Lec 08: Nonlinear problems

- Newton's method

- Advanced topics: Material / Geometric nonlinearity, buckling, contact

Newton's method

Newton's method is the most important method for nonlinear FEM.

Intuition: Newton's method in 1D.

Goal: Find the root of a function $f(x)$, i.e., find x^* s.t. $f(x^*)=0$.

Algorithm: Start with x_0 (initial guess)

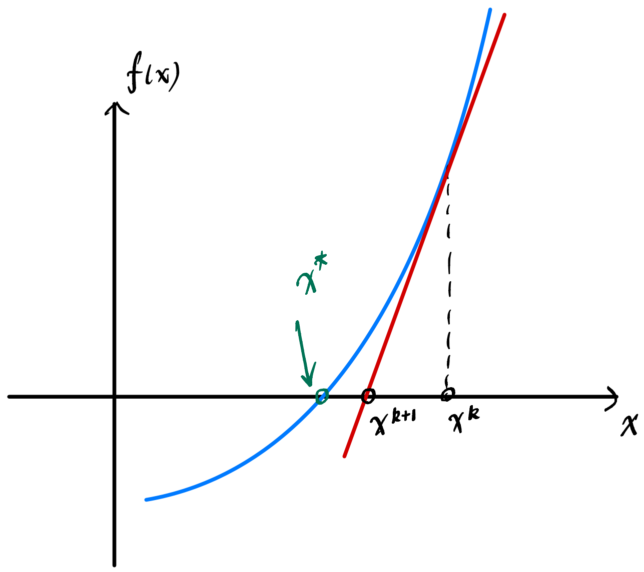
While $|f(x^k)| >$ tolerance:

$$\left.\frac{df}{dx}\right|_{x=x^k} \cdot \delta x + f(x^k) = 0$$

$$\Rightarrow \quad \delta x = -\frac{f(x^k)}{f'(x^k)}$$

update $x^{k+1} = x^k + \delta x$

Return x^{k+1} as x^*



More intuition: Newton's method in finite dimensions.

Goal: Find the root $\underline{x}^*$ such that $\underline{F}(\underline{x}^*) = \underline{0}$, where $\underline{F}: \mathbb{R}^N \to \mathbb{R}^N$.

Key update: $\underline{x}^{k+1} = \underline{x}^k + \delta \underline{x}$

Jacobian matrix

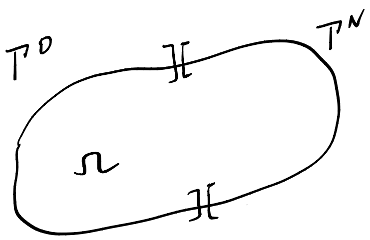
where $\left.\frac{\partial \underline{F}}{\partial \underline{x}}\right|_{\underline{x}=\underline{x}^k} \cdot \delta \underline{x} + \underline{F}(\underline{x}^k) = \underline{0}$ $\left(\left.\frac{\partial \underline{F}}{\partial \underline{x}}\right|_{\underline{x}=\underline{x}^k} = \underline{\underline{J}}_{\underline{F}}(\underline{x}^k) \right)$

High-level ideas: When to apply Newton's method in FEM?

strong form ← Newton's method weak form Galerkin approximation	strong form weak form ← Newton's method Galerkin approximation	strong form weak form Galerkin approximation ← Newton's method
Newton's method at the PDE level (I)	Newton's method at the weak form level (II)	Newton's method at the discretized level (III)

The three approaches will eventually yield equivalent solutions, but the implementation is quite different. JAX-FEM uses approach III.

A model problem to demonstrate the three approaches



Nonlinear Poisson's problem:

$$-\underline{\nabla}\cdot(q(u)\underline{\nabla}u) = f \quad \text{in } \Omega \qquad \text{(governing equation)}$$

$$u = g \quad \text{on } \Gamma^D \qquad \text{(Dirichlet B.C.)}$$

$$q\,\underline{\nabla}u\cdot\underline{n} = h \quad \text{on } \Gamma^N \qquad \text{(Neumann B.C.)}$$

Observation: $q(u)$ makes the problem nonlinear (unless $q(u) = \text{const.}$)

Approach I: Newton's method at the PDE level

We apply Newton's method to "$\underline{\nabla}\cdot(q(u)\underline{\nabla}u) + f = 0$" directly.

