and small ϵ

$$
\begin{aligned}
\delta F(\eta, z) &= \lim_{\epsilon \to 0} \frac{F\{z + \epsilon\eta\} - F\{z\}}{\epsilon} \\
&= \iint_{\Omega} \left[\eta \frac{\partial f}{\partial z} + \eta_x \frac{\partial f}{\partial z_x} + \eta_y \frac{\partial f}{\partial z_y} \right] \, dx \, dy.
\end{aligned}
$$

We next need to do the equivalent of integration by parts, but it's a bit more complicated — we need to use Green's theorem.

Green's theorem

One form of Green's theorem states

$$\iint_{\Omega} \left(\frac{\partial \phi}{\partial x} + \frac{\partial \psi}{\partial y} \right) \, dx \, dy = \oint_{\delta\Omega} \phi \, dy - \oint_{\delta\Omega} \psi \, dx$$

for $\phi, \psi : \bar{\Omega} \to \mathbb{R}$ such that ϕ, ψ, ϕ_x and ψ_y are continuous.

This converts an area integral over a region into a line integral around the boundary.

Green's theorem in use

Green's theorem: $\iint \Omega \left(\frac{\partial \phi}{\partial x} + \frac{\partial \psi}{\partial y} \right) dx\, dy = \oint_{\delta\Omega} \phi\, dy - \oint_{\delta\Omega} \psi\, dx$

For instance, take

$$\phi = \eta \frac{\partial f}{\partial z_x} \quad \text{and} \quad \psi = \eta \frac{\partial f}{\partial z_y}$$

$$\begin{aligned} \frac{\partial \phi}{\partial x} &= \eta_x \frac{\partial f}{\partial z_x} + \eta \frac{\partial}{\partial x} \frac{\partial f}{\partial z_x} \\ \frac{\partial \psi}{\partial y} &= \eta_y \frac{\partial f}{\partial z_y} + \eta \frac{\partial}{\partial y} \frac{\partial f}{\partial z_y} \end{aligned}$$

Green's theorem in use

Green's theorem: $$\iint_{\Omega}\left(\frac{\partial\phi}{\partial x}+\frac{\partial\psi}{\partial y}\right)dx\,dy=\int_{\delta\Omega}\phi\,dy-\int_{\delta\Omega}\psi\,dx$$

So

$$\begin{aligned}\iint_{\Omega}&\left(\eta_x\frac{\partial f}{\partial z_x}+\eta_y\frac{\partial f}{\partial z_y}+\eta\frac{\partial}{\partial x}\frac{\partial f}{\partial z_x}+\eta\frac{\partial}{\partial y}\frac{\partial f}{\partial z_y}\right)dx\,dy\\ &=\oint_{\delta\Omega}\eta\frac{\partial f}{\partial z_x}\,dy-\oint_{\delta\Omega}\eta\frac{\partial f}{\partial z_y}\,dx\end{aligned}$$

Notice that $\eta(x,y)=0$ for all $(x,y)\in\delta\Omega$, and so the right hand side integrals are both zero.

Given the RHS of the equation was zero, we can rearrange to get

$$\iint_\Omega \left(\eta_x \frac{\partial f}{\partial z_x} + \eta_y \frac{\partial f}{\partial z_y} \right) \, dx\, dy = - \iint_\Omega \eta \left[\frac{\partial}{\partial x} \frac{\partial f}{\partial z_x} + \frac{\partial}{\partial y} \frac{\partial f}{\partial z_y} \right] \, dx\, dy$$

With the result that the First Variation can be written

$$\delta F(\eta, z) = \iint_\Omega \eta \left[\frac{\partial f}{\partial z} - \frac{\partial}{\partial x} \frac{\partial f}{\partial z_x} - \frac{\partial}{\partial y} \frac{\partial f}{\partial z_y} \right] \, dx\, dy$$

This step is the analogy of integration by parts in the derivation of the standard Euler-Lagrange equation.

