Master in Seismic Engineering— E.T.S.I. Industriales (U.P.M.)

Discretization Methods in Engineering

# Variational principles and the Rayleigh-Ritz method

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1. Motivation.
2. Minimization principles in Mechanics.
3. Finite dimensional minimization problems.
4. Infinite dimensional minimization problems.
5. The Rayleigh-Ritz method.
6. The Rayleigh-Ritz Finite Element method.

Things to learn in this class:

- ▷ The importance of convex minimization in mechanics.
- ▷ Calculus of variations.
- ▷ The basic idea of the Raleigh-Ritz method.

Many, many problems in Mechanics are described by minimization principles:

- **Example 1:** Consider an elastic string aligned with the $x$ axis, of length $L$, with stiffness $EA$, fixed at the end $x = 0$ and with forces $f : (0, L) \to \mathbb{R}$, and a force $h$ at $x = L$. Then, in the equilibrium position, the displacement $\boldsymbol{u} : [0, L] \to \mathbb{R}$ minimizes the potential energy

$$\Pi = \int_0^L \left(\tfrac{1}{2}EA(u')^2 - f \cdot u\right) \mathrm{d}x - hu(L)$$

- **Example 2:** Consider a domain $\Omega \subset \mathbb{R}^3$, with boundary $\partial\Omega = \partial_d\Omega \cup \partial_n\Omega$. If a body occupies $\Omega$, is subjected to a heat supply $r : \Omega \to \mathbb{R}$ and a boundary heat flux $h : \partial_n\Omega \to \mathbb{R}$, the temperature field in the equilibrium is the minimizer of the energy

$$\Pi_2 = \int_\Omega \left(\tfrac{1}{2}\kappa|\nabla\theta|^2 - r \cdot \theta\right) \mathrm{d}\Omega - \int_{\partial_n\Omega} h\, \theta\, \mathrm{d}\Gamma$$

- **Example 3:** (Constrained minimization) The state variables $\boldsymbol{X} \in \mathbb{R}^N$ that define the equilibrium position of a thermodynamic system with energy $E$ are those which maximize the entropy $S(E, \boldsymbol{X})$ subject to the restriction that the energy is equal to $E$.

- **Example 4:** The path taken between two points by a ray of light is the path that can be traversed in the least time (Fermat's principle)

- **Example 5:** A bubble adopts a shape that minimizes its surface energy.
- **Example 6:** A structure under imposed loads and displacements deforms in such a way that its total potential energy is a minimum.

- ▷ In general, these problems are nonlinear, difficult to solve, and their solution need not be unique.
- ▷ In this course we only consider quadratic (convex) potentials which have unique solutions.
- ▷ When the unknown is a vector, the classical first order optimality condition $D\Pi = \mathbf{0}$ provides a solution. One may check that $D^2\Pi \geq 0$, the second order condition for minima.
- ▷ When the unknown is a function, we need to use the calculus of variations.

Many finite dimensional equilibrium problems can be stated as:

$$\text{Find } \boldsymbol{X} = \text{arg min. } \Pi(\boldsymbol{X}), \quad \text{with} \quad \Pi(\boldsymbol{X}) = \tfrac{1}{2}\boldsymbol{X}^T\boldsymbol{K}\boldsymbol{X} - \boldsymbol{X}^T\boldsymbol{F} \ ,$$

where $\boldsymbol{X}, \boldsymbol{F} \in \mathbb{R}^N$, $\boldsymbol{K}$ is an $N \times N$ symmetric, positive definite matrix.

