Optimal packing problems in the modeling of filaments

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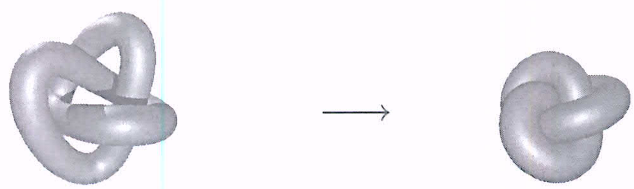
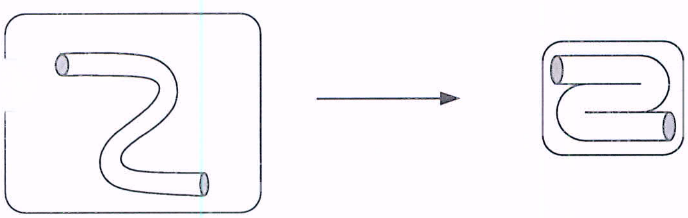
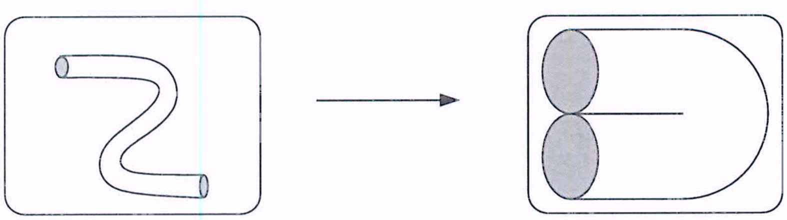
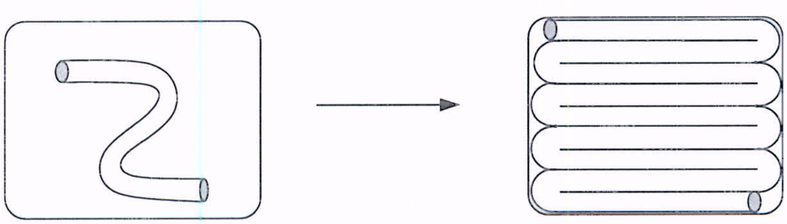
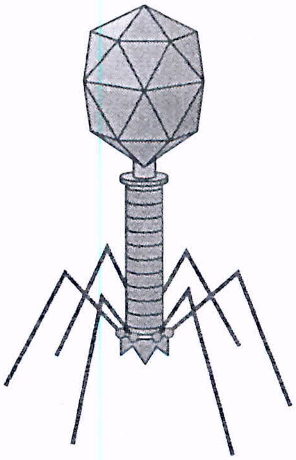
Outline

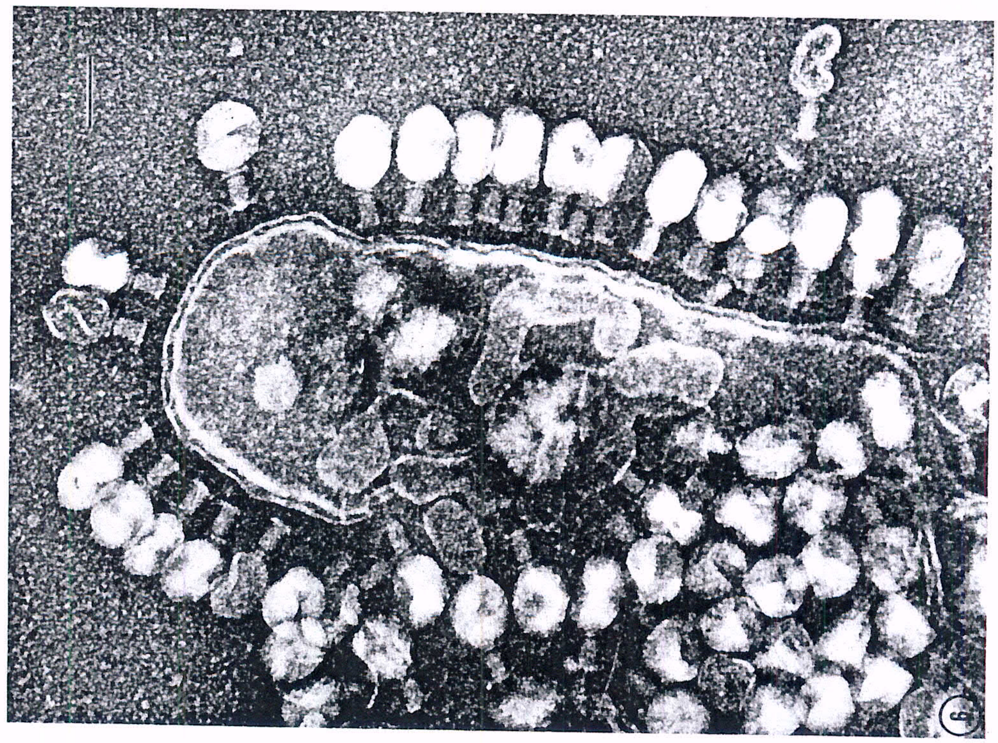
General problem

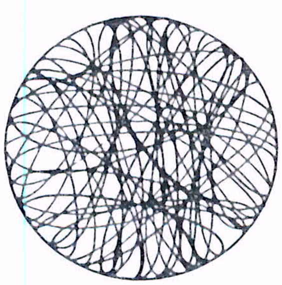
- optimize energy of a curve
- insist that curve be centerline of a solid tube

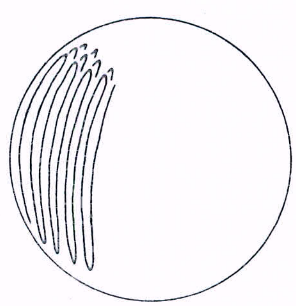
example	energy	constraints
	Len	Thk, Knot
	Box	Thk, Len, Knot
	Thk	Box, Len, Knot
	Len	Box, Thk, Knot

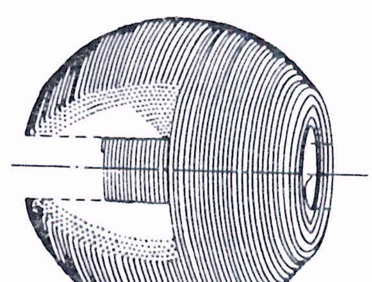
Motivation
DNA packing in bacteriophages











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Encapsidated Conformation of Bacteriophage T7 DNA

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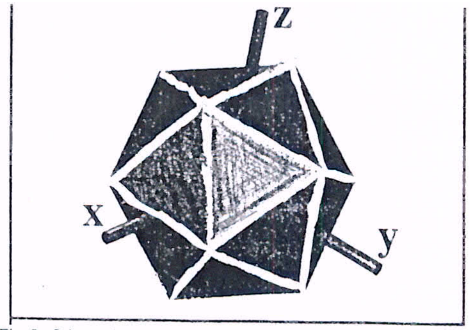
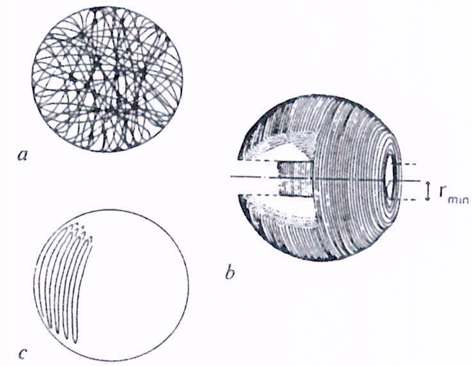


Fig. 5 Schematic representation of various models discussed in the text. *a* Ball-of-string. *b* Coaxial spool. *c* Chain-folded structure (with 180° folds at each end).