Euler-Lagrange equation

Given that $\delta F(\eta, z) = 0$ for all allowable η, Lemma 2.2.2 (see last page) can be extended directly to the 2D case, with the result that

$$\boxed{\frac{\partial f}{\partial z} - \frac{\partial}{\partial x}\frac{\partial f}{\partial z_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial z_y} = 0}$$

This is also called the Euler-Lagrange equation.

The general case of the Euler-Lagrange equations with 2 independent variables (and the boundary conditions) produces a Dirichlet boundary value problem.
These can be very hard to solve.

Simple example

Let Ω be the disk defined by $x^2 + y^2 < 1$, and the functional of interest be

$$F\{z\} = \iint_\Omega \left(1 + \frac{1}{2} z_x^2 + \frac{1}{2} z_y^2\right) \, dx \, dy$$

with boundary conditions

$$z_0(x, y) = 2x^2 - 1$$

for all (x, y) such that $x^2 + y^2 = 1$.

Simple example: solution

The Euler-Lagrange equation is

$$\frac{\partial f}{\partial z} - \frac{\partial}{\partial x}\frac{\partial f}{\partial z_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial z_y} = 0$$

Note that in this example, f has no explicit dependence on x, y or z, and so we get

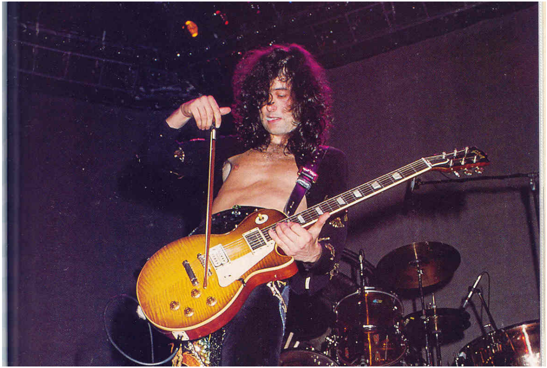
$$\frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2} = 0$$

This equation is called **Laplace's equation**.

Consider the function $z = x^2 - y^2$. This satisfies Laplace's equation, and on the boundary $y^2 = 1 - x^2$, so $z = 2x^2 - 1$, which satisfies our boundary condition.

Example: vibrating string

- Imagine a taut string
  - flexible
  - uniform mass
  - small deflections
- Equilibrium solution
  - the string sits in a straight line
  - consider small perturbations

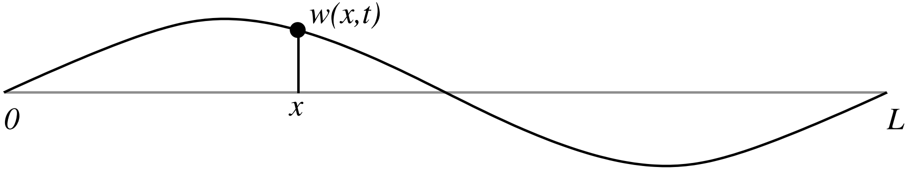


Example: vibrating string

Model:

- length of string is L
- position along the string is $x \in [0, L]$
- constant tension τ
- points on string move up/down perpendicular to x-axis
- displacement at x at time t is $w(x, t) \ll L$
- no friction or other damping
- only force occurs to stretch string
- constant density σ along the string's length