Question: How does Newton's method work for infinite dimensions?

For the operator $S(u) = \underline{\nabla}\cdot(q(u)\underline{\nabla}u) + f$, we can define the operator differential of $S(u)$ at u^k acting on δu as:

$$DS(u^k)[\delta u] := \lim_{\alpha \to 0} \frac{S[u^k + \alpha \delta u] - S[u^k]}{\alpha} = \frac{d}{d\alpha} S[u^k + \alpha \delta u] \Big|_{\alpha = 0}$$

(Analogous to $\left.\frac{\partial \underline{S}}{\partial \underline{u}}\right|_{\underline{u} = \underline{u}^k} \cdot \delta \underline{u}$ if $\underline{S}$ is a finite-dimensional function)

Therefore, $DS(u^k)[\delta u] = \frac{d}{d\alpha} \left(\underline{\nabla} \cdot (q(u^k + \alpha \delta u) \underline{\nabla}(u^k + \alpha \delta u)) + f \right) \Big|_{\alpha = 0}$

$$= \underline{\nabla} \cdot (q'(u^k) \, \delta u \, \underline{\nabla} u^k) + \underline{\nabla} \cdot (q(u^k) \, \underline{\nabla} \delta u)$$

Apply Newton's method to the governing equation: $DS(u^k)[\delta u] + S(u^k) = 0$

$$\Rightarrow \boxed{\underline{\nabla} \cdot (q'(u^k) \, \underline{\delta u} \, \underline{\nabla} u^k) + \underline{\nabla} \cdot (q(u^k) \, \underline{\nabla} \, \underline{\delta u}) + \underline{\nabla} \cdot (q(u^k) \underline{\nabla} u^k) + f = 0}$$

Note that we get a linear PDE in $\underline{\delta u}$.

Incremental linear problem

Apply Newton's method to the boundary conditions:

$$\boxed{\begin{array}{c} \underline{\delta u} + u^k - g = 0 \quad \text{(Dirichlet B.C.)} \\ q(u^k) \underline{\nabla} \, \underline{\delta u} \cdot \underline{n} + q'(u^k) \underline{\delta u} \, \underline{\nabla} u^k \cdot \underline{n} + q(u^k) \underline{\nabla} u^k \cdot \underline{n} - h = 0 \quad \text{(Neumann B.C.)} \end{array}}$$

Standard FEM procedure requires weak form:

Trial space: $\delta u \in S_k = \{ \delta u \in H^1 : \delta u = g - u^k \text{ on } \Gamma^D \}$

Test space: $v \in V_k = \{ v \in H^1 : v = 0 \text{ on } \Gamma^D \}$

and $\quad LHS = - \int_\Omega q'(u^k) \, \delta u \, \underline{\nabla} u^k \cdot \underline{\nabla} v + \int_{\Gamma^N} q'(u^k) \, \delta u \, \underline{\nabla} u^k \cdot \underline{n} \, v$

$$- \int_\Omega q(u^k) \, \underline{\nabla} \delta u \cdot \underline{\nabla} v + \int_{\Gamma^N} q(u^k) \, \underline{\nabla} \delta u \cdot \underline{n} \, v$$

$$RHS = \int_\Omega q(u^k)\,\nabla u^k \cdot \nabla v - \int_{\Gamma^N} q(u^k)\,\nabla u^k \cdot \underline{n}\; v - \int_\Omega f v$$

$LHS = RHS \Rightarrow$

$$\underbrace{\int_\Omega q'(u^k)\,\delta u\,\nabla u^k \cdot \nabla v + \int_\Omega q(u^k)\,\nabla \delta u \cdot \nabla v}_{a(v,\,\delta u)} = \underbrace{-\int_\Omega q(u^k)\,\nabla u^k \cdot \nabla v + \int_{\Gamma^N} h v + \int_\Omega f v}_{L(v)}$$

Solve for δu and do the update: $u^{k+1} = u^k + \delta u$.