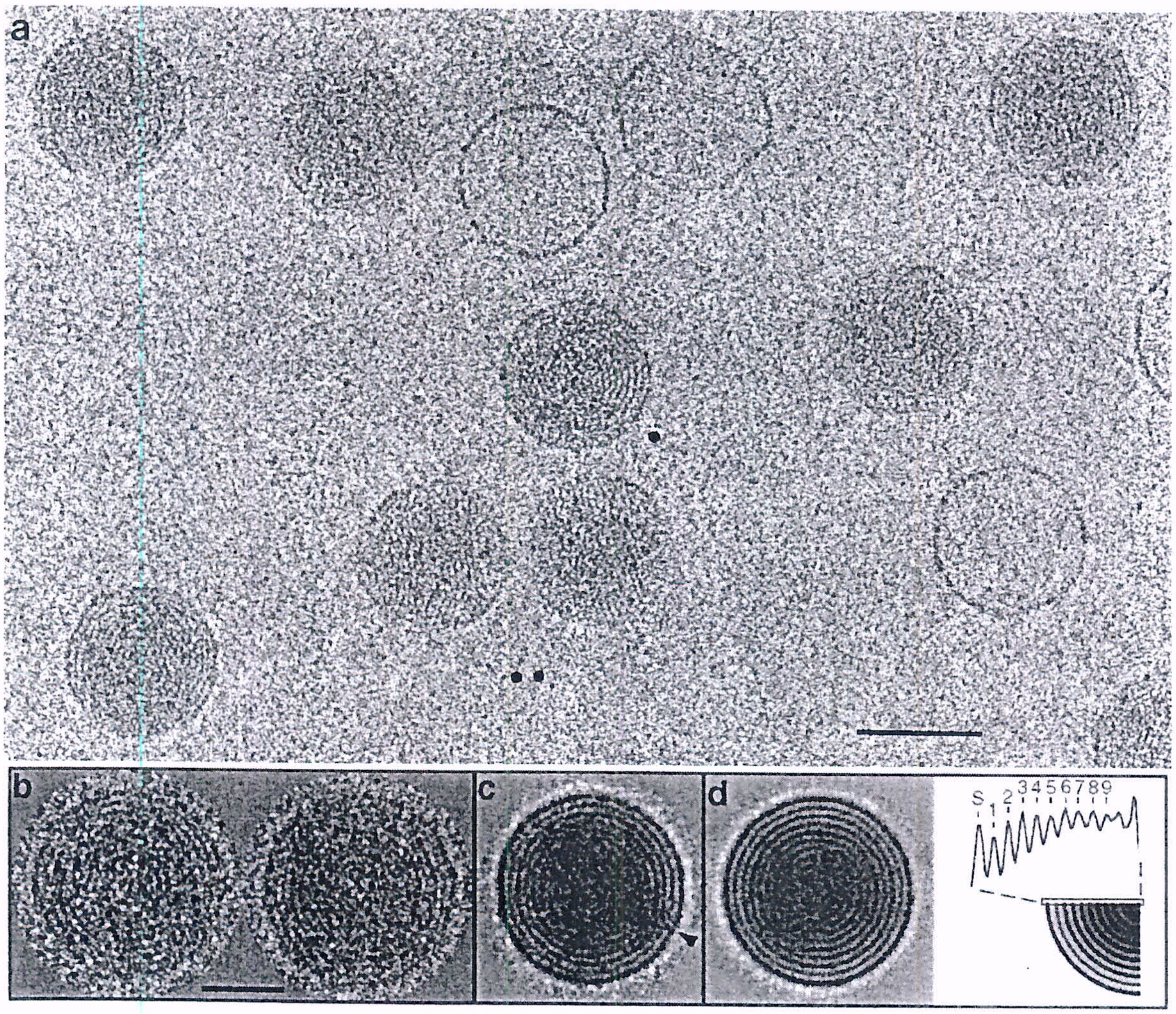


Figure 1. Cryo-electron Micrograph and Computer-Processed Images of T7 Heads from the Complete Tail-Deletion Mutant

(a) Cryo-electron micrograph of a field of bacteriophage T7 heads from the complete tail-deletion mutant. Empty capsids appear as thin-walled particles. Full capsids exhibit the characteristic 2.5 nm spacing of densely packed DNA duplexes in motifs that vary according to viewing direction (see Results). The concentric ring motif (e.g., particle indexed with a closed circle) is the view along the axis through the connector-core vertex and the center of the particle. Particles paired via their connector vertices present side views perpendicular to this axis (e.g., particles indexed with double closed circles). Bar = 50 nm.

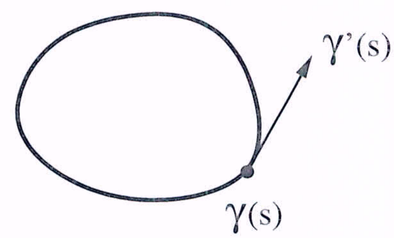
(b) Two examples of axial views, at higher magnification. Bar = 25 nm.

(c and d) Images obtained by averaging 21 and 77 particles, respectively. The closed triangle (c) marks the location of the discontinuity between the second and third DNA-associated rings. Also shown in (d) is a scan obtained by azimuthally averaging the accompanying image: it exhibits an outer dense ring (S) corresponding to the protein shell, then at least nine equally spaced DNA-associated rings.

Curves and tubular neighborhoods

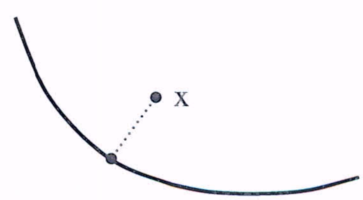
Curves $\gamma \in Q$

$$Q = \{\gamma \in C^1(S, \boldsymbol{R}^3) \mid \quad |\gamma'(s)| = 1, \quad s \in S \text{ (unit circ)}\}$$

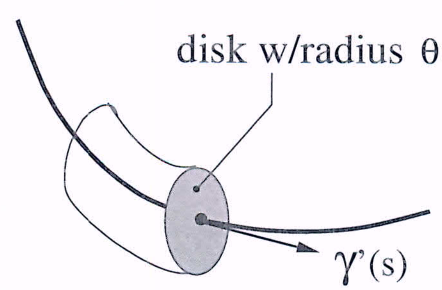


Tubular neighborhood $T_\theta(\gamma)$

$$T_\theta(\gamma) = \{\boldsymbol{x} \in \boldsymbol{R}^3 \mid \operatorname{dist}(\boldsymbol{x}, \gamma) < \theta\}$$

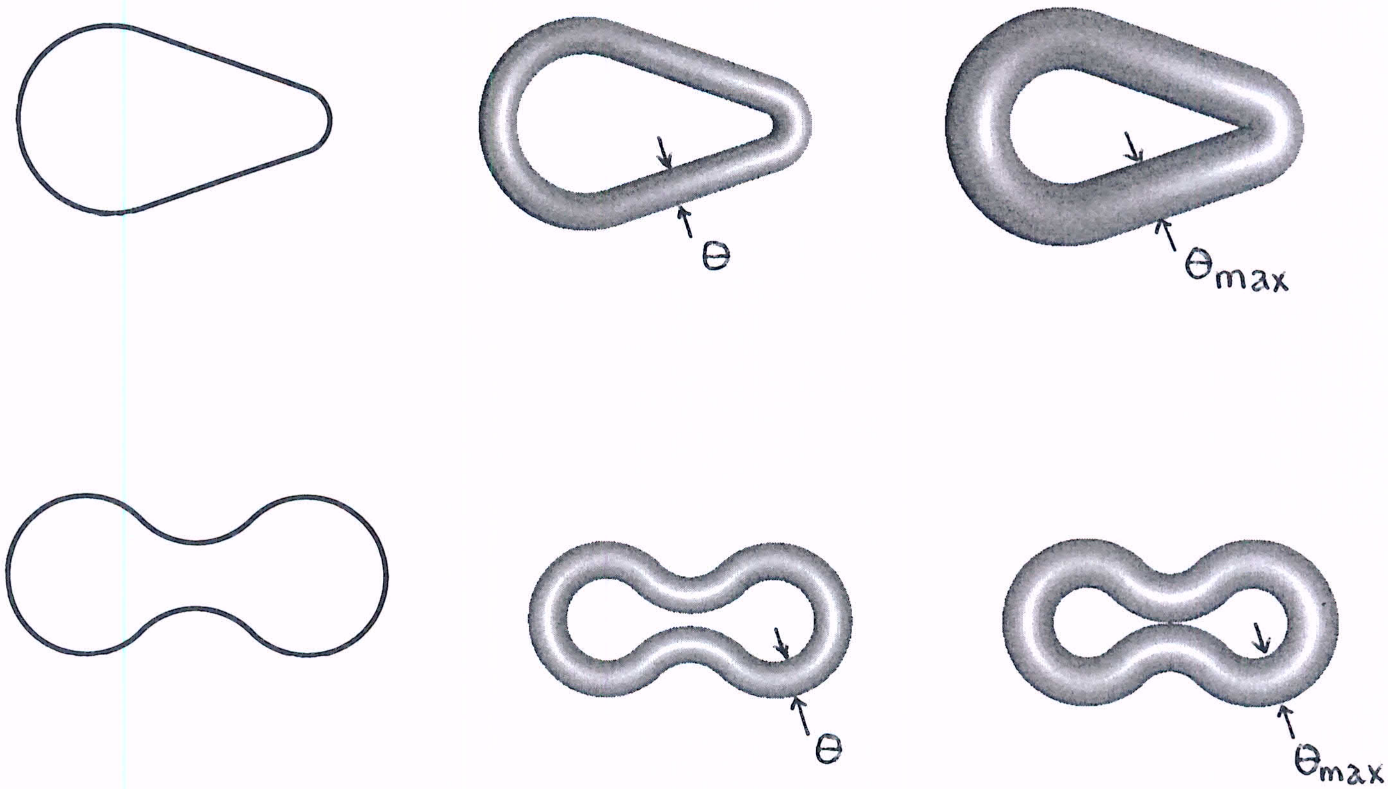


$$\gamma \in Q \quad \Rightarrow \quad T_\theta(\gamma) = \text{union of disks}$$



Curve thickness

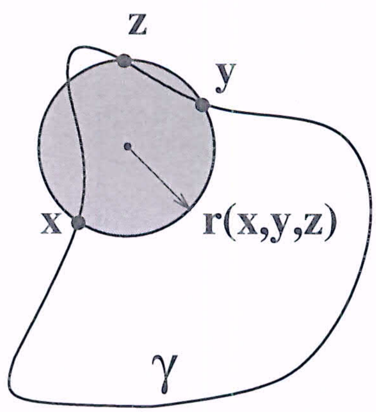
For each curve γ there is a maximum radius θ.