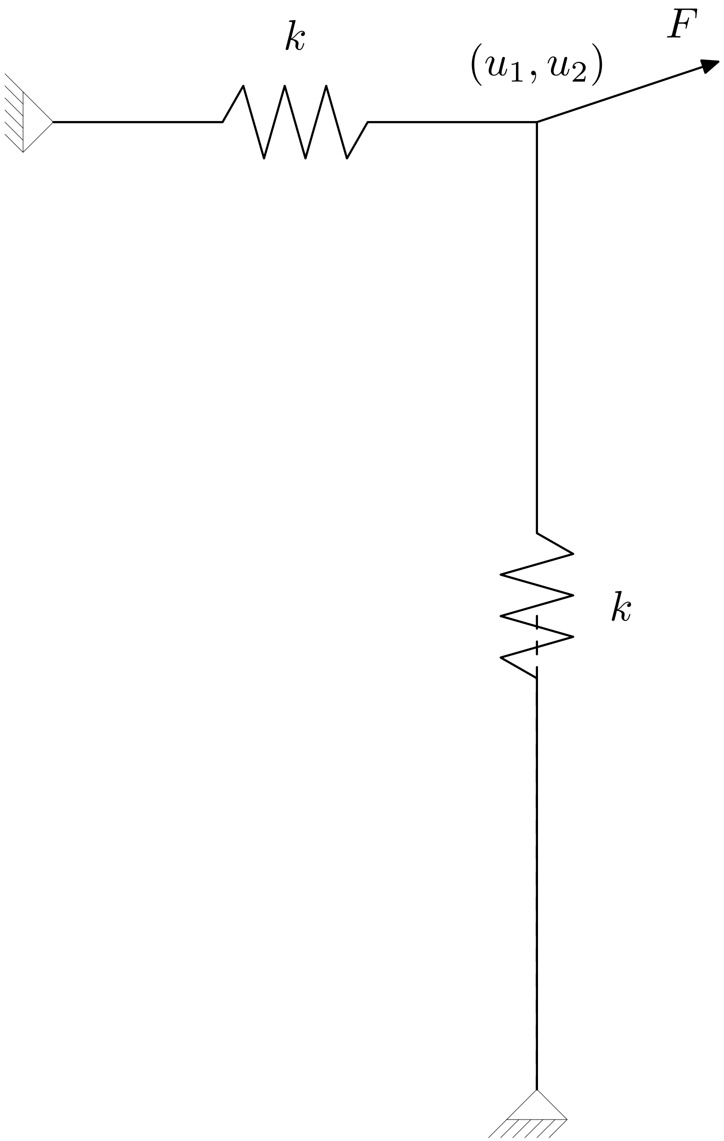
- **Solution:** Considering the first order optimality condition $D\Pi = \mathbf{0}$ we get

$$\mathbf{0} = D\Pi(\boldsymbol{X}) = \boldsymbol{K}\boldsymbol{X} - \boldsymbol{F} \ ,$$

  which is a system of linear equations, with $\boldsymbol{K}$ invertible.

- **Result:** Solving an unconstrained, quadratic minimization problem is identical to solving the system of linear equations

$$\boldsymbol{K}\boldsymbol{X} = \boldsymbol{F}$$




For a truss of this type

$$\Pi(u_1, u_2) = \Pi_{int}(u_1, u_2) - \Pi_{ext}(u_1, u_2)$$

$$\Pi_{int}(u_1, u_2) = \sum_{i=1}^{2} \frac{k}{2} \varepsilon_i^2$$

$$\Pi_{int}(u_1, u_2) = F_1 \cdot u_1 + F_2 \cdot u_2$$

- Determine $\Pi(u_1, u_2)$
- Calculate $D\Pi$
- Check $D^2\Pi \geq 0$

**Definition:** A functional is a mapping $\mathcal{F}$ from a space of functions to $\mathbb{R}$.

**Vague definition:** A functional is a "function of functions".

**Examples:**

1) $\mathcal{F}_1[g] = \int_0^1 g(x)\,\mathrm{d}x$ (the area of a function).

2) $\mathcal{F}_2[\boldsymbol{v}] = \int_\Omega \frac{1}{2}\rho|\boldsymbol{v}|^2\,\mathrm{d}V$ (the kinetic energy of a body $\Omega$).

3) $\mathcal{F}_3[u] = \int_o^L \frac{1}{2}EA|u'|^2\,\mathrm{d}x$ (the potential energy of a deformed string).

There are also minimization problems where the unknown is precisely the function that minimizes a functional

$$\text{Find } g = \text{arg min. } \mathcal{F}[g],$$

We need to find a first order condition for infinite dimensional problems:

- Let $\delta g$ be a variation of the function $g$, which is just any function with zero value at those points of $\Omega$ where $g$ is known. Then, the first order condition is:

$$\delta\mathcal{F}[g] = 0 \,, \quad \text{with} \quad \delta\mathcal{F}[g] := \left.\frac{\mathrm{d}}{\mathrm{d}\,\epsilon}\right|_{\epsilon=0} \mathcal{F}[g + \epsilon\,\delta g]$$

- **Justification:** if $g$ is a minimizer of $\mathcal{F}$ then $\mathcal{F}[g + \epsilon\,\delta g]$ must reach its minimum when $\epsilon = 0$.

The equation $\delta\mathcal{F}[g] = 0$ leads to a differential equation, which we can try to solve, which is called the Euler-Lagrange equation of the problem.