Approach II : Newton's method at the weak form level

The weak form for the nonlinear Poisson's problem is:

Trial space: $u \in S = \{ u \in H^1 : u = g \text{ on } \Gamma^D \}$

Test space: $v \in V = \{ v \in H^1 : v = 0 \text{ on } \Gamma^D \}$

$$R(u) = \int_\Omega q(u)\,\nabla u \cdot \nabla v - \int_{\Gamma^N} h v - \int_\Omega f v = 0 \qquad \forall\, v \in V$$

Note that $R(u)$ is a (nonlinear) functional in u.

Apply Newton's method to the weak form residual: $\delta R(u^k)[\delta u] + R(u^k) = 0$

$$\text{where } \delta R(u^k)[\delta u] = \lim_{\alpha \to 0} \frac{R(u^k + \alpha\,\delta u) - R(u^k)}{\alpha} = \left. \frac{d\, R(u^k + \alpha\,\delta u)}{d\alpha} \right|_{\alpha = 0}$$

Incremental linear problem

$$\Rightarrow \boxed{\begin{aligned} &\int_\Omega q'(u^k)\,\delta u\,\nabla u^k \cdot \nabla v + \int_\Omega q(u^k)\,\nabla \delta u \cdot \nabla v = -\int_\Omega q(u^k)\,\nabla u^k \cdot \nabla v + \int_{\Gamma^N} h v + \int_\Omega f v \quad \forall\, v \in V \\ &\text{Trial space: } \delta u \in S_k = \{ \delta u \in H^1 : \delta u = g - u^k \text{ on } \Gamma^D \} \end{aligned}}$$

Solve for δu and do the update: $u^{k+1} = u^k + \delta u$.

Approach III: Newton's method at the discretized level

For the weak form residual:

$$R(u, v) = \int_\Omega q(u) \nabla u \cdot \nabla v - \int_{\Gamma^N} h v - \int_\Omega f v = 0 \quad \forall v \in V$$

Consider Galerkin approximation:

Galerkin trial space: $u^h \in S^h = \{ u^h \in H^1 : u^h = \sum_{i=1}^N u_i \phi_i(\underline{x}),\ u^h = g \text{ on } \Gamma^D \} \subset S$

Galerkin test space: $v^h \in V^h = \{ v^h \in H^1 : v^h = \sum_{i=1}^N v_i \phi_i(\underline{x}),\ v^h = 0 \text{ on } \Gamma^D \} \subset V$

Then we have $R(u^h, v^h) = 0,\ \forall v^h \in V$. That is:

arbitrary

$$[v_1\ v_2 \cdots v_N] \cdot \begin{bmatrix} r_1(\underline{U}) \\ r_2(\underline{U}) \\ \vdots \\ r_N(\underline{U}) \end{bmatrix} = 0, \quad \text{where } \underline{U} := \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{bmatrix} \text{ is the unknown solution}$$

$$r_i(\underline{U}) = \int_\Omega q\left(\sum_{j=1}^N u_j \phi_j\right) \nabla\left(\sum_{j=1}^N u_j \phi_j\right) \cdot \nabla \phi_i - \int_{\Gamma^N} h \phi_i - \int_\Omega f \phi_i = 0$$

Apply Newton's method to the discretized system $\underline{R}(\underline{U}) = \underline{0}$ to get

$$\boxed{\left.\frac{\partial \underline{R}}{\partial \underline{U}}\right|_{\underline{U} = \underline{U}^k} \cdot \delta \underline{U} + \underline{R}(\underline{U}^k) = 0}$$

linear incremental problem

$$\text{where } \left[\frac{\partial \underline{R}}{\partial \underline{U}}\right]_{ij} = \frac{\partial r_i}{\partial u_j} = \int_\Omega q'\left(\sum_{k=1}^N u_k \phi_k\right) \phi_j \nabla\left(\sum_{k=1}^N u_k \phi_k\right) \cdot \nabla \phi_i + \int q\left(\sum_{k=1}^N u_k \phi_k\right) \nabla \phi_j \cdot \nabla \phi_i$$

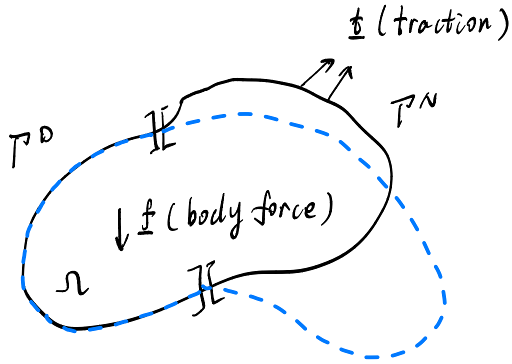
Solve for $\delta \underline{U}$ and do the update: $\underline{U}^{k+1} = \underline{U}^k + \delta \underline{U}$.