Given γ what is thickness $\theta_{\max}$?

Characterization of thickness

Circumradius function $r : \gamma \times \gamma \times \gamma \to R$



$$r(x, y, z) = \frac{|x - y||x - z||y - z|}{4A(x, y, z)}$$

Global (radius of) curvature $\rho_G : \gamma \to R$

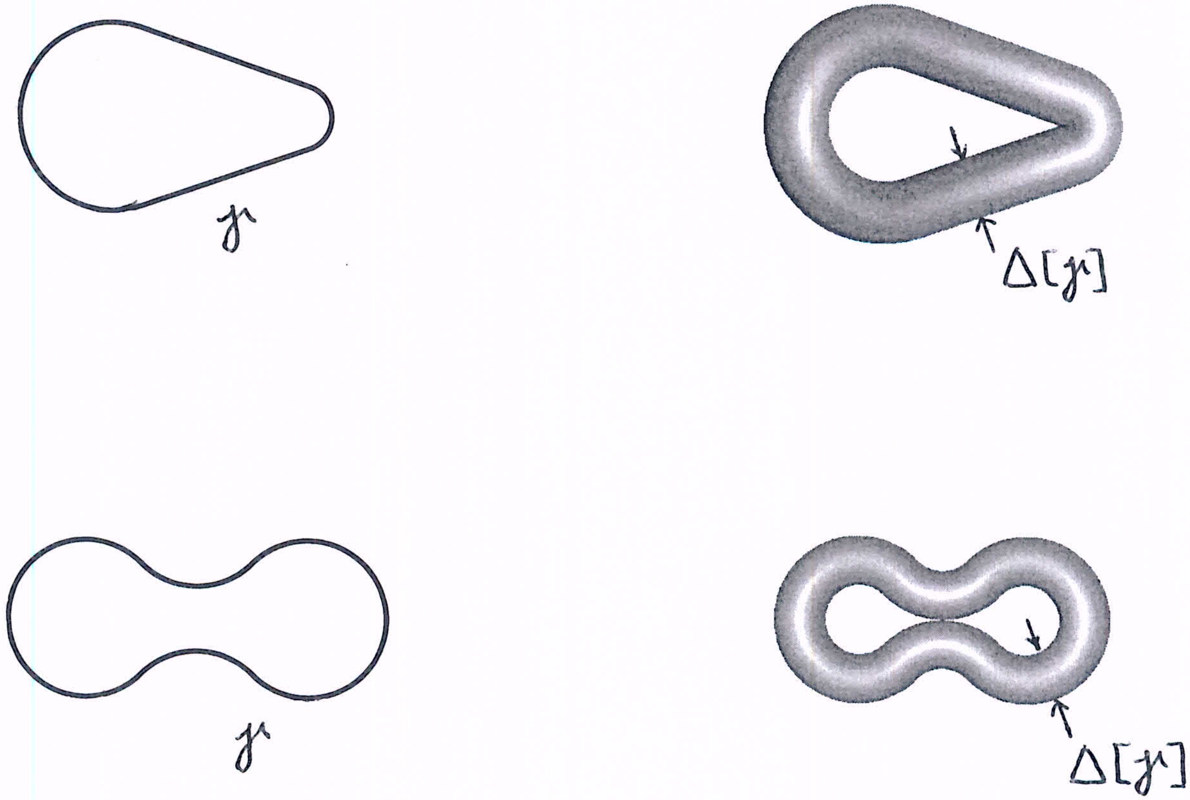
$$\rho_G(x) = \min_{y,z \in \gamma} r(x, y, z)$$

