Optimal Functions and Nanomechanics III

APP MTH 3022/7106

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Lecture 18

Last lecture

- Derived the Euler-Lagrange equation for several independent variables
- Look at the problem of a vibrating string
- Approximately solved the problem of minimal surfaces
- Approximations were needed because the full PDE

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

is hard.

Numerical Solutions

The E-L equations may be hard to solve

Natural response is to find numerical methods

- Numerical solution of E-L DE
  - we won't consider these here (see other courses)
- Euler's finite difference method
- Ritz (Rayleigh-Ritz)
  - In 2D: Kantorovich's method

Euler's finite difference method

We can approximate our function (and hence the integral) onto a finite grid. In this case, the problem reduces to a standard multivariable maximization (or minimization) problem, and we find the solution by setting the derivatives to zero. In the limit as the grid gets finer, this approximates the E-L equations.

Numerical Approximation

Numerical approximation of integrals:

- use an arbitrary set of mesh points $a = x_0 < x_1 < x_2 < \cdots < x_n = b$.
- approximate

$$y'(x_i) = \frac{y_{i+1} - y_i}{x_{i+1} - x_i} = \frac{\Delta y_i}{\Delta x_i}$$

- rectangle rule

$$F\{y\} = \int_a^b f(x, y, y')\, dx \simeq \sum_{i=0}^{n-1} f\left(x_i, y_i, \frac{\Delta y_i}{\Delta x_i}\right) \Delta x_i = \bar{F}(\mathbf{y})$$

$\bar{F}(\cdot)$ is a function of the vector $\mathbf{y} = (y_1, y_2, \ldots, y_n)$.

Finite Difference Method (FDM)

Treat this as a maximization of a function of n variables, so that we require

$$\frac{\partial \bar{F}}{\partial y_i} = 0$$

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

Typically use uniform grid so $\Delta x_i = \Delta x = (b - a)/n$.

Simple Example

Find extremals for

$$F\{y\} = \int_0^1 \left[\frac{1}{2} y'^2 + \frac{1}{2} y^2 - y \right] dx$$

with $y(0) = 0$ and $y(1) = 0$.

E-L equations $y'' - y = 1$.

Simple Example: direct solution

E-L equations $y'' - y = -1$
Solution to homogeneous equations $y'' - y = 0$ is given by $e^{\lambda x}$ giving characteristic equation $\lambda^2 - 1 = 0$, so $\lambda = \pm 1$.
Particular solution $y = 1$
Final solution is

$$y(x) = Ae^x + Be^{-x} + 1$$

The boundary conditions $y(0) = y(1) = 0$ constrain $A + B = -1$ and $Ae + Be^{-1} = -1$, so $Ae + (1 - A)e^{-1} = 1$, so $A = \frac{e^{-1}-1}{e-e^{-1}}$ and $B = \frac{1-e}{e-e^{-1}}$.
Then the exact solution to the extremal problem is

$$y(x) = \frac{e^{-1} - 1}{e - e^{-1}} e^x + \frac{1 - e}{e - e^{-1}} e^{-x} - 1$$

Simple Example: Euler's FDM

Find extremals for

$$F\{y\} = \int_0^1 \left[\frac{1}{2} y'^2 + \frac{1}{2} y^2 - y \right] dx$$

Euler's FDM.

- Take the grid $x_i = i/n$, for $i = 0, 1, \ldots, n$ so
  - end points $y_0 = 0$ and $y_n = 0$
  - $\Delta x = 1/n$
  - $\Delta y_i = y_{i+1} - y_i$
- So
  - $y_i' = \Delta y_i / \Delta x = n(y_{i+1} - y_i)$
  - and

$$y_i'^2 = n^2 \left(y_i^2 - 2 y_i y_{i+1} + y_{i+1}^2 \right)$$

Simple Example: Euler's FDM

Find extremals for

$$F\{y\} = \int_0^1 \left[\frac{1}{2}y'^2 + \frac{1}{2}y^2 - y\right] dx$$

Its FDM approximation is

$$\begin{aligned}
\bar{F}(\mathbf{y}) &= \sum_{i=0}^{n-1} f\left(x_i, y_i, y_i'\right) \Delta x \\
&= \sum_{i=0}^{n-1} \frac{1}{2} n^2 \left(y_i^2 - 2y_i y_{i+1} + y_{i+1}^2\right) \Delta x + (y_i^2/2 - y_i)\Delta x \\
&= \sum_{i=0}^{n-1} \frac{1}{2} n \left(y_i^2 - 2y_i y_{i+1} + y_{i+1}^2\right) + \frac{y_i^2/2 - y_i}{n}
\end{aligned}$$