Advanced topics

We will present how Newton's method (Approach II) applies to a hyperelasticity problem. Then we discuss special treatment for two prominent nonlinear problems: bucking and contact.

Material / geometric nonlinearity

We will use hyperelasticity as the example for demonstration:



deformed configuration

Find displacement $\underline{u}(\underline{X})$ for $\underline{X} \in \Omega$, s.t.

$$-\underline{\underline{P}} \cdot \underline{\nabla} = \underline{f} \text{ in } \Omega \quad (\text{equilibrium})$$

$$\underline{u} = \underline{g} \text{ on } \Gamma^D \quad (\text{Dirichlet B.C.})$$

$$\underline{\underline{P}} \cdot \underline{n} = \underline{h} \text{ on } \Gamma^N \quad (\text{Neumann B.C.})$$

$\underline{\underline{P}} = \dfrac{\partial W}{\partial \underline{\underline{F}}}$: first Piola-Kirchhoff stress (constitutive law) Material nonlinearity

$\underline{\underline{F}} = \dfrac{\partial \underline{x}}{\partial \underline{X}} = \underline{\underline{I}} + \dfrac{\partial \underline{u}}{\partial \underline{X}}$: deformation gradient (kenematic relationship) Geometric nonlinearity

For a compressible neo-Hookean material : $W(\underline{\underline{F}}) = \dfrac{\mu}{2}(J^{-2/3} I_1 - 3) + \dfrac{\kappa}{2}(J-1)^2$,

with $J = \det(\underline{\underline{F}})$ (volume ratio), $I_1 = tr(\underline{\underline{F}}^T \underline{\underline{F}})$ (first invariant), μ (shear modulus) and κ (bulk modulus).

Verify that $\underline{\underline{P}} = \dfrac{\partial W}{\partial \underline{\underline{F}}} = \mu J^{-2/3}\left(\underline{\underline{F}} - \frac{1}{3} tr(\underline{\underline{F}}^T \underline{\underline{F}}) \underline{\underline{F}}^{-T}\right) + \kappa (J-1) J \underline{\underline{F}}^{-T}$.

Weak form:

$$\int_\Omega \underline{\underline{P}} : \underline{v}\underline{\nabla} - \int_{\Gamma^N} \underline{h} \cdot \underline{v} - \int_\Omega \underline{f} \cdot \underline{v} = 0 \quad \forall \underline{v}$$

or $$\int_\Omega P_{ij} v_{i,j} - \int_{\Gamma^N} h_i v_i - \int_\Omega f_i v_i = 0$$

Apply Newton's method to get the linear incremental problem (solve for $\delta \underline{u}$):

$$\underbrace{\int_\Omega \left.\frac{\partial P_{ij}}{\partial F_{kl}}\right|_{\underline{u}=\underline{u}^k} \delta F_{kl} v_{i,j}}_{\displaystyle \parallel \atop \displaystyle \int_\Omega \left.\frac{\partial P_{ij}}{\partial F_{kl}}\right|_{\underline{u}=\underline{u}^k} \delta u_{k,l} v_{i,j}} + \int_\Omega P_{ij}(\underline{u}^k) v_{i,j} - \int_{\Gamma^N} h_i v_i - \int_\Omega f_i v_i = 0$$

by DeepSeek

Modulus tensor:

$$\frac{\partial \underline{\underline{P}}}{\partial \underline{\underline{F}}} = \underline{\underline{\underline{\underline{C}}}} = \mu J^{-2/3}\left(\underline{\underline{I}} \otimes \underline{\underline{I}} - \frac{1}{3}\left(\underline{\underline{F}}^{-T} \otimes \underline{\underline{F}} + 2\underline{\underline{F}} \otimes \underline{\underline{F}}^{-T}\right)\right)$$
$$+ \kappa\left((2J-1)\underline{\underline{F}}^{-T} \otimes \underline{\underline{F}}^{-T} - (J-1)J\underline{\underline{F}}^{-T}\underline{\underline{F}}^{-T}\right)$$

You should let Automatic Differentiation (AD) tools do this task!