Thickness functional $\Delta : Q \to R$

$$\Delta[\gamma] = \min_{x \in \gamma} \rho_G(x)$$

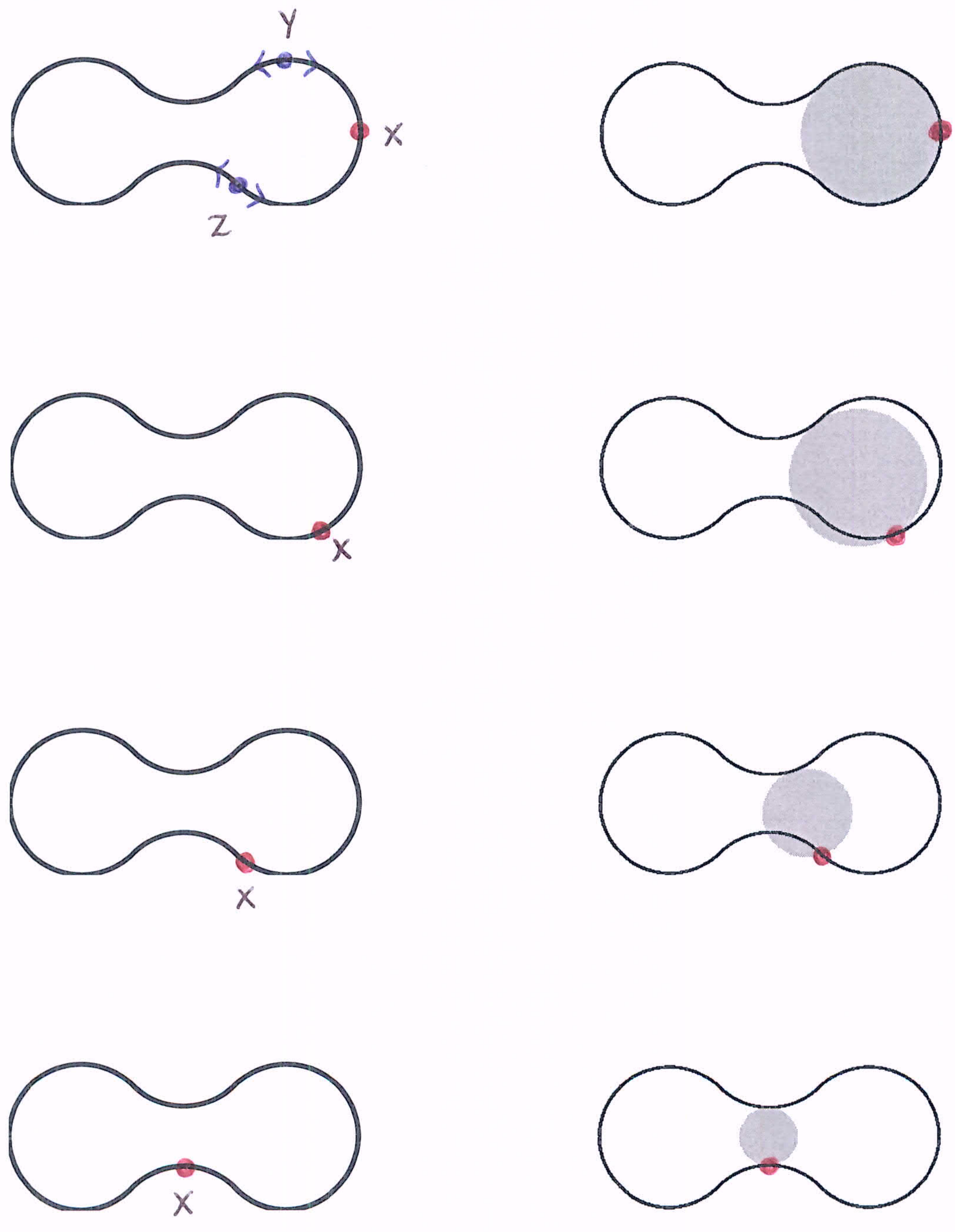
Fundamental result

$$\Delta[\gamma] := \min_{x \in \gamma} \rho_G(\boldsymbol{x}) = \theta_{\max}$$



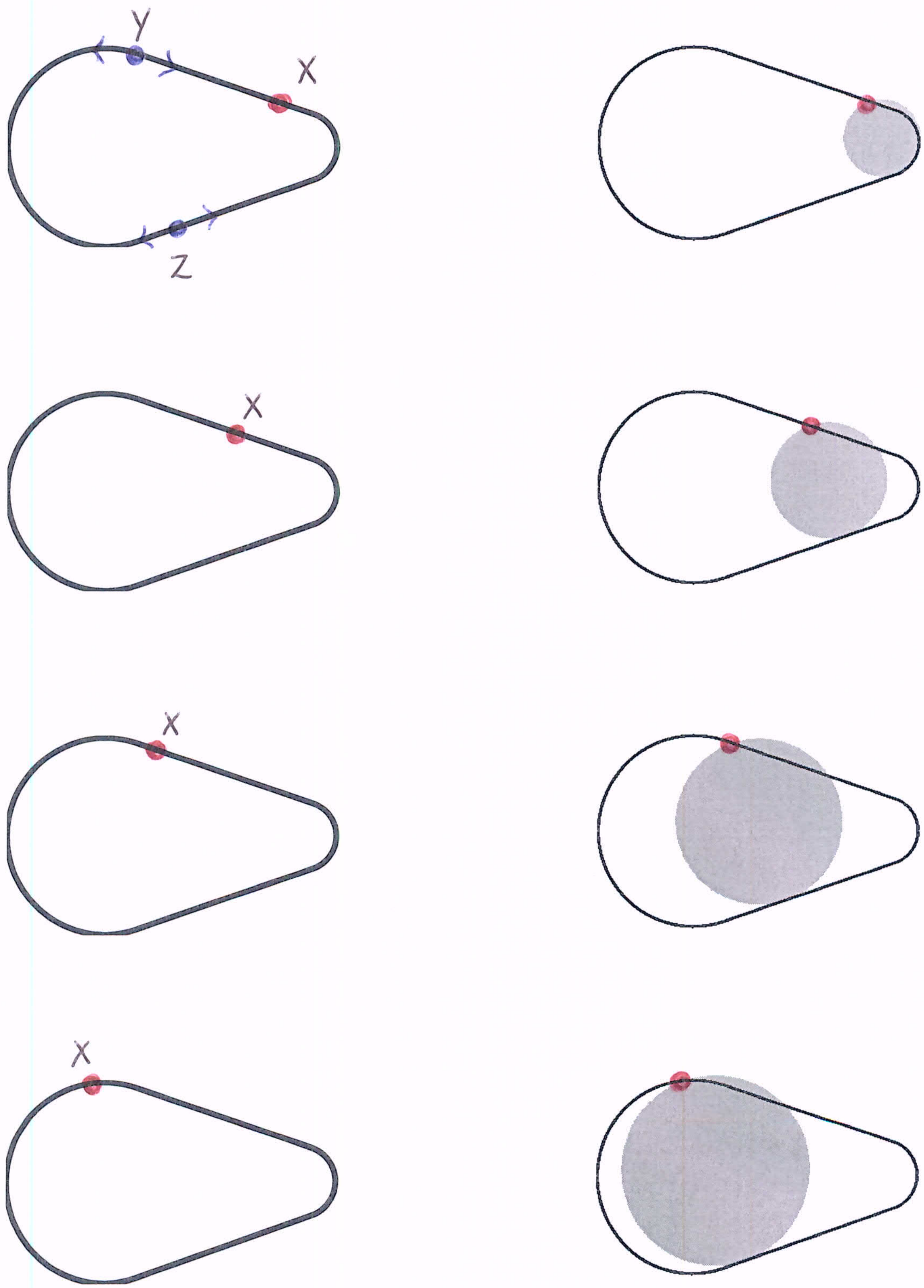
Example

$$\rho_G(\boldsymbol{x}) = \min_{\boldsymbol{y},\boldsymbol{z}\in\gamma} r(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$$



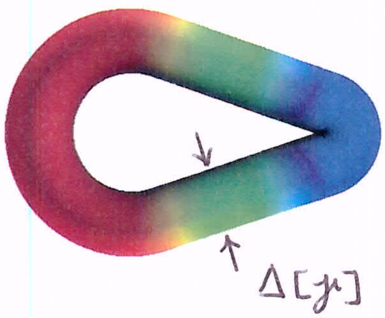
Example

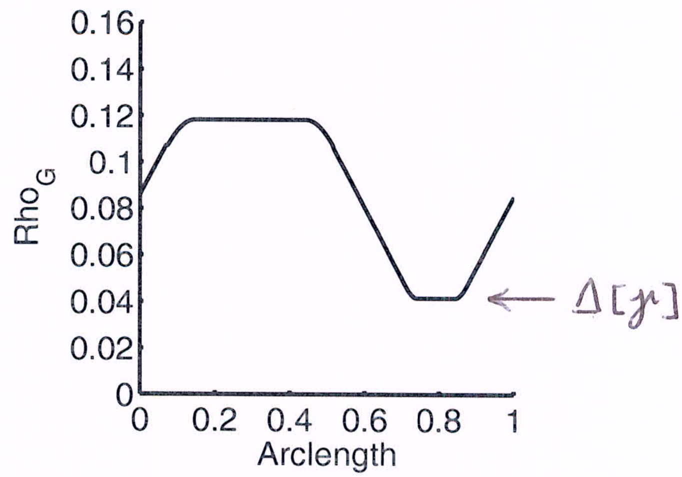
$$\rho_G(\boldsymbol{x}) = \min_{\boldsymbol{y},\boldsymbol{z}\in\gamma} r(\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})$$

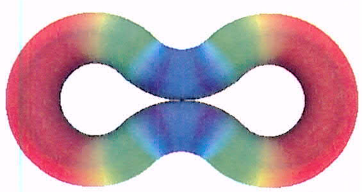


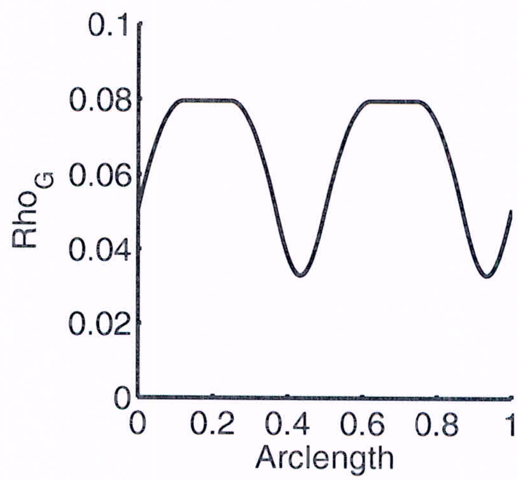
Example

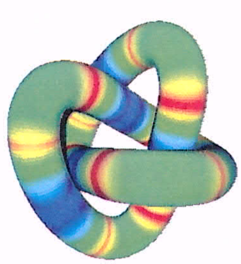
$$\Delta[\gamma] = \min_{x \in \gamma} \rho_G(x)$$

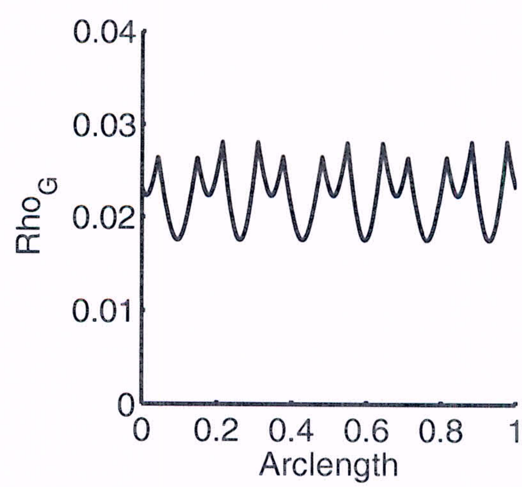












Ideal knots

Intuitive definition

$$\left.\begin{array}{l}\text{fix radius, knot type}\\ \\ \text{minimize length}\end{array}\right\} \quad \text{or} \quad \left\{\begin{array}{l}\text{fix length, knot type}\\ \\ \text{maximize radius}\end{array}\right.$$

Ideal knots

Variational definition

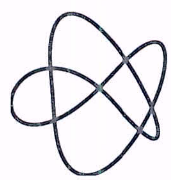
Consider curves with knot type specified by a given curve $\boldsymbol{k} \in Q$

$$Q_{\boldsymbol{k}} = \{\gamma \in Q \mid \quad \gamma \simeq \boldsymbol{k}, \quad \gamma(0) = 0\}.$$

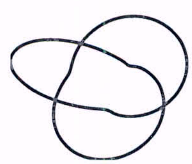
A curve $\gamma_* \in Q_{\boldsymbol{k}}$ is an ideal shape if

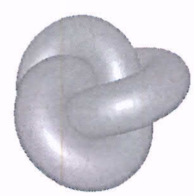
$$\Delta[\gamma_*] = \sup_{\gamma \in Q_{\boldsymbol{k}}} \Delta[\gamma].$$

$\boldsymbol{k}$:



γ_* :





Results for ideal knots

$$\Delta[\gamma_*] = \sup_{\gamma \in Q_k} \Delta[\gamma]$$

Existence/regularity

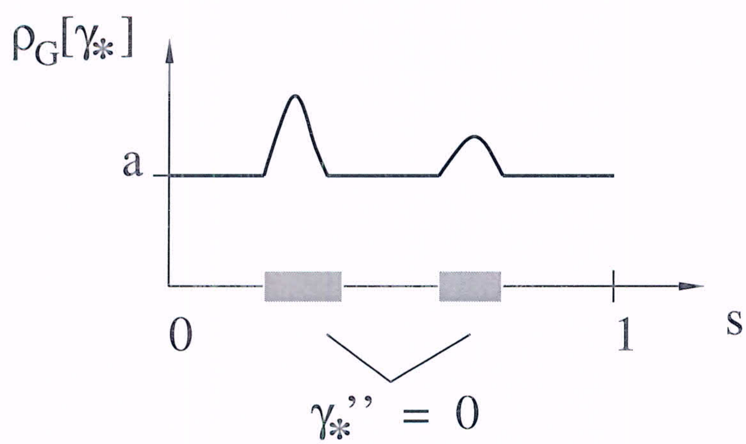
There is an ideal shape $\gamma_* \in Q_k$ for any given simple curve $k \in Q$. Every ideal shape is in the class $C^{1,1}(S, R^3)$.