Consider the minimization of the potential energy of a stretched string

$$V(u) = \int_0^L \left(\tfrac{1}{2} EA(u')^2 - f \cdot u\right) \, \mathsf{d}x - g \cdot u(L) \ ,$$

where $u$ is the unknown displacement, and $u(0) = 0$.

- **Solution:** The variation $\delta u$ is any function that satisfies $\delta u(0) = 0$. Then, the variation of the potential energy is

$$\begin{aligned} \delta V &= \int_0^L (EA\, u' \cdot \delta u' - f \cdot \delta u) \, \mathsf{d}x - g \cdot \delta u(L) \\ &= \int_0^L (-EA\, u'' - f) \cdot \delta u \, \mathsf{d}x + (EA\, u'(L) - g) \cdot \delta u(L) \end{aligned}$$

Since $\delta u$ is arbitrary, we choose $\delta u = m \cdot (EA\, u'' - f)$, with $m$ a non-negative function with $m(0) = m(1) = 0$. Then,

$$0 = \int_0^L m \cdot (-EA\, u'' - f)^2 \, \mathrm{d}x \Rightarrow -EA\, u'' - f = 0$$

Hence, for any $\delta u$

$$0 = (EA\, u'(L) - g) \cdot \delta u(L)$$

and thus the terms in parenthesis must vanish too.

The minimizer $u$ must verify

$$\boxed{-EAu'' = f \ , \quad EA\, u'(L) = g \ , \quad u(0) = 0}$$

If we are satisfied with an approximate solution for an infinite dimensional problem we can obtain one in a simple way. For example, for the string problem:

Let $N^1, N^2, N^3, \ldots, N^r$ be $r$ linearly independent functions that satisfy $N^i(0) = 0$. Let the solution $u$ be approximated by a function

$$u^h(x) = \sum_{a=1}^{r} N_a(x) d_a$$

where $d_a$ are unknowns. Let $\boldsymbol{d} = \{d_1, d_2, \ldots, d_r\}$. Then the "best" coefficients $d_a$ are those that solve the minimization problem

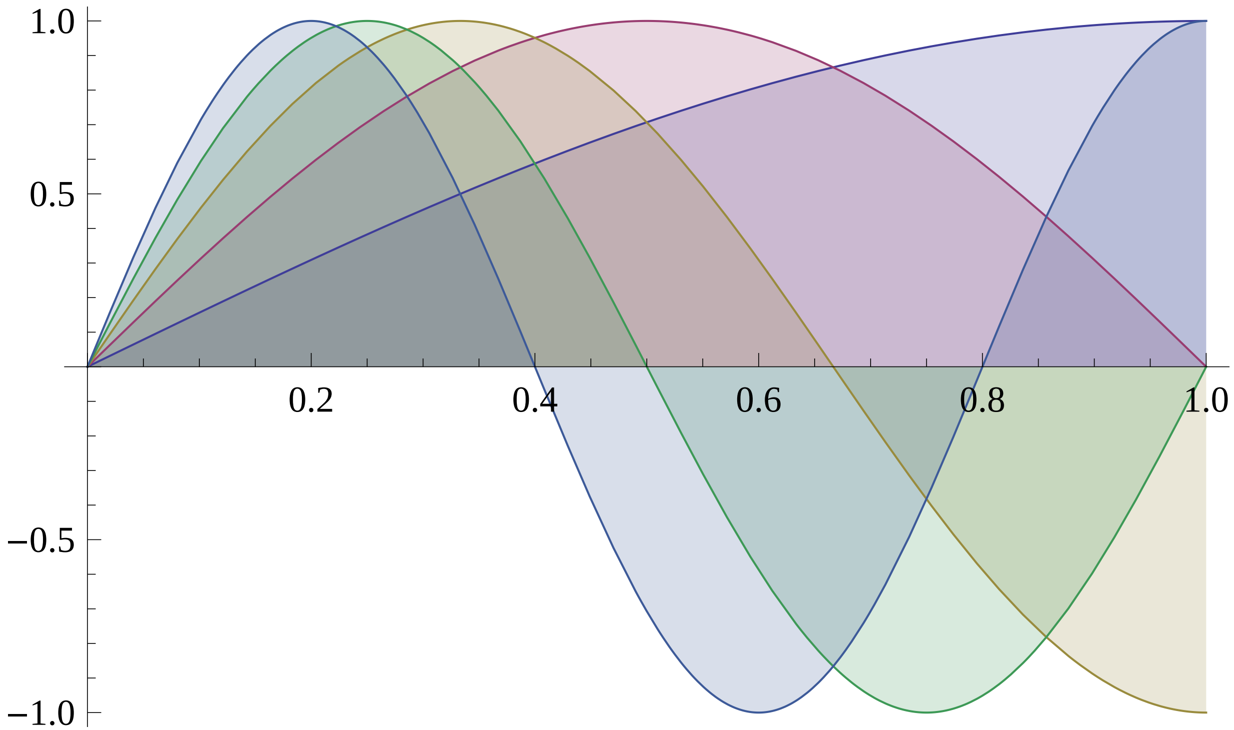
$$\boldsymbol{d} = \text{arg min. } \mathcal{F}[\sum_{i=a}^{r} N_a(x) d_a]$$