Simple Example: end-conditions

- We know the end conditions $y(0) = y(1) = 0$, which imply that

$$y_0 = y_n = 0$$

- Include them into the objective using Lagrange multipliers

$$\bar{H}(\mathbf{y}) = \sum_{i=0}^{n-1} \frac{1}{2} n \left(y_i^2 - 2 y_i y_{i+1} + y_{i+1}^2 \right) + \frac{y_i^2/2 - y_i}{n} + \lambda_0 y_0 + \lambda_n y_n$$

Simple Example: Euler's FDM

Taking derivatives, note that y_i only appears in two terms of the FDM approximation

$$
\begin{aligned}
\bar{H}(\mathbf{y}) &= \sum_{i=0}^{n-1} \frac{1}{2} n \left(y_i^2 - 2 y_i y_{i+1} + y_{i+1}^2 \right) + \frac{y_i^2/2 - y_i}{n} + \lambda_0 y_0 + \lambda_n y_n \\
\frac{\partial \bar{H}(\mathbf{y})}{\partial y_i} &= \begin{cases} n\left(y_0 - y_1\right) + \frac{y_0 - 1}{n} + \lambda_0 & \text{for } i = 0 \\ n\left(2y_i - y_{i+1} - y_{i-1}\right) + \frac{y_i}{n} - \frac{1}{n} & \text{for } i = 1, \ldots, n-1 \\ n\left(y_n - y_{n-1}\right) + \lambda_n & \text{for } i = n \end{cases}
\end{aligned}
$$

We need to set the derivatives to all be zero, so we now have $n+3$ linear equations, including $y_0 = y_n = 0$, and $n+3$ variables including the two Lagrange multipliers. We can solve this system numerically using, e.g., MATLAB.

Simple Example: Euler's FDM

Example: $n = 4$, solve

$$A\boldsymbol{z} = \boldsymbol{b}$$

where

$$A = \begin{pmatrix} 4.25 & -4.00 & & & & 1.00 & \\ -4.00 & 8.25 & -4.00 & & & & \\ & -4.00 & 8.25 & -4.00 & & & \\ & & -4.00 & 8.25 & -4.00 & & \\ & & & -4.00 & 4.00 & & 1.00 \\ 1.00 & & & & & & \\ & & & & 1.00 & & \end{pmatrix} \quad \text{and} \quad \boldsymbol{b} = \begin{pmatrix} 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.00 \\ 0.00 \\ 0.00 \end{pmatrix}$$

- first $n+1$ terms of $\boldsymbol{z}$ give $\boldsymbol{y}$
- last two terms give the Lagrange multipliers λ_0 and λ_n

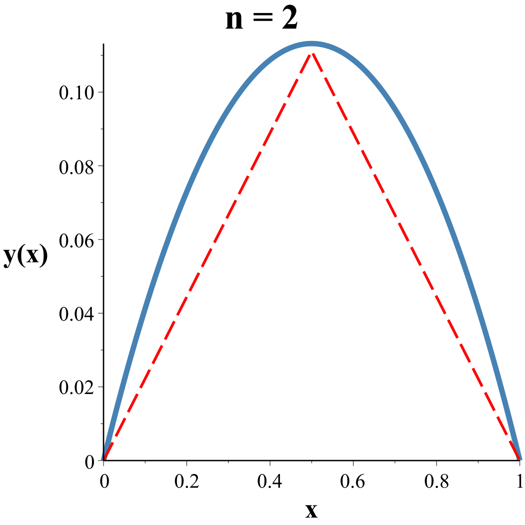
Simple Example: Euler's FDM

Note that with some rearrangement we can express the system from the previous page in the following equivalent form

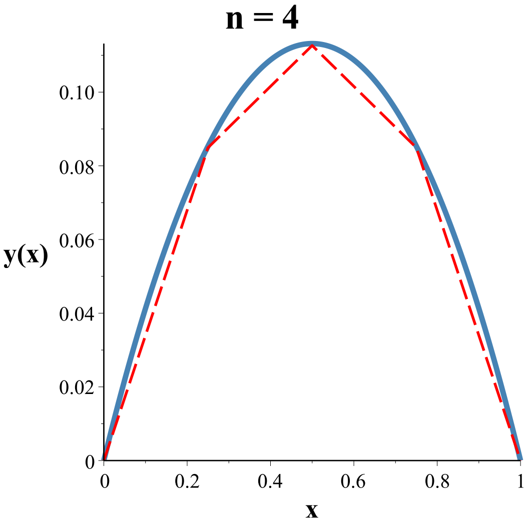
$$
A = \begin{pmatrix}
-4.00 & & & & & & \\
8.25 & -4.00 & & & & 1.00 & \\
-4.00 & 8.25 & -4.00 & & & & \\
 & -4.00 & 8.25 & -4.00 & & & \\
 & & -4.00 & 8.25 & -4.00 & & \\
 & & & -4.00 & 8.25 & & 1.00 \\
 & & & & -4.00 & &
\end{pmatrix}
\quad \text{and} \quad
\boldsymbol{b} = \begin{pmatrix}
0.00 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.00 \\ 0.00
\end{pmatrix}
$$

