Optimal Functions and Nanomechanics III

APP MTH 3022/7106

Barry Cox

Lecture 19

Last lecture

- Looked at numerical approximation
- Euler's Finite Difference Method
- Convergence of Euler's FDM
- Ritz's method

Example: the Catenary, again

The functional of interest (the potential energy) is

$$W_p\{y\} = mg \int_{x_0}^{x_1} y\sqrt{1+y'^2}\,dx$$

Take symmetric problem with fixed end points

$$y(-1) = a \text{ and } y(1) = a$$

and we know the solution looks like

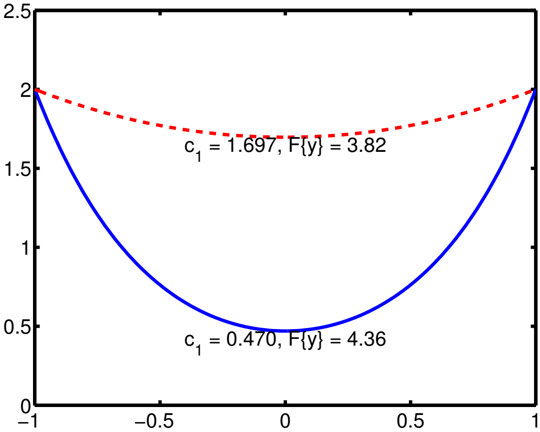
$$y(x) = c_1 \cosh\left(\frac{x}{c_1}\right)$$

where c_1 is chosen to match the end points.

Example: the Catenary, again

$y(1) = 2$ gives $c_1 = 0.47$ or $c_1 = 1.697$

- are they both local minima?



Ritz and the Catenary

Let's try approximating the curve by a polynomial

$$y(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + \cdots$$

Note that symmetry of problem implies y is an even function, and hence the odd terms $a_1 = a_3 = \cdots = 0$. So, to second order we can approximate

$$y(x) \simeq a_0 + a_2 x^2$$

We have fixed $y(1) = y_1$, so we can simplify to get

$$y(x) \simeq a_0 + (y_1 - a_0)x^2$$

Ritz and the Catenary

$$\begin{aligned} y &\simeq a_0 + (y_1 - a_0)x^2 \\ y' &\simeq 2(y_1 - a_0)x \end{aligned}$$

We can substitute into the functional

$$W_p\{y\} = mg \int_{x_0}^{x_1} y\sqrt{1 + y'^2}dx$$

and integrate to get a function $W_p(a_1)$ with respect to a_0.

But this is getting complicated.

Ritz and the Catenary

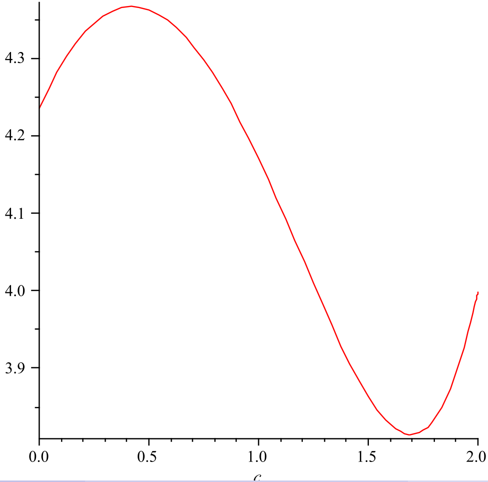
From Maple

$$
\begin{aligned}
W_p(a_0) = \quad & -1/4\, a_0 (-8\sqrt{\pi}(4 - 4\,a_0 + {a_0}^2) + (-4\,\ln(2) - 1 - \ln(4 - 4\,a_0 + {a_0}^2))\sqrt{\pi} \\
& -\sqrt{\pi}(4 - 4\,a_0 + {a_0}^2)(-(4 - 4\,a_0 + {a_0}^2)^{-1} - 8) \\
& -8\sqrt{\pi}(4 - 4\,a_0 + {a_0}^2) sqrt(1 + (16 - 16\,a_0 + 4\,{a_0}^2)^{-1}) \\
& -1/16\, \frac{\sqrt{\pi}(128 - 128\,a_0 + 32\,{a_0}^2)\ln(1/2 + 1/2\, sqrt(1 + (16 - 16\,a_0 + 4\,{a_0}^2)^{-1}))}{4 - 4\,a_0 + {a_0}^2})(\sqrt{\pi})^{-1}(sqrt(4 - 4\,a_0 + \\
& -1/16\,(2 - a_0)(-16\sqrt{\pi}(4 - 4\,a_0 + {a_0}^2)^2 - 4\sqrt{\pi}(4 - 4\,a_0 + {a_0}^2) \\
& -1/4\,(1/2 - 4\,\ln(2) - \ln(4 - 4\,a_0 + {a_0}^2))\sqrt{\pi} \\
& +2\sqrt{\pi}(4 - 4\,a_0 + {a_0}^2)^2(1/16\,(4 - 4\,a_0 + {a_0}^2)^{-2} + 2\,(4 - 4\,a_0 + {a_0}^2)^{-1} + 8) \\
& +2\sqrt{\pi}(4 - 4\,a_0 + {a_0}^2)^2(-(4 - 4\,a_0 + {a_0}^2)^{-1} - 8) sqrt(1 + (16 - 16\,a_0 + 4\,{a_0}^2)^{-1}) \\
& +1/32\, \frac{\sqrt{\pi}(64 - 64\,a_0 + 16\,{a_0}^2)\ln(1/2 + 1/2\, sqrt(1 + (16 - 16\,a_0 + 4\,{a_0}^2)^{-1}))}{4 - 4\,a_0 + {a_0}^2})(4 - 4\,a_0 + {a_0}^2)^{-3/2}\sqrt{\pi}
\end{aligned}
$$