This is now a finite dimensional problem (in the unknown $\boldsymbol{d}$) whose solution can be obtained from the first order condition

$$D_{\boldsymbol{d}} \mathcal{F}[u^h] = \boldsymbol{0}$$

For the string problem, one might chose

$$N_a(x) = sin(a\frac{\pi}{2L}x)$$



- For the string problem:

$$\begin{aligned}\mathcal{F}[u^h] &= \int_0^L \frac{EA}{2}((u^h)')^2 \,\mathsf{d}x - \int_0^L f \cdot u^h \,\mathsf{d}x \\ &= \int_0^L \frac{EA}{2} \sum_{a,b=1}^{r} (N_a' \, N_b' \, d_a \, d_b) \,\mathsf{d}x - \int_0^L f \cdot \sum_{a=1}^{r} N_a \, d_a \,\mathsf{d}x \\ &= \frac{1}{2} \sum_{a,b=1}^{r} \left( \int_0^L EA \, N_a' N_b' \,\mathsf{d}x \right) d_a \, d_b - \sum_{a=1}^{r} \int_0^L f \cdot N_a \,\mathsf{d}x \, d_a \\ &= \frac{1}{2} \boldsymbol{d}^T \boldsymbol{K} \boldsymbol{d} - \boldsymbol{d}^T \boldsymbol{F}\end{aligned}$$

if we identify the components of $\boldsymbol{F}$ and $\boldsymbol{K}$ as:

$$F_a = \int_0^L f \cdot N_a \,\mathsf{d}x$$

$$K_{ab} = \int_0^L EA \, N_a' \, N_b' \,\mathsf{d}x$$

Is the system $\boldsymbol{K}\boldsymbol{d} = \boldsymbol{F}$ solvable when using Ritz method with sines? Difficult to say looking at

$$K_{ab} = \int_0^L EA\ sin'(a\frac{\pi}{2L}x)\ sin'(b\frac{\pi}{2L}x)\,\mathrm{d}x$$

Check positive definiteness of $\boldsymbol{K}$: Take any $u^h \neq 0$:

$$\begin{aligned}\{\boldsymbol{u}\}\cdot\boldsymbol{K}\{\boldsymbol{u}\} &= \sum_{a,b=1}^{r}\int_0^L EA\ sin'(a\frac{\pi}{2L}x)\ sin'(b\frac{\pi}{2L}x)u_a\ u_b\,\mathrm{d}x \\ &= \int_0^L EA\ ((u^h)')^2\,\mathrm{d}x \\ &> 0\end{aligned}$$

By proving that $\boldsymbol{K}$ is positive definite, we know that $\boldsymbol{K}\boldsymbol{d} = \boldsymbol{F}$ has a unique solution

Maybe, when $r \to \infty$, the matrix $\boldsymbol{K}$ becomes ill-conditioned. Again, difficult to say looking at

$$K_{ab} = \int_0^L EA \ sin'(a\frac{\pi}{2L}x) \ sin'(b\frac{\pi}{2L}x)\,\mathrm{d}x$$

We prove the stability of the problem in the $H_1(0,L)$ norm. For that we need a "matrix norm" $\boldsymbol{H}$ such that $\|\boldsymbol{u}\|_1 = \sqrt{\boldsymbol{u}\cdot\boldsymbol{H}\boldsymbol{u}}$.