which might be easier to code.

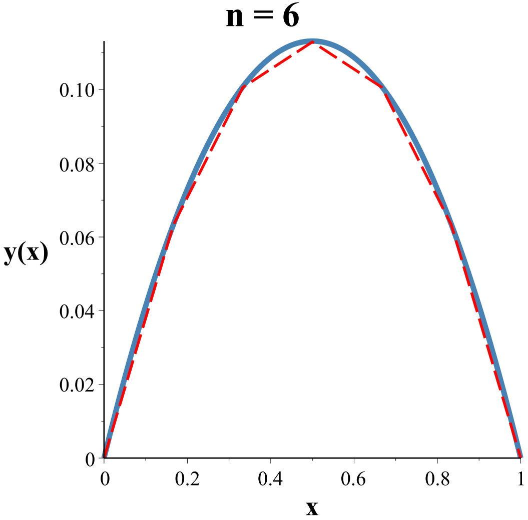
Simple example: results



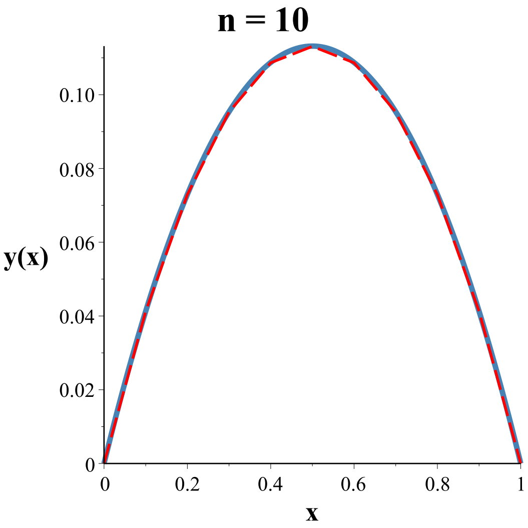
Simple example: results



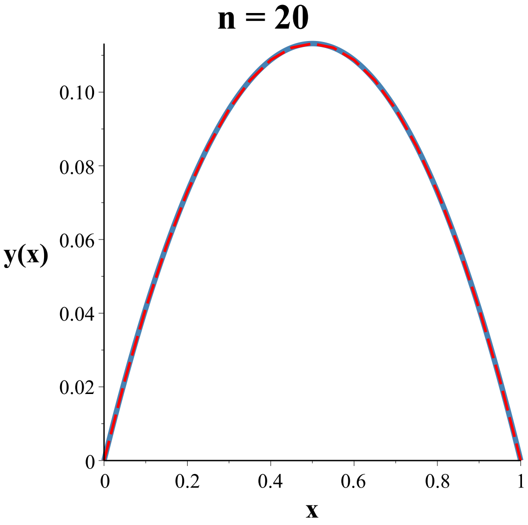
Simple example: results



Simple example: results



Simple example: results



Convergence of Euler's FDM

$$\bar{F}(\mathbf{y}) = \sum_{i=0}^{n-1} f\left(x_i, y_i, \frac{\Delta y_i}{\Delta x}\right) \Delta x \quad \text{and} \quad \Delta y_i = y_{i+1} - y_i$$

Only and two terms in the sum involve y_i, so

$$\begin{aligned}
\frac{\partial \bar{F}}{\partial y_i} &= \frac{\partial}{\partial y_i} f\left(x_{i-1}, y_{i-1}, \frac{\Delta y_{i-1}}{\Delta x}\right) + \frac{\partial}{\partial y_i} f\left(x_i, y_i, \frac{\Delta y_i}{\Delta x}\right) \\
&= \frac{1}{\Delta x} \frac{\partial f}{\partial y_i'}\left(x_{i-1}, y_{i-1}, \frac{\Delta y_{i-1}}{\Delta x}\right) \\
&\quad + \frac{\partial f}{\partial y_i}\left(x_i, y_i, \frac{\Delta y_i}{\Delta x}\right) - \frac{1}{\Delta x} \frac{\partial f}{\partial y_i'}\left(x_i, y_i, \frac{\Delta y_i}{\Delta x}\right) \\
&= \frac{\partial f}{\partial y_i}\left(x_i, y_i, y_i'\right) - \frac{\frac{\partial f}{\partial y_i'}\left(x_i, y_i, \frac{\Delta y_i}{\Delta x}\right) - \frac{\partial f}{\partial y_i'}\left(x_{i-1}, y_{i-1}, \frac{\Delta y_{i-1}}{\Delta x}\right)}{\Delta x}
\end{aligned}$$