Buckling

Buckling can occur for both linear and nonlinear problems, indicating the loss of stabilities of a structure. We will consider "snap-through" buckling under large deformation and show that Newton's method will fail. We will show the arc-length method as an effective strategy.

Problem setup: Introduce a loading parameter λ in the weak form:

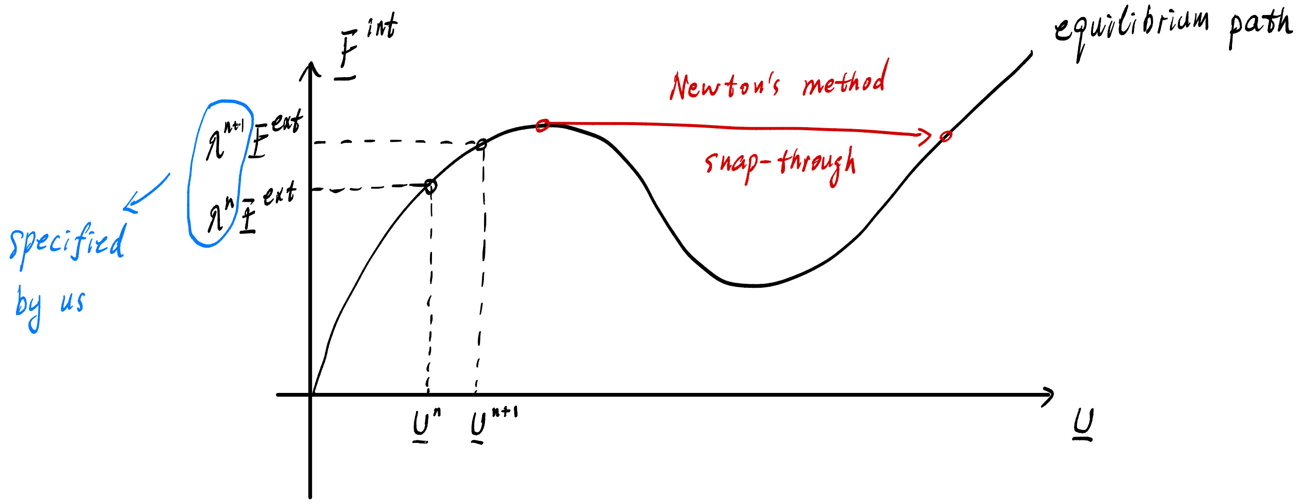
$$\int_\Omega \underline{\underline{P}} : \nabla \underline{v} - \int_{\Gamma^N} \lambda \, \underline{h} \cdot \underline{v} - \cancel{\int_\Omega \underline{f} \cdot \underline{v}} = 0 \quad \forall \underline{v}$$

neglected

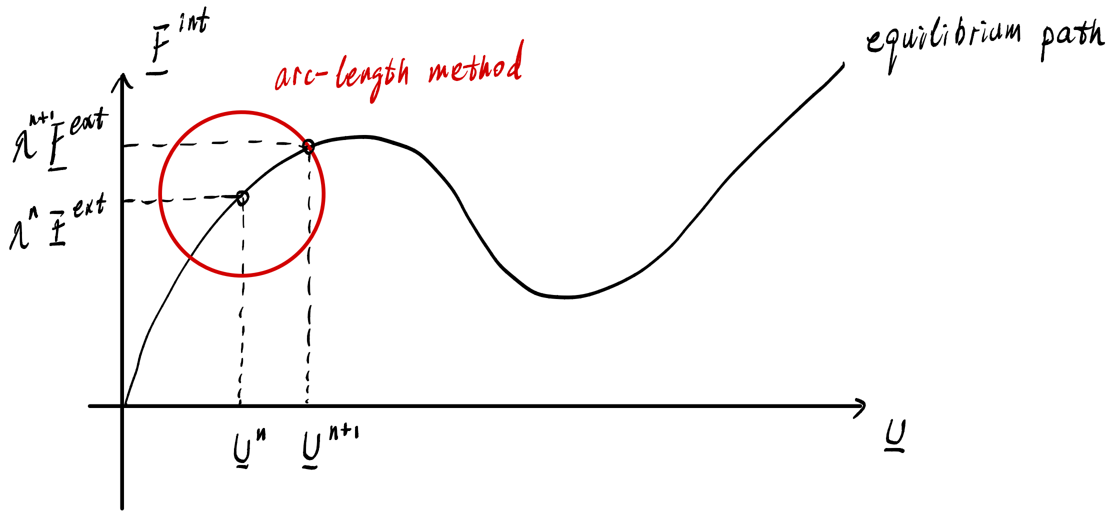
$$\Rightarrow \int_\Omega \underline{\underline{P}} : \nabla \underline{v} = \lambda \int_{\Gamma^N} \underline{h} \cdot \underline{v} \quad (\text{internal force} = \text{external force})$$

