Stability Results for Elastic Rods with Electrostatic Self-Repulsion

Contact Stability

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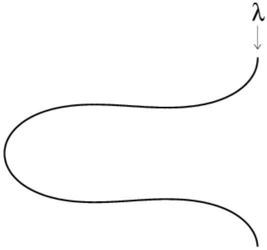
Outline



Consider a two dimensional elastic rod, whose configuration is described by an angle $\theta(s)$ and a position $\mathbf{r}(s) = (x, z)$, for $0 \leq s \leq 1$. We assume the rod to be inextensible and unshearable,

$$\mathbf{r}'(s) = \mathbf{d}_3(\theta) = (\cos(\theta), \sin(\theta)).$$

and satisfy the following boundary conditions

$$\theta(0) = \theta(1) = 0, \quad \mathbf{r}(0) = (0, 0), \mathbf{r}(1) = (0, *)$$

Variational Formulation

The energy functional of the two-dimensional elastic strut is

$$J[\theta] = \int_0^1 \frac{K}{2}(\theta'(s) - g(s))^2 + \lambda \cos\theta(s) ds,$$

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Remarks

- $g(s)$ specifies the intrinsic shape of the elastic rod
- assume linear elasticity but only for computational convenience

First Variation

Substitute $\theta = \theta_0 + \epsilon$ into the functional and collect terms that are first order in ϵ

$$\delta J \;\; = \;\; \int_0^1 \left[K\epsilon'(s)(\theta_0'(s) - g(s)) - \lambda \sin\theta_0(s)\epsilon(s) \right] ds$$

A necessary condition for a minimum is that the first variation δJ vanish for all admissible variations that satisfy the linearized boundary conditions

$$\epsilon(0) = \epsilon(1) = 0$$

and the linearized constraints

$$\int_0^1 \cos(\theta_0(s))\epsilon(s)\; ds = 0.$$

Equilibrium Equations

Integrating δJ by parts,

$$\delta J = \langle \epsilon, -K(\theta_0''(s) - g'(s)) - \lambda \sin\theta_0(s) \rangle \equiv 0$$

for all ϵ such that $\langle \epsilon, \cos(\theta_0) \rangle = 0$. Then,

$$\mu \cos(\theta_0) = -K(\theta_0''(s) - g'(s)) - \lambda \sin\theta_0(s)$$

Define $\mathbf{n} = [-\mu, \lambda]^T$, so then,

$$\mathbf{n}(s)^T (\mathbf{d}_3)_\theta(\theta(s)) = K\theta'' - Kg'(s)$$

Thus, the equilibrium equations are:

$$\begin{aligned} \mathbf{n}(s)^T(\mathbf{d}_3)_\theta(\theta(s)) &= K\theta'' - Kg'(s), \\ \mathbf{n}'(s) &= 0 \\ \mathbf{r}'(s) &= \mathbf{d}_3(\theta(s)) \end{aligned}$$

Second Variation

The quadratic form of the second variation of J is

$$\delta^2 J[\epsilon] = \frac{1}{2}\langle \epsilon(s), \mathcal{S}\epsilon(s)\rangle$$

where $\mathcal{S}$ is the second-order differential operator

$$\mathcal{S}\epsilon = (-K\epsilon''(s) - \lambda \cos\theta(s)\epsilon(s) + \mu \sin\theta(s)\epsilon(s))$$

A necessary condition for a minimum is that the second variation $\delta^2 J[\epsilon] \geq 0$ for all admissible variations.

Jacobi Conjugate Points

Classical calculus of variations theory states that under the condition that $K > 0$ (Legendre's strengthen condition), a solution that satisfies the equilibrium equations satisfies $\delta^2 J[\epsilon] \geq 0$, provided there are no values of $0 < \sigma \leq 1$ such that

$$\mathcal{S}\epsilon = \mathbf{0}$$
$$\epsilon(0) = 0 = \epsilon(\sigma)$$

Such points are called **Jacobi Conjugate Points**.

Jacobi Conjugate Points

Embed Jacobi conjugate condition in an eigenvalue problem

$$\mathcal{S}\epsilon(\sigma) = \rho(\sigma)\epsilon(\sigma)$$
$$\epsilon(0) = 0 = \epsilon(\sigma),$$

for each $0 < \sigma \leq 1$.