Convergence of Euler's FDM

The condition for a stationary point becomes

$$\frac{\partial \bar{F}}{\partial y_i} = \frac{\partial f}{\partial y_i}(x_i, y_i, y_i') - \frac{\frac{\partial f}{\partial y_i'}\left(x_i, y_i, \frac{\Delta y_i}{\Delta x}\right) - \frac{\partial f}{\partial y_i'}\left(x_{i-1}, y_{i-1}, \frac{\Delta y_{i-1}}{\Delta x}\right)}{\Delta x} = 0$$

In limit $n \to \infty$, then $\Delta x \to 0$, and so we get

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

which are the Euler-Lagrange equations.

- i.e., the finite difference solution converges to the solution of the E-L equations

Comments

- There are lots of ways to improve Euler's FDM
  - use a better method of numerical quadrature (integration)
    - trapezoidal rule
    - Simpson's rule
    - Romberg's method
  - use a non-uniform grid
    - make it finer where there is more variation
- We can use a different approach that can be even better

Ritz's method

In Ritz's method (called Kantorovich's methods where there is more than one independent variable), we approximate our functions (the extremal in particular) using a family of simple functions. Again we can reduce the problem into a standard multivariable maximization problem, but now we seek coefficients for our approximation.

Ritz's method

Assume we can approximate $y(x)$ by

$$y(x) = \phi_0(x) + c_1\phi_1(x) + c_2\phi_2(x) + \cdots + c_n\phi_n(x)$$

where we choose a convenient set of functions $\phi_j(x)$ and find the values of c_j which produce an extremal.

For fixed end-point problem:

- Choose $\phi_0(x)$ to satisfy the end conditions.
- Then $\phi_j(x_0) = \phi_j(x_1) = 0$ for $j = 1, 2, \ldots, n$

The ϕ can be chosen from standard sets of functions, e.g. power series, trigonometric functions, Bessel functions, etc. (but must be linearly independent)

Ritz's method

- select $\{\phi_j\}_{j=0}^{n}$
- Approximate $y_n(x) = \phi_0(x) + c_1\phi_1(x) + c_2\phi_2(x) + \cdots + c_n\phi_n(x)$
- Approximate $F\{y\} \simeq F\{y_n\} = \int_{x_0}^{x_1} f(x, y_n, y_n')\,dx$
- Integrate to get $F\{y_n\} = F_n(c_1, c_2, \ldots, c_n)$
- F_n is a known function of n variables, so we can maximize (or minimize) it as usual by

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

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

Upper bounds

Assume the extremal of interest is a minimum, then for the extremal

$$F\{y\} < F\{\hat{y}\}$$

for all $\hat{y}$ within the neighborhood of y. Assume our approximating function y_n is close enough to be in that neighborhood, then

$$F\{y\} \leq F\{y_n\} = F_n(\boldsymbol{c})$$

so the approximation provides an **upper bound** on the minimum $F\{y\}$.
Another way to think about it is that we optimize on a smaller set of possible functions y, so we can't get quite as good a minimum.

Simple Example

Find extremals for

$$F\{y\} = \int_0^1 \left[\frac{1}{2}y'^2 + \frac{1}{2}y^2 - y\right] dx$$

with $y(0) = 0$ and $y(1) = 0$.

E-L equations $y'' - y = -1$, but we shall bypass the E-L equations to use Ritz's method.

$$y_n(x) = \phi_0(x) + \sum_{i=1}^{n} c_i \phi_i(x)$$

where we take $\phi_0(x) = 0$ and $\phi_i(x) = x^i(1-x)^i$.