Necessary condition

A smooth curve $\gamma_* \in Q_k$ can be ideal only if

$$\left.\begin{array}{ll} \rho_G[\gamma_*](s) = a, & \forall s : \gamma_*''(s) \neq 0 \\ \rho_G[\gamma_*](s) \geq a, & \forall s : \gamma_*''(s) = 0 \end{array}\right\}$$

where $a > 0$ is curve thickness.



Outline of existence/regularity proof

$$\Delta[\gamma_*] = \sup_{\gamma \in Q_k} \Delta[\gamma]$$

- $\Delta : Q_k \to R$ bounded.

$$\Delta[\gamma] \geq M \quad \Rightarrow \quad \text{diam}(\gamma) \geq 2M.$$

$$\therefore \quad \sup_{Q_k} \Delta < \infty.$$

- Maximizing sequence $\{\gamma_n\} \subset Q_k$ equicont/bdd in C^1.

$$\Delta[\gamma_n] \geq \theta > 0 \quad \Rightarrow \quad \begin{cases} |\gamma_n(s) - \gamma_n(\sigma)| \leq |s - \sigma| \\ |\gamma_n'(s) - \gamma_n'(\sigma)| \leq |s - \sigma|\theta^{-1}. \end{cases}$$

$$\therefore \quad \gamma_{n_j} \to \gamma_* \quad C^1.$$

- $\Delta : Q_k \to R$ upper semi-cont wrt/C^1 convergence.

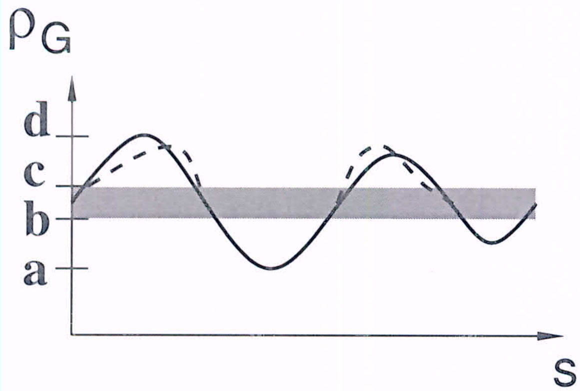
$$\Delta[\gamma_{n_j}] \to \sup_{Q_k} \Delta \leq \Delta[\gamma_*].$$

$$\therefore \quad \Delta[\gamma_*] = \sup_{Q_k} \Delta.$$

Outline of necessary condition proof

For contradiction suppose

- $\gamma_* \in Q_k$ ideal $\quad \Leftrightarrow \quad \Delta[\gamma_*] = \sup_{\gamma \in Q_k} \Delta[\gamma]$
- $\rho_G[\gamma_*]$ not constant
- $a = \min \rho_G[\gamma_*], \quad d = \max \rho_G[\gamma_*].$



$$F = \{s \in S \mid \rho_G[\gamma_*](s) > c\}$$

$$E = \{s \in S \mid \rho_G[\gamma_*](s) < b\}$$

Then

- curve shorten in F: $\quad \gamma_* \to \gamma_{**}, \quad L[\gamma_{**}] < L[\gamma_*]$
- "isolation" of E: $\quad \Delta[\gamma_{**}] = \Delta[\gamma_*]$
- rescale length to get $\gamma_{**} \in Q_k$ and $\Delta[\gamma_{**}] > \Delta[\gamma_*]$
- contradiction since $\Delta[\gamma_*] = \sup_{\gamma \in Q_k} \Delta[\gamma]$

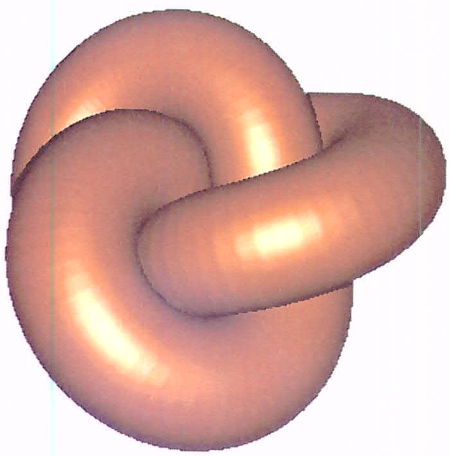
Note

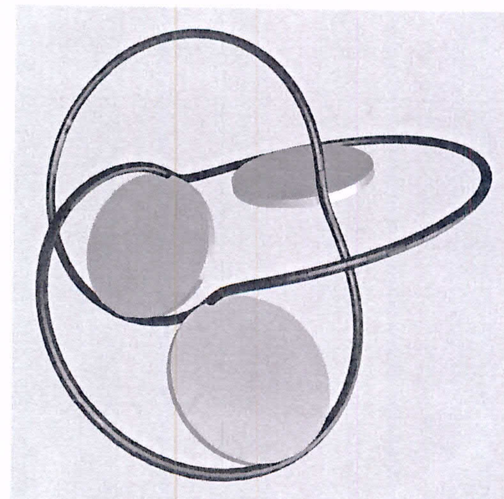
- curve shortening possible only if $\gamma_*'' \neq 0$ in F.

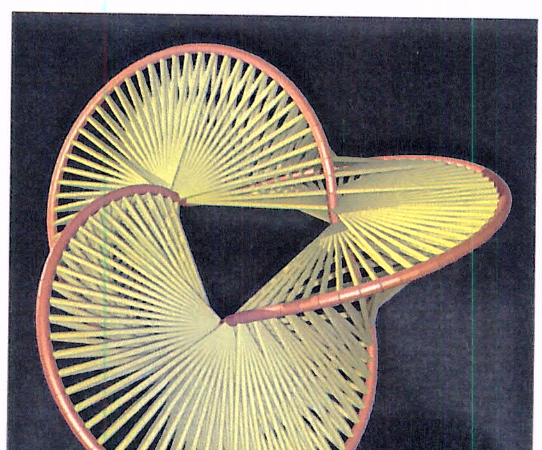
Ideal K31 Knot

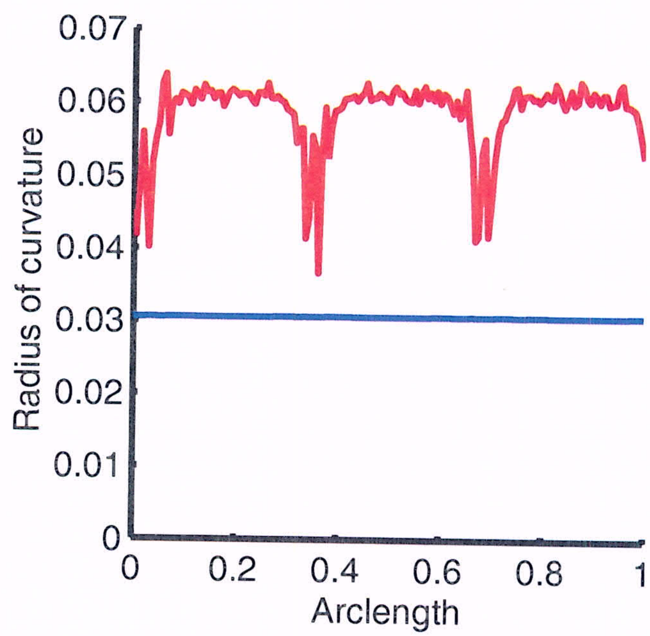
V. Katritch et. al., Nature 384 (1996) 142 – 145