Property 1: For prescribed σ, the spectrum of $\mathcal{S}$ consists of isolated eigenvalues $\rho_1(\sigma) \leq \rho_2(\sigma) \leq \cdots$, each with finite multiplicity,
Property 2: Each eigenvalue $\rho_j(\sigma)$ is a monotonically decreasing function of σ, and
Property 3: For σ sufficiently close to 0, $\rho_j(\sigma) > 0$ for all j

The number of conjugate points corresponds to the (Morse) **index** of the equilibrium solutions. Solutions with index zero correspond to minima.

Jacobi Conjugate Points with Constraints

The relationship between the number of Jacobi conjugate points and the index can be expanded to include isoperimetric constraints, provided the operator

$$\mathcal{S} \rightarrow \mathcal{QSQ}$$

is replaced with the a projected operator $\mathcal{QSQ}$, where $\mathcal{Q}$ is a self-adjoint orthogonal projection that maps $L^2(0, \sigma)$ onto the orthogonal complement of the constraints.

Properties 1-3 hold for the operator $\mathcal{QSQ}$, (provided they hold for $\mathcal{S}$), and the corresponding index theory holds.

Property 2 does not hold for elastic rods with electrostatic repulsion.

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II. Stability of Elastic Rods with Electrostatic Repulsion
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Consider a function

$$f(\chi, \rho) : \mathbb{R}^2 \to \mathbb{R}$$

to be the energy density for electrostatic self-repulsion.
This could take on many forms, such as: Coulomb repulsion, Debye-Huckel, Lennard-Jones. For computational purposes we are using

$$f(\chi, \rho) = \iota \frac{\chi^4}{\rho},$$

where $\chi = |s - t|$ and $\rho = |\mathbf{r}(s) - \mathbf{r}(t)|$.

Variational Formulation

The energy functional of the two-dimensional elastic strut with an electrostatic repulsion is

$$J[\theta, \mathbf{r}] = \int_0^1 \left\{ \frac{K}{2}(\theta'(s) - g(s))^2 + \lambda \cos\theta(s) + \int_0^1 f(\chi, \rho)\, dt \right\} ds,$$

with the boundary conditions

$$\theta(0) = \theta(1) = 0, \quad \mathbf{r}(0) = (0,0), \mathbf{r}(1) = (0, *)$$

and the constraint

$$\mathbf{r}'(s) = \mathbf{d}_3(\theta) = (\cos(\theta), \sin(\theta)).$$

Thus, the equilibrium equations are:

$$\begin{aligned}\mathbf{n}(s)^T(\mathbf{d}_3)_\theta(\theta(s)) &= K\theta'' - Kg'(s),\\ \mathbf{n}'(s) &= -2\int_0^1 f_\rho(\chi,\rho)\frac{\mathbf{r}(s)-\mathbf{r}(t)}{|\mathbf{r}(s)-\mathbf{r}(t)|}dt,\\ \mathbf{r}'(s) &= \mathbf{d}_3(\theta(s))\end{aligned}$$

Numerical Implementation

Subdivide $[0, 1]$ into N equal pieces of length $\Delta s = \frac{1}{N}$. The approximation of the equilibrium equations at $s = \frac{i}{N}$ is:

$$\begin{aligned}
\mathbf{n}_i^T(\mathbf{d}_3)_\theta(\theta_i) &= K\frac{\theta_{i+1} - 2\theta_i + \theta_{i-1}}{(\Delta s)^2}, \\
\frac{\mathbf{n}_{i+1} - \mathbf{n}_i}{\Delta s} &= -2\sum_{j=0, j\neq i}^{N-1}\left[f_\rho\left(\left|\frac{i}{N} - \frac{j}{N}\right|, |\mathbf{r}_i - \mathbf{r}_j|\right)\frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|}\right], \\
\frac{\mathbf{r}_{i+1} - \mathbf{r}_i}{\Delta s} &= \mathbf{d}_3(\theta_i),
\end{aligned}$$

where the integral has been approximated using a trapezoid rule.

The NOX/LOCA algorithms were used to solve the resulting non-linear system and perform the continuation in λ.