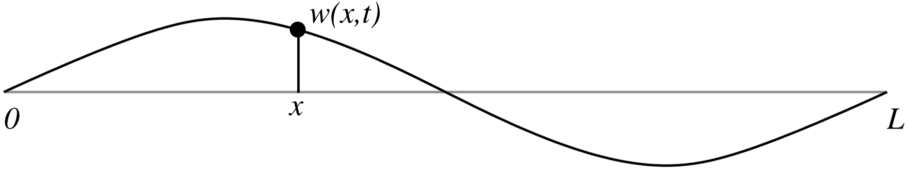
Example: vibrating string



- end points are fixed so $w(0,t) = w(L,t) = 0$
- velocity of particle is $w_t = \frac{\partial w}{\partial t}$
- kinetic energy of string

$$T = \frac{\sigma}{2} \int_0^L w_t^2 \, dx$$

Example: vibrating string



- slope of string $\frac{\partial w}{\partial x}$
- potential energy of the string depends on how much it is stretch from its original length L
- length at time t is given by

$$J(t) = \int_0^L \sqrt{1 + w_x^2}\, dx$$

Example: vibrating string

- potential is $V = \tau(J - L)$, so

$$V(t) = \tau \int_0^L \sqrt{1 + w_x^2} - 1 \, dx$$

- we assumed that w is small, so we can approximate

$$\sqrt{1 + w_x^2} \simeq 1 + \frac{1}{2} w_x^2$$

- so we use

$$V(t) = \frac{\tau}{2} \int_0^L w_x^2 \, dx$$

Example: vibrating string

Now we apply the "principle of stationary action" (Hamilton's principle), which says the shape will be an extremum with respect to

$$F\{w\} = \int_{t_1}^{t_2} (T - V)\, dt = \frac{1}{2} \int_{t_1}^{t_2} \int_0^L \left(\sigma w_t^2 - \tau w_x^2\right)\, dx\, dt$$

The Euler-Lagrange equation is

$$\frac{\partial f}{\partial w} - \frac{\partial}{\partial x}\frac{\partial f}{\partial w_x} - \frac{\partial}{\partial t}\frac{\partial f}{\partial w_t} = 0$$

which gives

$$\frac{\partial}{\partial x}\tau w_x = \frac{\partial}{\partial t}\sigma w_t$$

Example: vibrating string

$$\frac{\partial}{\partial x}\tau w_x = \frac{\partial}{\partial t}\sigma w_t,$$

or, if we denote $c^2 = \tau/\sigma$, then

$$\frac{\partial^2 w}{\partial t^2} = c^2 \nabla^2 w,$$

which is the classic wave equation, which you have no doubt seen and solved in other contexts.

Example: Plateau's problem

We want to find the surface with minimal area stretched between a boundary.

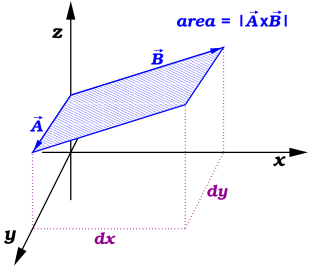
- this is what a soap film does
- architecture influenced by minimal surfaces
  - architect Frei Otto
  - Munich Olympic Stadium

Surface area minimization

The functional of interest is the surface area

$$F\{z\} = \iint_\Omega dA$$

As before, we can't compute this integral, so we must convert it to a convenient form:



$$\begin{aligned}
\mathbf{A} &= (0, dy, z_y\, dy) \\
\mathbf{B} &= (dx, 0, z_x\, dx) \\
\mathbf{A}\times\mathbf{B} &= (z_x\, dx\, dy, z_y\, dx\, dy, -dx\, dy)
\end{aligned}$$

$$\begin{aligned}
dA &= |\mathbf{A}\times\mathbf{B}| = \sqrt{(z_x\, dx\, dy)^2 + (z_y\, dx\, dy)^2 + (-dx\, dy)^2} \\
&= \sqrt{1 + z_x^2 + z_y^2}\, dx\, dy
\end{aligned}$$

Surface area minimization

So we may rewrite the functional as

$$F\{z\} = \iint_{\Omega} \sqrt{1 + z_x^2 + z_y^2}\, dx\, dy$$

The Euler-Lagrange equation is

$$\frac{\partial f}{\partial z} - \frac{\partial}{\partial x}\frac{\partial f}{\partial z_x} - \frac{\partial}{\partial y}\frac{\partial f}{\partial z_y} = 0$$