original Monte Carlo data



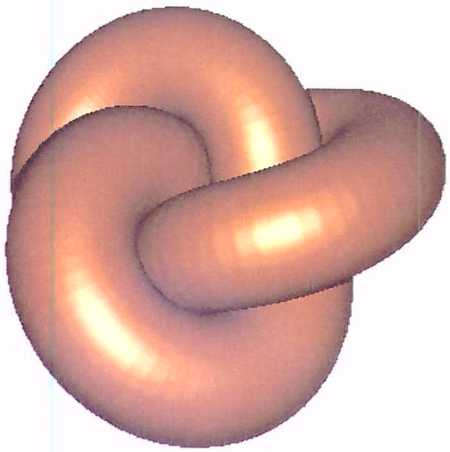


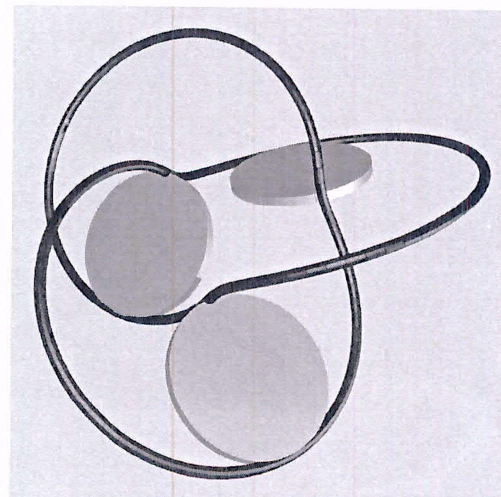


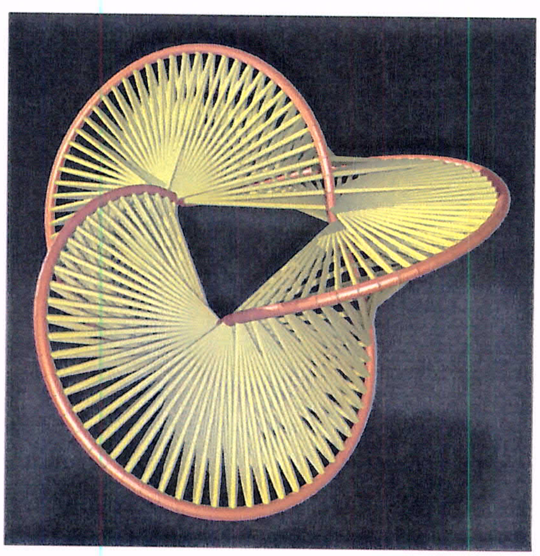


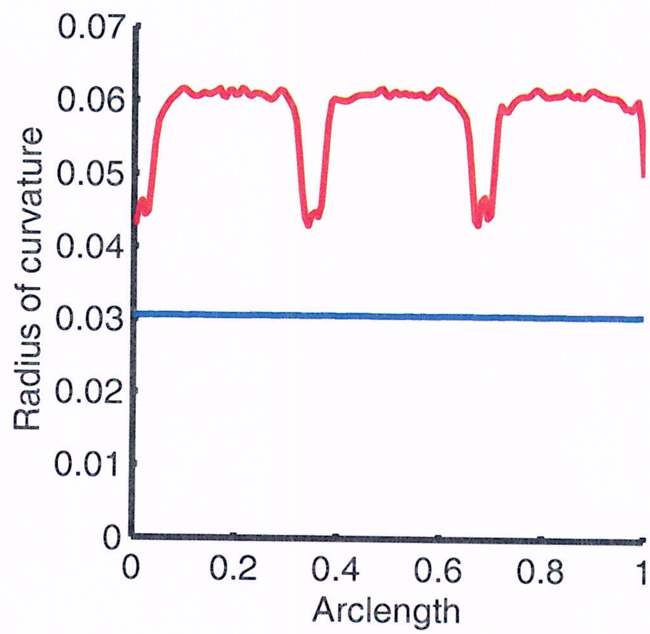
Ideal K31 Knot

smoothened data





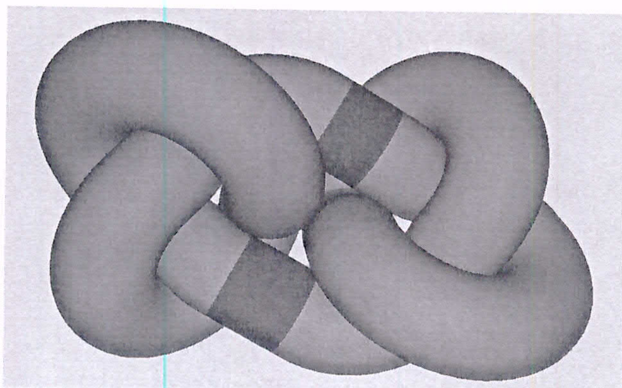


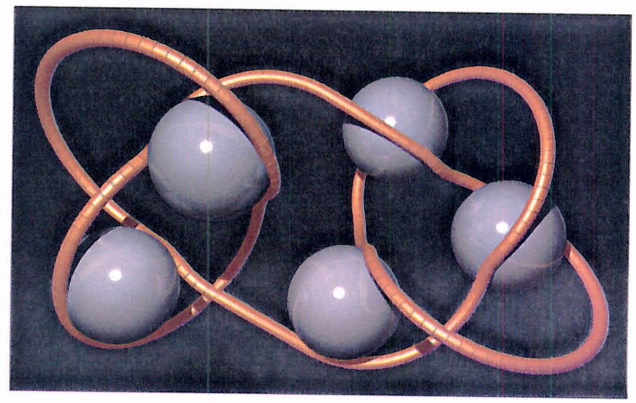


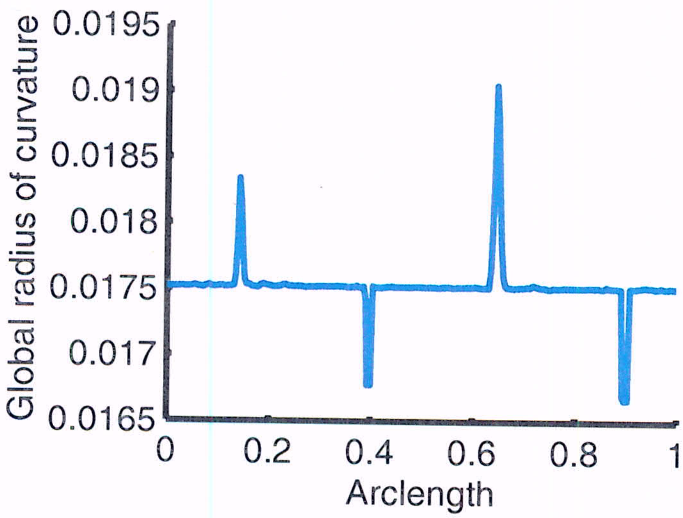
Ideal Composite P31P31 Knot

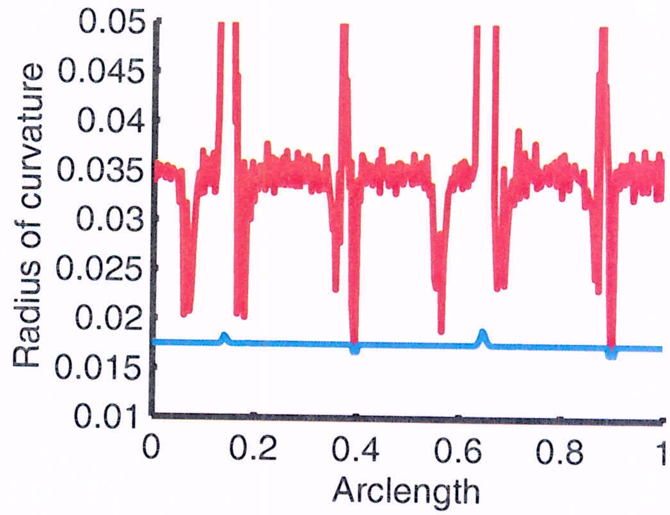
V. Katritch et. al., Nature 388 (1997) 148 – 151