Second Variation

The second variation of J consists of two parts:

- the familiar non-contact term $\langle \epsilon, \mathcal{S}\epsilon \rangle$ described for the non-contact elastic strut
- the contributions from the contact term in the functional:

$$= \frac{1}{2}\int_0^1 \int_0^1 \left\{ \left(\int_t^s (\mathbf{d}_3)_\theta(\tau)\epsilon(\tau)d\tau \right)^T \mathbf{M} \left(\int_t^s (\mathbf{d}_3)_\theta(\rho)\epsilon(\rho)d\rho \right) + \int_t^s \left[f_\rho(|s-t|, |\mathbf{x}|)\frac{\mathbf{x}^T}{|\mathbf{x}|} \right] \epsilon^2(w)(\mathbf{d}_3)_{\theta\theta}(w)dw \right\} dtds,$$

where $\mathbf{x} \equiv \mathbf{r}_0(s) - \mathbf{r}_0(t)$ and $\mathbf{M}(s,t) \in \mathbb{R}^{2\times 2}$

$$\left[f_{\rho\rho}(|s-t|, |\mathbf{x}|)\frac{\mathbf{x}\mathbf{x}^T}{|\mathbf{x}|^2} + f_\rho(|s-t|, |\mathbf{x}|)\frac{\mathbf{I}}{|\mathbf{x}|} - f_\rho(|s-t|, |\mathbf{x}|)\frac{\mathbf{x}\mathbf{x}^T}{|\mathbf{x}|^3} \right]$$

Second Variation

The second variation can be written as a quadratic form:

$$\delta^2 J[\epsilon] = \frac{1}{2}\langle \epsilon, \mathcal{O}\epsilon \rangle,$$

where the operator $\mathcal{O}$ is defined by

$$\mathcal{O}z(\tau) = \mathcal{S}(\theta_0(\tau))z(\tau) + \int_0^1 K(\rho,\tau)z(\rho)d\rho.$$

We note that ϵ satisfies the the linearized boundary conditions $\epsilon(1) = 0 = \epsilon(1)$ and the linearized constraints, that is, ϵ is in the orthogonal complement of $T \equiv (\mathbf{d}_{31})_\theta(\theta_0)$. These two conditions define the space of allowed variations:

$$\mathcal{A}_d = \left\{ \epsilon \in \mathcal{H}^2(0,1) | \epsilon(0) = 0 = \epsilon(1) \text{ and } \int_0^1 \cos(\theta(s))\epsilon(s)\, ds = 0 \right\}$$

The Operator $\mathcal{O}$

Consider the eigenvalue problem

$$\begin{aligned} \mathcal{O}_\sigma \epsilon(\sigma) =& \rho(\sigma)\epsilon(\sigma) \\ \epsilon(0) =& 0 = \epsilon(\sigma). \end{aligned}$$

Properties of $\mathcal{O}$:

- $\mathcal{O}$ is a densely defined operator: $\mathcal{O} : \mathcal{A}_d \subset L^2(0, \sigma) \to L^2(0, \sigma)$
- $\mathcal{O}_\sigma$ is symmetric
- $\mathcal{O}_\sigma$ is self-adjoint and bounded below

The Operator $\mathcal{O}$

Assumption 1 $\mathcal{O}$ consists of isolated eigenvalues $\rho_1(\sigma) \leq \rho_2(\sigma) \leq \cdots$, each with finite multiplicity

Assumption 2 the eigenvalues of $\mathcal{O}$ are continuously dependent on σ,

Assumption 3 the number of negative eigenvalues of $\mathcal{O}$ for σ sufficiently small, is known.

Index Theory

A non-negative integer called an index measures the size of the space on which the second variation is negative.

$$
\begin{aligned}
\text{Index} \;&=\; \begin{pmatrix} \text{the number of negative eigenvalues of } \mathcal{O} \\ \text{for } \sigma \text{ sufficiently close to zero} \end{pmatrix} \\
&+\; \begin{pmatrix} \text{additional negative eigenvalues} \\ \text{gained as } \sigma \text{ varies in the interval} \end{pmatrix} \\
&-\; \begin{pmatrix} \text{additional negative eigenvalues} \\ \text{lost as } \sigma \text{ varies in the interval} \end{pmatrix}
\end{aligned}
$$

The direction in which the eigenvalues cross zero can be determined using a perturbation expansion.