- Result 1: $\|\boldsymbol{K}\|_1 \leq EA$. Proof

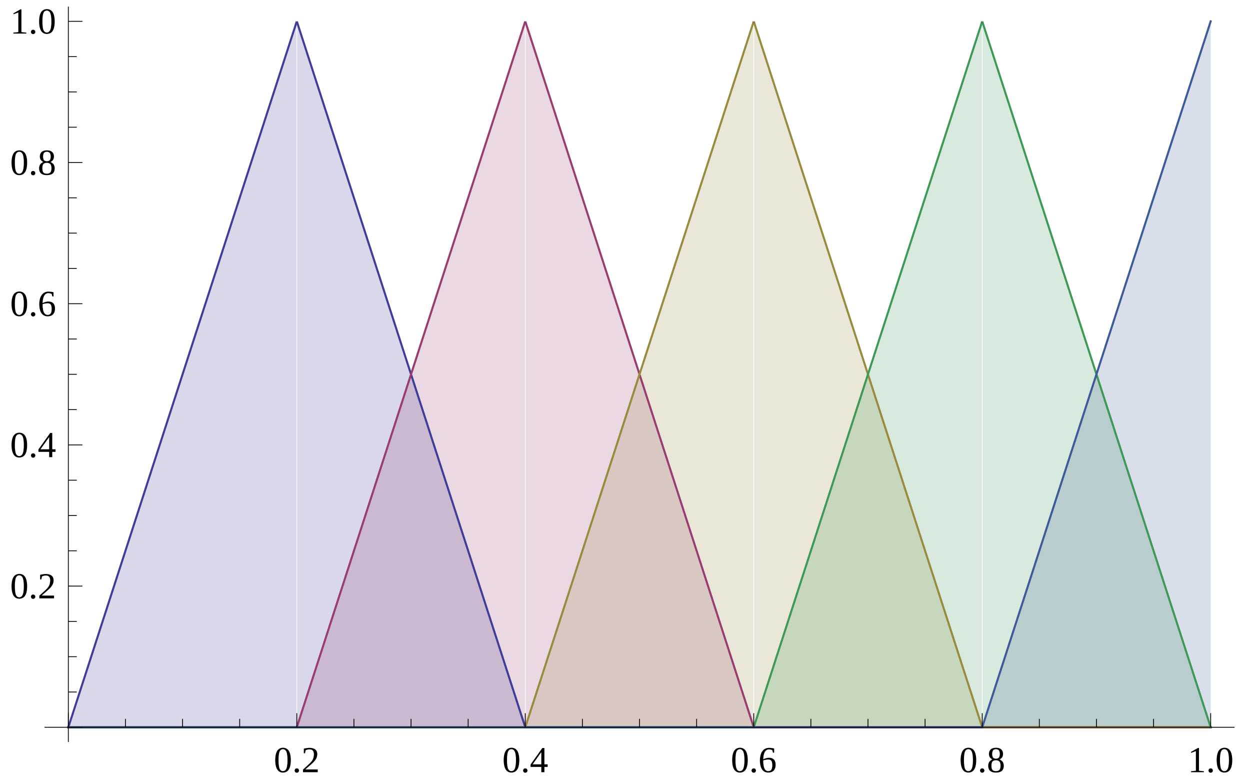
$$\|\boldsymbol{K}\|_1 = \max_{\boldsymbol{u}} \frac{\|\boldsymbol{K}\boldsymbol{u}\|_1}{\|\boldsymbol{u}\|_1} = \max_{\boldsymbol{v}} \max_{\boldsymbol{u}} \frac{|\boldsymbol{v}\cdot\boldsymbol{K}\boldsymbol{u}|}{\|\boldsymbol{u}\|_1\|\boldsymbol{v}\|_1} = \max_{\boldsymbol{v}} \max_{\boldsymbol{u}} \frac{\int_0^L EA\, u_h'\, v_h'\,\mathrm{d}x}{\|\boldsymbol{u}\|_1\|\boldsymbol{v}\|_1} \leq EA$$

- Result 2: $\boldsymbol{u}\cdot\boldsymbol{K}\boldsymbol{u} \geq EA\|\boldsymbol{u}\|_1^2$.

Using results 1 & 2:

$$\kappa(\boldsymbol{K})_1 = \|\boldsymbol{K}\|_1 \ \|\boldsymbol{K}^{-1}\|_1 \leq 1$$

- There are infinite possible sets of “trial” functions $N_a$.
- Reasonable choices: sines, splines, polynomials, NURBS.
- The Finite Element Method (FEM) is the particularization of the Rayleigh-Ritz method when the trial space of functions is the set of piecewise polynomials.



- Minimization problems are ubiquitous in Mechanics.
- Finite dimensional convex problems are "easy" to solve, but infinite dimensional ones might be very difficult.
- The idea of first order optimality condition might be extended to infinite dimensional problems, but still we are left with a boundary value problem.
- If an approximate minimizer is acceptable, the Rayleigh-Ritz method provides a simple methodology to obtain one.
- There are many possible choices for solution spaces. The choice of piecewise polynomials results in the Finite Element Method (FEM).

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