Its a pain to find the zeros of dW/da_0, but its easy to plot, and find them numerically.

Ritz and the Catenary

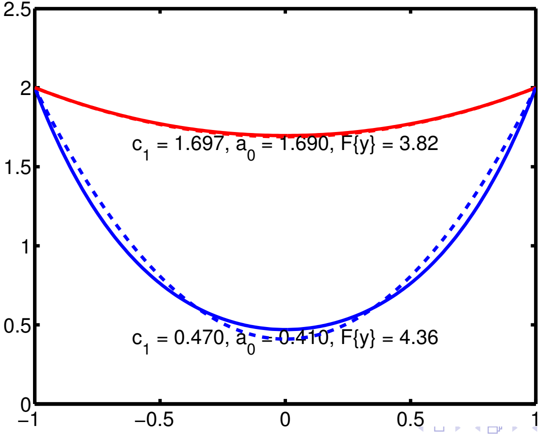
It's a function, and I can plot it, or use simple numerical techniques to find its stationary points.



Ritz and the Catenary

Stationary points

- local max: $a_0 \simeq 0.41$
- local min: $a_0 \simeq 1.69$



Ritz and the Catenary

Doesn't just give us an approximation to the extremal curves, its also gives us some insight into the nature of these extremals. If

- approximations are near to the actual extrema
- There are no other extrema so close by
- The functional is smooth (it can't have jumps either)

Then the type of extrema we get for the approximation will be the same for the real extrema, i.e.,

- local max: $a_0 \simeq 0.41 \Rightarrow$ local max for $c_1 = 0.47$
- local min: $a_0 \simeq 1.69 \Rightarrow$ local min for $c_1 = 1.697$

More than one indep. var

2D case: we are approximating a surface with series of functions, e.g.

$$z(x,y) \simeq z_n(x,y) = \phi_0(x,y) + \sum_{i=1}^{n} c_i \phi_i(x,y)$$

where $\phi_0(x,y)$ satisfies the boundary conditions, e.g. $\phi_0(x,y) = z_0(x,y)$ for $(x,y) \in \delta\Omega$, the boundary of the region on interest Ω, and the $\phi_i(x,y)$ satisfy the homogeneous boundary conditions $\phi_i(x,y) = 0$ for $(x,y) \in \delta\Omega$.

More than one indep. var

As before, we approximate the functional by

$$F\{z\} \simeq F\{z_n\} = F_n(c_1, \ldots, c_n)$$

As before we determine the c_j by requiring that the partial derivatives are zero, e.g.

$$\frac{\partial F_n}{\partial c_i} = 0$$

for all $i = 1, 2, \ldots, n$

Kantorovich's method

Approximate with

$$z(x,y) \simeq z_n(x,y) = \phi_0(x,y) + \sum_{i=1}^{n} c_i(x)\phi_i(x,y)$$

Again the ϕ_i are suitably chosen, but the c_i are no longer constants, but rather functions of one independent variable. This allows a larger class of functions to be used.

Kantorovich's method

Note that the integral function

$$F\{z_n\} = \iint_\Omega z_n(x,y)\,dx\,dy = \sum_{i=0}^{n} \int c_i(x) \left[\int_{y_0(x)}^{y_1(x)} \phi_i(x,y)\,dy \right] dx$$

We integrate the inner integral, and get

$$F\{z_n\} = \sum_{i=0}^{n} \int c_i(x)\Phi_i(x)\,dx$$

Now we just have a function of x, and so we may apply the Euler-Lagrange machinery.

The method approx. separates the variables x and y.

Example

Find the extremals of

$$F\{z(x,y)\} = \int_{-b}^{b}\int_{-a}^{a} \left(z_x^2 + z_y^2 - 2z\right)\, dx\, dy$$

with $z = 0$ on the boundary.