original Monte Carlo data



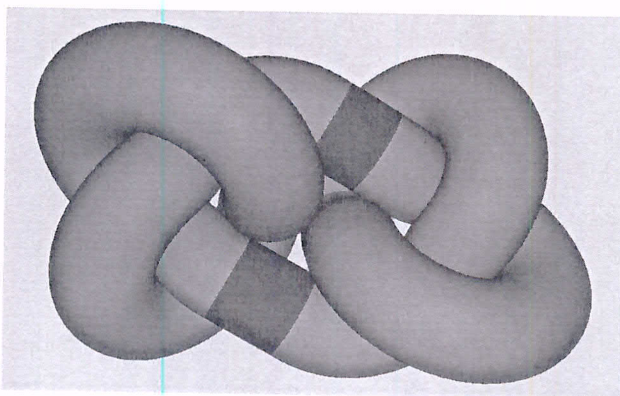


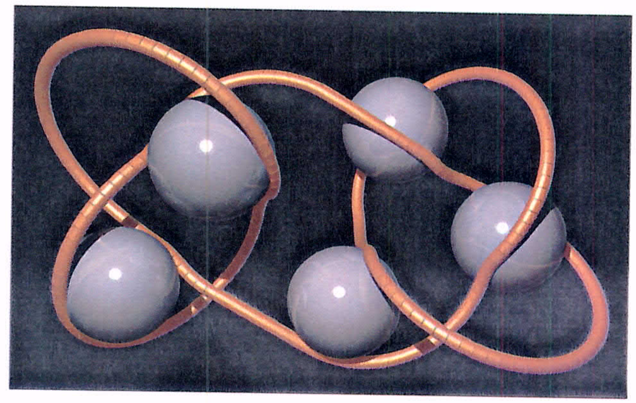


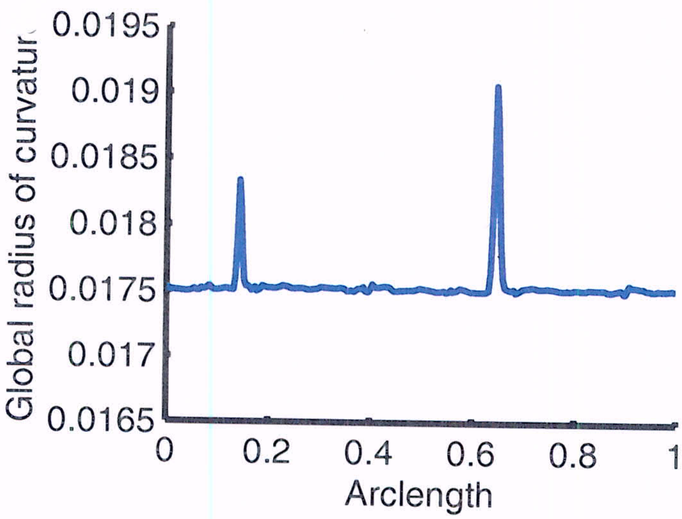


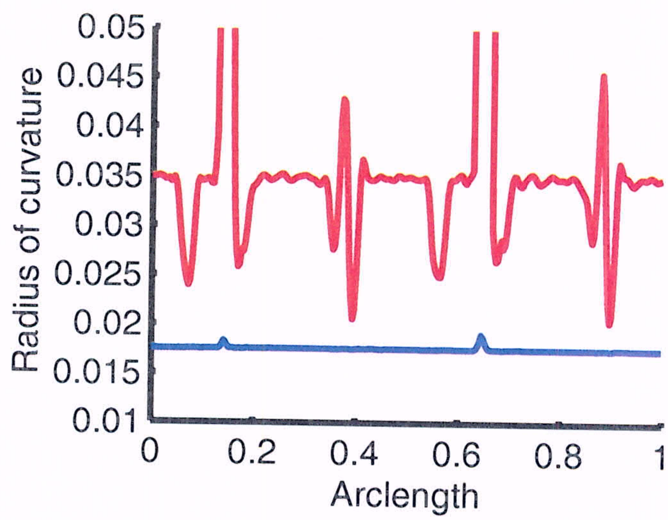
Ideal Composite P31P31 Knot

smoothened data







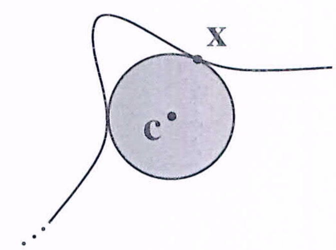


Local curvature on ideal knots

$$\Delta[\gamma_*] = \sup_{\gamma \in Q_k} \Delta[\gamma]$$

At each $x \in \gamma_*$ let

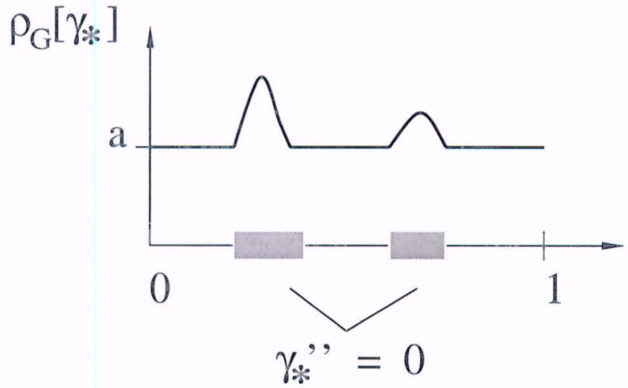
C_x = all centers c associated with $\rho_G(x)$

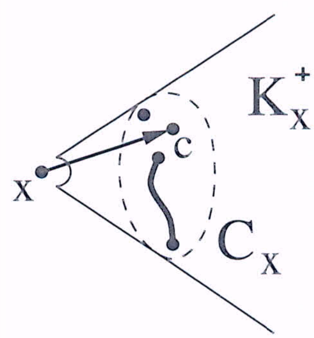


K_x^+ = positive cone defined by C_x.

Then a smooth curve $\gamma_* \in Q_k$ can be ideal only if

$$\left.\begin{array}{llll} \rho_G(x) = a, & \gamma_*''(x) \in K_x^+, & & \forall x : \gamma_*''(x) \neq 0 \\ \rho_G(x) \geq a, & & & \forall x : \gamma_*''(x) = 0 \end{array}\right\}$$

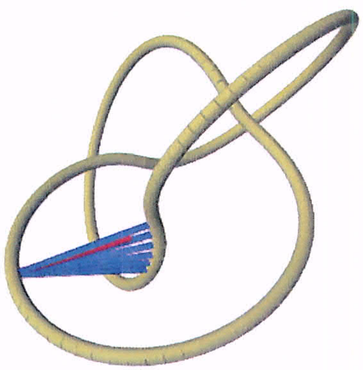


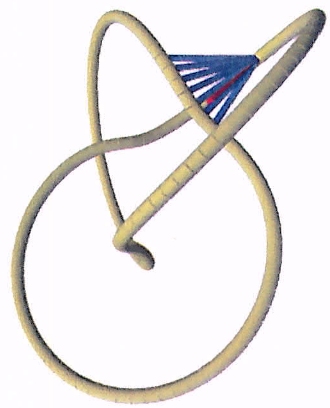


Proven for $C^{1,1}$ case by F. Schuricht and H. von der Mosel (2004)

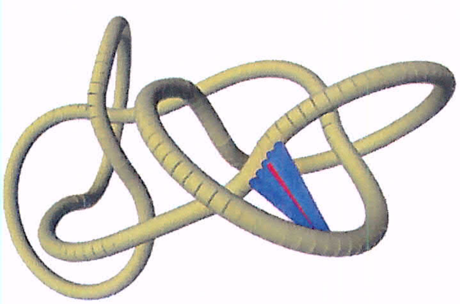
Local curvature on ideal knots

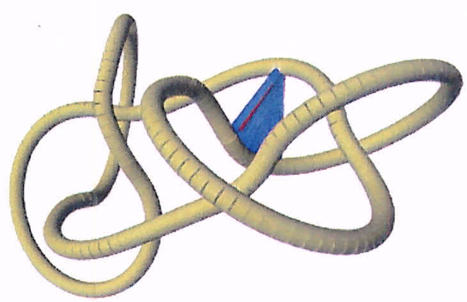
K31





P31P31

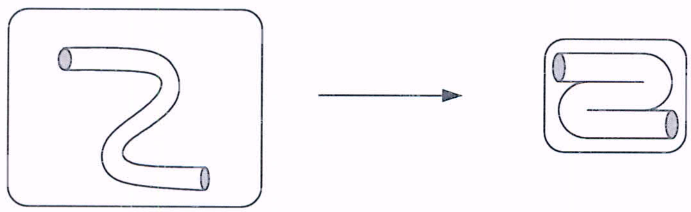




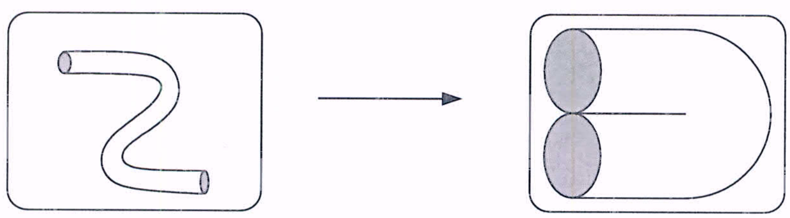
Optimal packing

Intuitive definitions

- fix tube radius, length, knot type
- minimize "packing energy"



- fix length, knot type, "box"
- maximize tube radius



Optimal packing problems

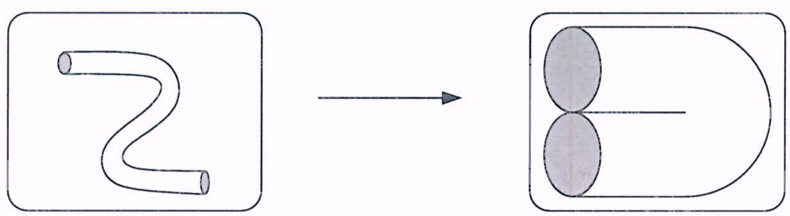
Variational definition

Consider

- packing functional $G[\gamma] = \mathrm{diam}(\gamma),\ \mathrm{rad\_of\_gyration}(\gamma), \ldots$
- knot representative $\boldsymbol{k} \in Q$
- admissible set $Q_{\boldsymbol{k},a} = \{\gamma \in Q \mid G[\gamma] \le a,\ \gamma \simeq \boldsymbol{k},\ \gamma(0) = 0\}.$

A curve $\gamma_* \in Q_{\boldsymbol{k},a}$ is an optimally packed shape if

$$\Delta[\gamma_*] = \sup_{\gamma \in Q_{\boldsymbol{k},a}} \Delta[\gamma].$$



Existence/regularity

If $G[\gamma]$ is lower semi-continuous in C^1, then there is an optimally packed shape $\gamma_* \in Q_{\boldsymbol{k},a}$ for any given simple curve $\boldsymbol{k} \in Q$. Every such shape is in the class $C^{1,1}(S, \boldsymbol{R}^3)$.