Which for this functional is

$$-\frac{\partial}{\partial x}\left[\frac{z_x}{\sqrt{1 + z_x^2 + z_y^2}}\right] - \frac{\partial}{\partial y}\left[\frac{z_y}{\sqrt{1 + z_x^2 + z_y^2}}\right] = 0$$

Surface area minimization

Continuing the derivation

$$\frac{\partial}{\partial x}\left[\frac{z_x}{\sqrt{1+z_x^2+z_y^2}}\right] = \frac{z_{xx}}{\sqrt{1+z_x^2+z_y^2}} - \frac{z_x\big(z_x z_{xx} + z_y z_{yx}\big)}{(1+z_x^2+z_y^2)^{3/2}}$$

$$= \frac{z_{xx}(1+z_x^2+z_y^2) - z_x\big(z_x z_{xx} + z_y z_{yx}\big)}{(1+z_x^2+z_y^2)^{3/2}}$$

$$= \frac{z_{xx}(1+z_y^2) - z_x z_y z_{yx}}{(1+z_x^2+z_y^2)^{3/2}}$$

$$\frac{\partial}{\partial y}\left[\frac{z_y}{\sqrt{1+z_x^2+z_y^2}}\right] = \frac{z_{yy}(1+z_x^2) - z_x z_y z_{yx}}{(1+z_x^2+z_y^2)^{3/2}}$$

Surface area minimization

Add the two terms above to get the E-L equation

$$2\mathcal{C} = \frac{z_{xx}(1+z_y^2) - 2z_x z_y z_{yx} + z_{yy}(1+z_x^2)}{(1+z_x^2+z_y^2)^{3/2}} = 0$$

where we call $\mathcal{C}$ the mean curvature (which is 0 on the extremals).

We multiply both sides of the E-L equation by the denominator to get

$$z_{xx}(1+z_y^2) - 2z_x z_y z_{yx} + z_{yy}(1+z_x^2) = 0$$

This is a hard PDE in general.

Approximate solutions

If the surfaces are almost planes (e.g. if z is small), then we can take **squared derivate** terms like z_x^2, z_y^2 and $z_x z_y$ to be zero. In this case the general equation

$$z_{xx}(1+z_y^2) - 2z_x z_y z_{yx} + z_{yy}(1+z_x^2) = 0$$

simplifies to give us

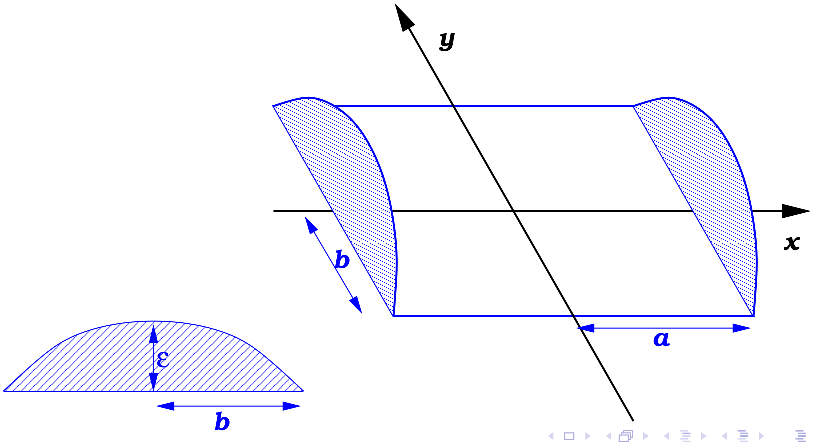
$$z_{xx} + z_{yy} = 0$$

the **Laplace equation** again. We know from the previous example that this is equivalent to approximating

$$f(x, y, z, z_x, z_y) = \sqrt{1 + z_x^2 + z_y^2} \simeq 1 + \frac{1}{2}z_x^2 + \frac{1}{2}z_y^2$$

Example

Design a surfaces of minimum surface area over a stadium with small curved walls, of shape $z = \epsilon \cos\left(\frac{\pi}{2}\frac{y}{b}\right)$, located at $x = \pm a$, and with no end walls at $y = \pm b$.