Simple Example

Simple approximation $y_1 = c_1\phi_1(x)$ we get

$$F_1(c_1) = F\{y_1\} = \int_0^1 \left[\frac{1}{2}c_1^2\phi_1'^2 + c_1^2\frac{1}{2}\phi_1^2 - c_1\phi_1\right] dx$$

Now $\phi_1 = x(1-x)$ so $\phi_1' = 1-2x$, and

$$\begin{aligned}
F_1(c_1) &= \int_0^1 \left[\frac{c_1^2}{2}(1-2x)^2 + \frac{c_1^2}{2}x^2(1-x)^2 - c_1x(1-x)\right] dx \\
&= \frac{c_1^2}{2}\int_0^1 \left[1 - 4x + 5x^2 - 2x^3 + x^4\right] dx + c_1\int_0^1 \left[-x + x^2\right] dx \\
&= \frac{c_1^2}{2}\left[x - 2x^2 + 5x^3/3 - x^4/2 + x^5/5\right]_0^1 + c_1\left[-x^2/2 + x^3/3\right]_0^1 \\
&= \frac{c_1^2}{2}\frac{11}{30} - \frac{c_1}{6}
\end{aligned}$$

Simple Example

We solve for c_1 by setting

$$\frac{dF_1}{dc_1} = \frac{11c_1}{30} - \frac{1}{6} = 0$$

to get $c_1 = 5/11$, so the approximate extremal is

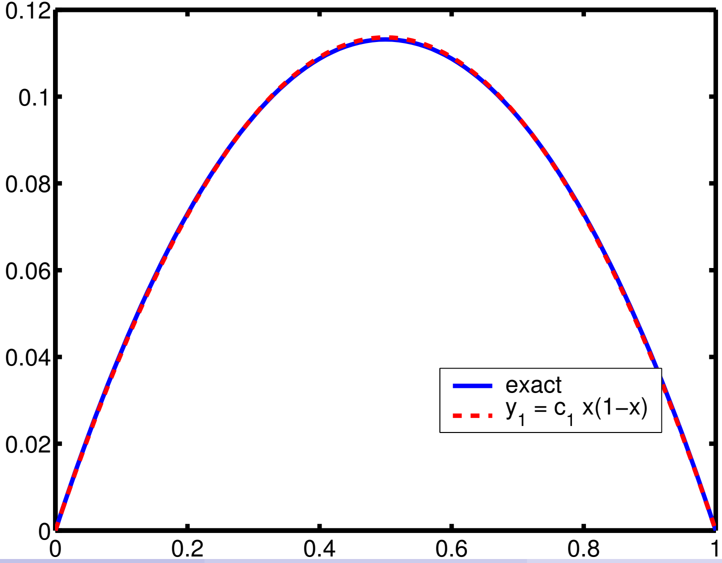
$$y_1(x) = \frac{5}{11}x(1-x)$$

The value of the approximate functional at this point is

$$F_1(5/11) = \frac{c_1^2}{2}\frac{11}{30} - \frac{c_1}{6} = -\frac{5}{132} = -0.0378787878\ldots$$

which is an upper bound on the true value of the functional on the extremal.

Simple example: results



Alternate approach

Choose $\phi_1(x) = \sin(\pi x)$ (use the first element of a trigonometric series to approximate y). Then, $\phi'(x) = \pi \cos(\pi x)$, and so the functional is

$$\begin{aligned} F_1(c_1) &= F\{c_1\phi_1\} = \int_0^1 \left[\frac{1}{2} c_1^2 \phi_1'^2 + c_1^2 \frac{1}{2} \phi_1^2 - c_1 \phi_1 \right] dx \\ &= \int_0^1 \left[\frac{c_1^2 \pi^2}{2} \cos^2(\pi x) + \frac{c_1^2}{2} \sin^2(\pi x) - c_1 \sin(\pi x) \right] dx \end{aligned}$$

Now $\int_0^1 \cos^2(\pi x)\, dx = \int_0^1 \sin^2(\pi x)\, dx = 1/2$,
and $\int_0^1 \sin(\pi x)\, dx = [-\frac{1}{\pi} \cos(\pi x)]_0^1 = 2/\pi$, so

$$F(c_1) = \frac{c_1^2}{2} \frac{1}{2} \left[\pi^2 + 1 \right] - \frac{2}{\pi} c_1$$

Alternate approach

Once again we solve for c_1 by setting

$$\frac{dF_1}{dc_1} = c_1 \frac{1}{2}\left[\pi^2 + 1\right] - \frac{2}{\pi} = 0$$

to get $c_1 = \frac{4}{\pi(\pi^2+1)}$, so the approximate extremal is

$$y_1(x) = \frac{4}{\pi(\pi^2+1)} \sin(\pi x)$$

In this case

$$F_1(c_1) = -\frac{4}{\pi^2(\pi^2+1)} \approx -0.0372860611\ldots$$

Alternate approach: results