Outline of existence/regularity proof

$$\Delta[\gamma_*] = \sup_{\gamma \in Q_{k,a}} \Delta[\gamma]$$

- $\Delta : Q_{k,a} \to R$ bounded.

$$\Delta[\gamma] \geq M \quad \Rightarrow \quad \mathrm{diam}(\gamma) \geq 2M.$$

$$\therefore \quad \sup_{Q_{k,a}} \Delta < \infty.$$

- Maximizing sequence $\{\gamma_n\} \subset Q_{k,a}$ equicont/bdd in C^1.

$$\Delta[\gamma_n] \geq \theta > 0 \quad \Rightarrow \quad \begin{cases} |\gamma_n(s) - \gamma_n(\sigma)| \leq |s - \sigma| \\ |\gamma_n'(s) - \gamma_n'(\sigma)| \leq |s - \sigma|\theta^{-1}. \end{cases}$$

$$\therefore \quad \gamma_{n_j} \to \gamma_* \quad C^1.$$

- $G : Q \to R$ lower semi-cont wrt/C^1 convergence.

$$\therefore \quad G[\gamma_*] \leq a.$$

- $\Delta : Q_{k,a} \to R$ upper semi-cont wrt/C^1 convergence.

$$\Delta[\gamma_{n_j}] \to \sup_{Q_{k,a}} \Delta \leq \Delta[\gamma_*].$$

$$\therefore \quad \Delta[\gamma_*] = \sup_{Q_{k,a}} \Delta.$$

Optimal packing problems

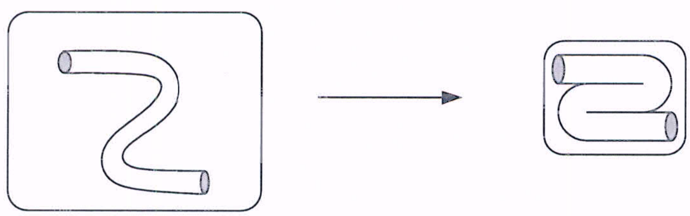
Variational definition

Consider

- packing functional $\quad G[\gamma] = \mathrm{diam}(\gamma),\ \mathrm{rad\_of\_gyration}(\gamma), \ldots$
- knot representative $\quad \boldsymbol{k} \in Q$
- admissible set $\quad Q_{\boldsymbol{k},a} = \{\gamma \in Q \mid \Delta[\gamma] \geq a,\ \gamma \simeq \boldsymbol{k},\ \gamma(0) = 0\}.$

A curve $\gamma_* \in Q_{\boldsymbol{k},a}$ is an optimally packed shape if

$$G[\gamma_*] = \inf_{\gamma \in Q_{\boldsymbol{k},a}} G[\gamma].$$



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Outline of existence/regularity proof

$$G[\gamma_*] = \inf_{\gamma \in Q_{k,a}} G[\gamma]$$

- Suppose $G : Q_{k,a} \to \boldsymbol{R}$ bounded from below.

$$\therefore \quad \inf_{Q_{k,a}} G \geq M.$$

- Minimizing sequence $\{\gamma_n\} \subset Q_{k,a}$ equicont/bdd in C^1.

$$\Delta[\gamma_n] \geq a > 0 \quad \Rightarrow \quad \begin{cases} |\gamma_n(s) - \gamma_n(\sigma)| \leq |s - \sigma| \\ |\gamma_n'(s) - \gamma_n'(\sigma)| \leq |s - \sigma| a^{-1}. \end{cases}$$

$$\therefore \quad \gamma_{n_j} \to \gamma_* \quad C^1.$$

- $\Delta : Q \to \boldsymbol{R}$ upper semi-cont wrt/C^1 convergence.

$$\therefore \quad \Delta[\gamma_*] \geq a.$$

- $G : Q_{k,a} \to \boldsymbol{R}$ lower semi-cont wrt/C^1 convergence.

$$G[\gamma_{n_j}] \to \inf_{Q_{k,a}} G \geq G[\gamma_*].$$

$$\therefore \quad G[\gamma_*] = \inf_{Q_{k,a}} G.$$

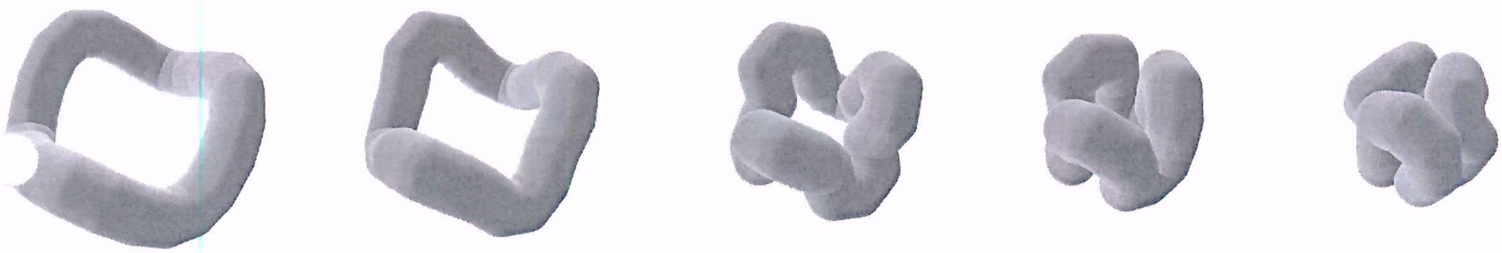
Numerical example

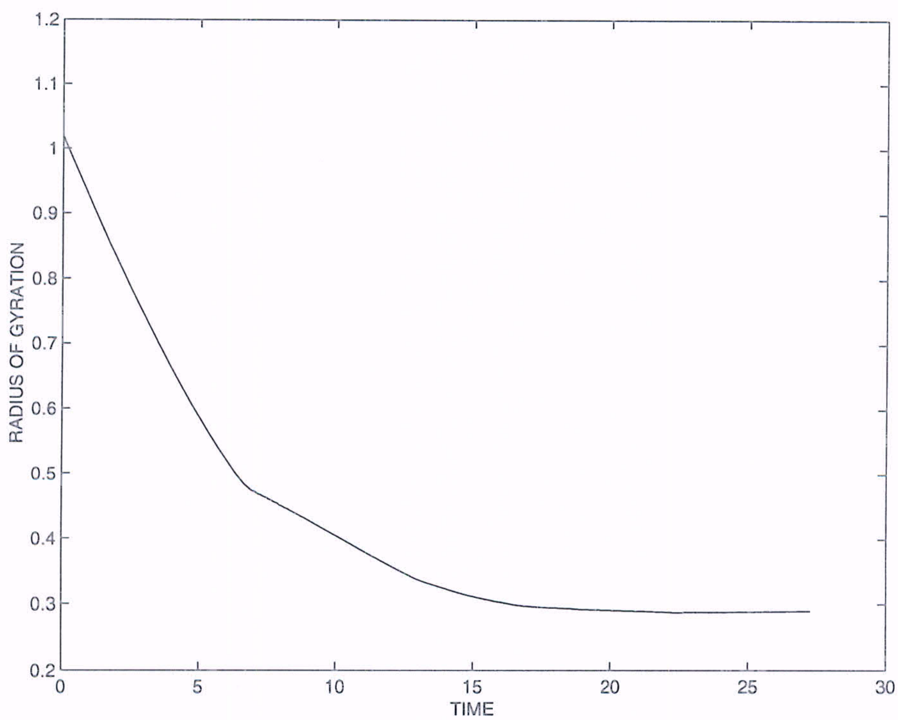
Optimal packing

Minimize radius of gyration $G[\gamma]$ subject to

- fixed center of mass: $\boldsymbol{c}[\gamma] = \mathbf{0}$ (for convenience).
- inextensibility: $|\gamma'| = 1$.
- lower bound on thickness: $\Delta[\gamma] \geq a$.

$$G[\gamma] = \frac{1}{L} \int_0^L |\gamma(s) - \boldsymbol{c}[\gamma]|^2 \, ds$$





Numerical scheme

Gradient flow approach

- interpret minimizers as fixed points of a gradient flow
- integrate the flow

$$\dot{\boldsymbol{r}} = -\nabla G(\boldsymbol{r}) + \sum_i \lambda_i \nabla E_i(\boldsymbol{r}) + \sum_a \mu_a \nabla I_a(\boldsymbol{r}) \qquad \text{grad flow}$$

$$0 = E_i(\boldsymbol{r}) \qquad \text{arcl, com}$$

$$0 \leq I_a(\boldsymbol{r}), \quad 0 \leq \mu_a, \quad 0 = \mu_a I_a(\boldsymbol{r}) \qquad \text{thickness}$$

Discretization

- space discretization: piecewise linear
- time discretization: fully implicit mid-point rule w/constraints

Concluding remarks

- Optimal packing of curves = interesting class of problems.
- Theory/analysis of problems is still in its infancy.
- Numerical analysis of problems is wide open.