Example

Use the approximation, so we wish to solve

$$\begin{aligned} z_{xx} + z_{yy} &= 0 \\ z(\pm a, y) &= \epsilon \cos\left(\frac{\pi}{2}\frac{y}{b}\right) \\ z(x, \pm b) &= 0 \end{aligned}$$

Assume a solution with separation of variables, e.g. $z(x,y) = X(x)Y(y)$, then the DE implies that

$$z \propto \begin{matrix}\cosh \\ \sinh\end{matrix}(\lambda x) \times \begin{matrix}\cos \\ \sin\end{matrix}(\lambda y)$$

Choose $\cos$ with $\lambda = \frac{\pi}{2b}$ to match the boundary conditions, and choose $\cosh$ because we expect the solution to be even.

Example: solution

So the solution is

$$z(x, y) = A \cos\left(\frac{\pi y}{2b}\right) \cosh\left(\frac{\pi x}{2b}\right)$$

Determine A using the end-points, e.g.

$$\epsilon \cos\left(\frac{\pi y}{2b}\right) = A \cos\left(\frac{\pi y}{2b}\right) \cosh\left(\frac{\pi a}{2b}\right)$$

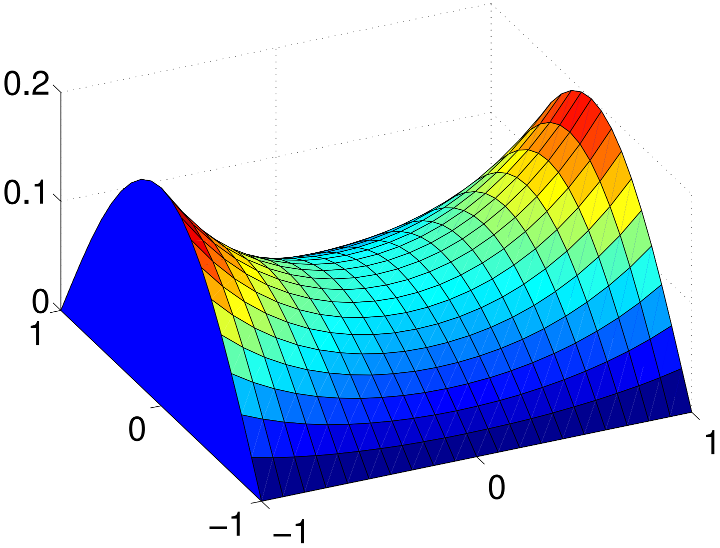
So

$$A = \epsilon / \cosh\left(\frac{\pi a}{2b}\right)$$

and

$$z(x, y) = \epsilon \cos\left(\frac{\pi y}{2b}\right) \cosh\left(\frac{\pi x}{2b}\right) / \cosh\left(\frac{\pi a}{2b}\right)$$

Example: solution



Example: solution

In fact, once we realize it will have a cosine cross-section, we know that the "area" of the curve for any given x will be proportional to the height, so we are in fact solving a problem that looks a lot like that of the catenary. So we should not be surprised to see that the result has the same $\cosh$ function.

But this is hard...

Solving the PDE form of the EL equations can be very hard. What can we do to make it easier? Surely computers can help?

Plateau's laws

A little bit extra:

- Soap films are made of entire smooth surfaces
- The average curvature of a portion of a soap film is always constant on any point on the same piece of soap film
- Soap films always meet in threes, and they do so at an angle of $cos^{-1}(-1/2) = 120$ degrees forming an edge called a Plateau Border.
- Plateau Borders meet in fours at an angle of $\cos^{-1}(-1/3) \simeq 109.47$ degrees (the tetrahedral angle) to form a vertex.