Numerical Implementation

The equation

$$\mathcal{Q}\mathcal{O}_\sigma\mathcal{Q}z = 0, \;\; z(0) = z(\sigma) = 0, \langle z, T\rangle = 0.$$

is equivalent to

$$\mathcal{S}(\theta_0(\tau))z(\tau) + \int_0^\sigma K_\sigma(\rho,\tau)z(\rho)d\rho = cT, \;\; z(0) = z(\sigma) = 0,$$

where c is any real number.

Numerical Implementation

The solution to this integro-differential equation is a linear combination of the solutions z^h to a homogeneous equation

$$\mathcal{S}(\theta_0(\tau))z(\tau) + \int_0^\sigma K_\sigma(\rho,\tau)z(\rho)d\rho = 0, \;\; z(0) = 0, \;\; z'(0) = 1$$

and the solutions z^n to a non-homogeneous equations

$$\mathcal{S}(\theta_0(\tau))z(\tau) + \int_0^\sigma K_\sigma(\rho,\tau)z(\rho)d\rho = T, \;\; z(0) = 0, \;\; z'(0) = 0.$$

The discretization of the differential operator $\mathcal{S}$ is analogous to the discretization of the equilibrium equations and the integral part of the operator is evaluated using the trapezoid rule.

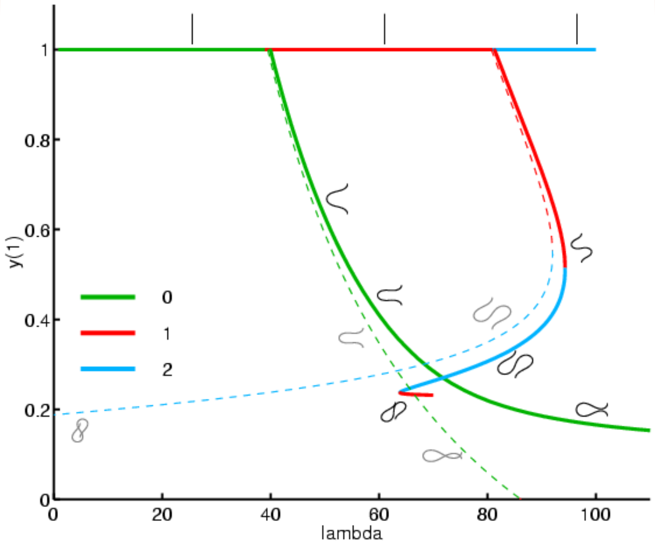
Stability Matrix

Any solution to the initial value problem can be written as $\check{c}z^h + cz^n$. The additional conditions that $z(\sigma) = 0$ and $\langle z, T \rangle = 0$ are enforced by solving the linear system:

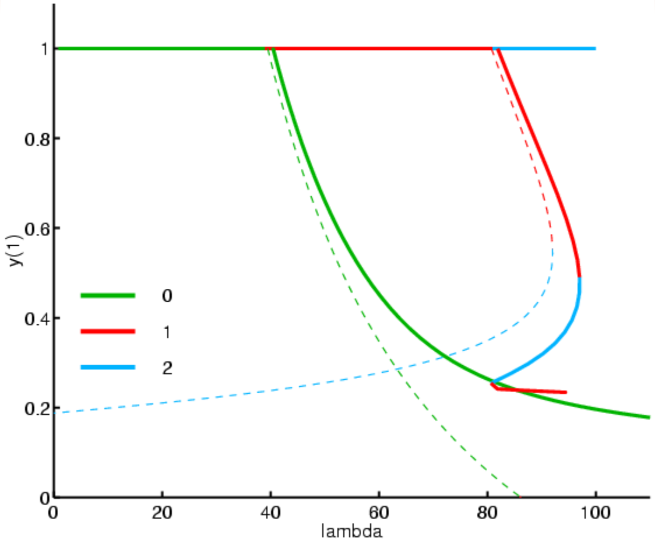
$$\begin{bmatrix} z^h & z^n \\ \langle z^h, T \rangle & \langle z^n, T \rangle \end{bmatrix} \begin{bmatrix} c \\ \check{c} \end{bmatrix} = \mathbf{0},$$

Conjugate points correspond to values of σ for which the determinant of the **stability matrix** is zero.

Results $\iota = 2$



Results $\iota = 4$



Verification

How do we know the results are correct?

- Distinguished diagrams
- Discrete Optimization Methods

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