The discretized weak form is: $\underline{F}^{int}(\underline{U}) = \lambda \underline{F}^{ext}$.

Assume the structure behaves like:



Goal: We want to travel along the equilibrium path.



Arc-length method: Solve for $(\underline{U}^{n+1}, \lambda^{n+1})$ at the same time:

$$(*) = \begin{cases} \underline{F}^{int}(\underline{U}^{n+1}) = \lambda^{n+1}\underline{F}^{ext} & \text{(equilibrium)} \\ \|\underline{U}^{n+1} - \underline{U}^{n}\|^2 + \psi^2 \|\lambda^{n+1}\underline{F}^{ext} - \lambda^{n}\underline{F}^{ext}\|^2 = \Delta l^2 & \text{(arc-length equation)} \end{cases}$$

where $(\underline{U}^n, \lambda^n)$ satisfying $\underline{F}^{int}(\underline{U}^n) = \lambda^n \underline{F}^{ext}$ are from the previous step, and ψ and Δl are numerical parameters.

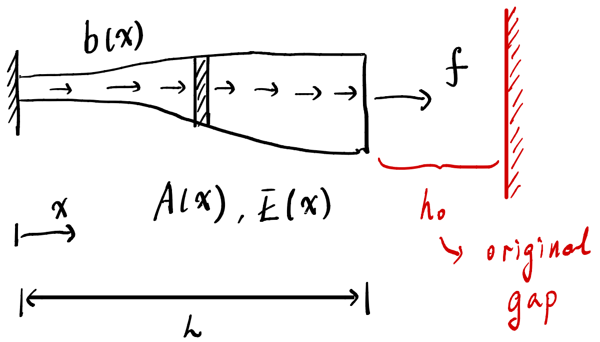
Remarks: You can apply Newton's method to solve $(*)$ directly. It is also possible to improve the workflow (check Crisfield's formulation).

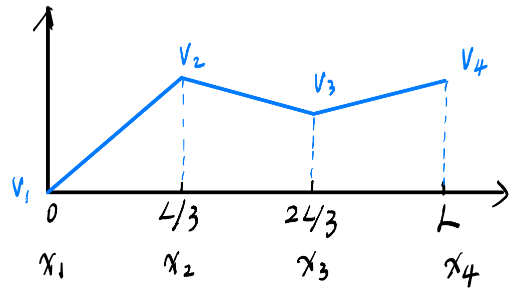
There are other numerical methods to deal with buckling, e.g., dynamic relaxation methods.

Contact

Contact problems are computationally challenging. Essentially, contact problems deal with constraints (inequality or equality).

Revisit our 1D problem, with a rigid wall placed near the right end:





$$u^h(x) = \sum_{i=1}^{4} v_i \phi_i(x) + g\, \phi_1(x)$$

In the optimization context:

$$\min_{[v]} \; E([v])$$
$$\text{s.t.} \quad g([v]) = 0$$
$$\boxed{h([v]) \geq 0} \quad (\text{contact constraint})$$

where $E([v]) = \frac{1}{2}[v]^T[K][v] - [v]^T[F]$ is the energy function to be minimized

$g([v]) = v_1 - 0 = 0$ is the constraint that must be satisfied

$h([v]) = h_0 - v_4 \geq 0$ is the contact constraint.

Penalty-based methods are popular: $\min_{[v]} \; E([v]) + \frac{\mu_g}{2} g^2([v]) + \frac{\mu_h}{2}\left(\langle -h([v])\rangle_+\right)^2,$

where $\langle x \rangle_+ = (|x| + x)/2$ is the positive function.