The Euler-Lagrange equation reduces to Poisson's equation, e.g.

$$\begin{aligned} \frac{d}{dx}\frac{\partial f}{\partial z_x} + \frac{d}{dy}\frac{\partial f}{\partial z_y} &= \frac{\partial f}{\partial z} \\ \frac{d}{dx}2z_x + \frac{d}{dy}2z_y &= -2 \\ \nabla^2 z(x,y) &= -1 \end{aligned}$$

Example

Approximate

$$z_1(x,y) = c(x)(b^2 - y^2)$$

Note $z_1(x, \pm b) = 0$ (as required) and

$$\begin{aligned}
\left(\frac{\partial z_1}{\partial x}\right)^2 &= \left(c'(x)(b^2 - y^2)\right)^2 \\
&= c'(x)^2(b^4 - 2b^2y^2 + y^4) \\
\left(\frac{\partial z_1}{\partial y}\right)^2 &= \left(c(x)2y\right)^2 \\
&= 4c(x)^2y^2
\end{aligned}$$

Example

Hence, we approximate

$$
\begin{aligned}
F\{z(x,y)\} &\simeq F\{z_1(x,y)\} \\
&= \int_{-b}^{b}\int_{-a}^{a}\left(z_x^2+z_y^2-2z\right)\,dx\,dy \\
&= \int_{-a}^{a}\left[\int_{-b}^{b}\left[c'(x)^2(b^2-y^2)^2+4c(x)^2y^2-2c(x)(b^2-y^2)\right]\,dy\right]\,dx \\
&= \int_{-a}^{a}\left[c'(x)^2(b^4y-2b^2y^3/3+y^5/5)+4c(x)^2y^3/3- \right. \\
&\qquad \left. 2c(x)(b^2y-y^3/3)\right]_{-b}^{b}\,dx \\
&= \int_{-a}^{a}\left[\frac{16}{15}b^5c'(x)^2+\frac{8}{3}b^3c(x)^2-\frac{8}{3}b^3c(x)\right]\,dx
\end{aligned}
$$

Example

So we can write

$$F\{z(x,y)\} \simeq F\{z_1(x,y)\} = F\{c(x)\} = \int_{-a}^{a} f(x,c,c')\,dx$$

We can use the simple Euler-Lagrange equations, where

$$\begin{aligned}
f(x,c,c') &= \frac{16}{15}b^5c'(x)^2 + \frac{8}{3}b^3c(x)^2 - \frac{8}{3}b^3c(x) \\
\frac{\partial f}{\partial c} &= \frac{16}{3}b^3c(x) - \frac{8}{3}b^3 \\
\frac{\partial f}{\partial c'} &= \frac{32}{15}b^5c'(x) \\
\frac{d}{dx}\frac{\partial f}{\partial c'} &= \frac{32}{15}b^5c''(x)
\end{aligned}$$

Example

Euler-Lagrange equations

$$\begin{aligned} \frac{d}{dx}\frac{\partial f}{\partial c'} - \frac{\partial f}{\partial c} &= 0 \\ \frac{32}{15}b^5 c''(x) - \frac{16}{3}b^3 c(x) + \frac{8}{3}b^3 &= 0 \\ c''(x) - \frac{5}{2b^2}c(x) &= -\frac{5}{4b^2} \end{aligned}$$

Solutions

$$c(x) = k_1 \cosh\left(\sqrt{\frac{5}{2}}\frac{x}{b}\right) + k_2 \sinh\left(\sqrt{\frac{5}{2}}\frac{x}{b}\right) + \frac{1}{2}$$

Example

Note that the function must be zero on the boundary so $z(\pm a, y) = 0$, and so we look for an even function $c(x)$, and so $k_2 = 0$, and also $c(\pm a) = 0$, so

$$\begin{aligned} c(a) &= k_1 \cosh\left(\sqrt{\frac{5}{2}}\frac{a}{b}\right) + \frac{1}{2} \\ -\frac{1}{2} &= k_1 \cosh\left(\sqrt{\frac{5}{2}}\frac{a}{b}\right) \\ k_1 &= -\frac{1}{2\cosh\left(\sqrt{\frac{5}{2}}\frac{a}{b}\right)} \end{aligned}$$

Example

Solution

$$z_1(x,y) = \frac{1}{2}(b^2 - y^2)\left(1 - \frac{\cosh\left(\sqrt{\frac{5}{2}}\frac{x}{b}\right)}{\cosh\left(\sqrt{\frac{5}{2}}\frac{a}{b}\right)}\right)$$

If we wanted a more exact approximation, we could try

$$z_2(x,y) = (b^2 - y^2)c_1(x) + (b^2 - y^2)^2 c_2(x)$$

Lower bounds

- Obviously, quality of solution depends on
  - family of functions chosen
  - number of terms used, n
- Could test convergence by increasing n and seeing the difference in $|F\{y_{n+1}\} - F\{y_n\}|$, but this is not guaranteed to be a good indication.
- A better way to assess convergence is to have a lower-bound

$$\text{lower bound } \leqslant F\{y\} \leqslant \text{ upper bound}$$

- use **complementary variation principle**
- but its a bit complicated for us to cover here.