Surface variations

Plan

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   ⊙ Helfrich's free-energy functionals for vecicle membranes
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3. General case. ⊙ perturbations.
   ⊙ $\delta_\Gamma \int_\Gamma f(x)\,dS_x$.
   ⊙ $\delta_\Gamma \int_\Gamma H(x)\,dS_x$.
   ⊙ Other formulas.
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1. Introduction

Hadwiger's Theorem (for $\mathbb{R}^3$)

Let C denote the ~~class~~ set of all convex and compact subsets of $\mathbb{R}^3$.

Let M denote the set of all finite unions of convex and compact subsets of $\mathbb{R}^3$.

Let $F: M \to \mathbb{R}$ ~~be such~~ satisfy the following conditions:

(1) F is translationally and rotationally invariant:

$$F(S+a) = F(S) \quad \forall S \in M, \ \forall a \in \mathbb{R}^3$$
$$F(RS) = F(S) \quad \forall S \in M, \ \forall R \in SO(3).$$

[$SO(3)$ = the set of all proper rotations in $\mathbb{R}^3$].

(2) $F(U \cup V) = F(U) + F(V) - F(U \cap V)$ $\forall U, V \in M$.

(3) $F(U_k) \to F(U)$ as $k \to \infty$ if $U_k, U \in C$ $(k = 1, 2, \cdots)$ and $U_k \to U$ w.r.t. the Hausdorff distance.

Then $\exists a_1, \cdots, a_4 \in \mathbb{R}$ such that

(*)
$$F(U) = a_1 \mathrm{Vol}(U) + a_2 \mathrm{Area}(\partial U) + a_3 \int_{\partial U} H\, dS + a_4 \int_{\partial U} K\, dS, \quad \forall U \in M$$

where H and K denote the mean and Gaussian curvatures, respectively.

Note: The Hausdorff distance between two sets A and B is defined by

$$d_H(A, B) = \max\left\{ \sup_{a \in A} d(a, B), \sup_{b \in B} d(b, A) \right\}$$

Here, $d(\cdot, \cdot)$ is the metric of some metric space.

Scales. Let $U = B(0, R) \subset \mathbb{R}^3$ be the ball of radius $R > 0$ centered at 0. Then

the mean curvature: $H = \frac{1}{R}$ at ∂U.

the Gaussian curvature: $K = \frac{1}{R^2}$ at ∂U.

The 4 terms in (*) are:

$$\mathrm{vol}(U) = \frac{4}{3}\pi R^3$$

$$\mathrm{Area}(\partial U) = 4\pi R^2$$

$$\int_{\partial U} H\, dS = 4\pi R$$

$$\int_{\partial U} K\, dS = 4\pi \quad \text{(indep. of } R\text{)}.$$

<u>Questions</u> How to define and calculate the variations $\delta_\Gamma E[\Gamma]$, ~~where~~ with respect to the (locally) location change of $\Gamma = \partial U$? Here $E[\Gamma] = E[\partial U]$ can be any term in the Hadwiger functional F.

The Helfrich free-energy functional

$$F = \frac{1}{2} k_c \oint (c_1 + c_2 - c_0)^2 dA + \Delta p \int dV + \lambda \oint dA$$

k_c = a const. ... bending rigidity

c_1, c_2 = the two principal curvatures

$c_1 + c_2 = 2H$ with H being the mean curvature

c_0 .... spontaneous curvature, describing the asymmetry of a membrane or its environment.

$\Delta p = p_{out} - p_{in}$ ... pressure difference, a Lagrange multiplier.

λ ... tensile stress, serving as a Lagrange multiplier

The first term is the curvature-elastic energy of the vesicle membrane. The second and third terms ~~are~~ describe the constant-volume and constant-surface area constraints, or can be viewed as actual work.

Again, we ask how to define and calculate the variation of this energy functional with respect to the location change of the membrane surface.

2. Special cases

The case of a graph. $z = h(x, y)$.

Recall:

the mean curvature is:

$$H = \frac{1}{2(1+h_x^2+h_y^2)^{3/2}}\left[h_{xx}(1+h_y^2) + h_{yy}(1+h_x^2) - 2h_x h_y h_{xy}\right].$$

the Gaussian curvature is:

$$K = \frac{h_{xx}h_{yy} - h_{xy}^2}{(1+h_x^2+h_y^2)^2}.$$

Write $H = H(h)$, $K = K(h)$.

Consider a bounded, nice region $D \subset \mathbb{R}^2$. Assume $h: D \to \mathbb{R}$ is smooth. Let Γ denote the surface $\Gamma = \{(x, y, h(x,y)) \mid (x,y) \in D\}$. Define

$$E[h] = \int_\Gamma dS = \int_D \sqrt{1+h_x^2+h_y^2}\, dx\,dy$$

Let $\varphi \in C_c^\infty(D)$.

$$\frac{d}{dt}\Big|_{t=0} E[h+t\varphi] = \frac{d}{dt}\Big|_{t=0} \int_D \sqrt{1+(h_x+t\varphi_x)^2+(h_y+t\varphi_y)^2}\, dx\,dy$$

$\nabla = \begin{pmatrix}\partial_x \\ \partial_y\end{pmatrix}$.

$$= \int_D \frac{1}{\sqrt{1+|\nabla h|^2}} \nabla h \cdot \nabla \varphi \, dx\,dy$$

$$= -\int_D \nabla \cdot \left(\frac{\nabla h}{\sqrt{1+|\nabla h|^2}}\right) \varphi \, dx\,dy.$$

students: ~~check it!~~

~~Let (formally)~~ $\boxed{\delta E[h] = -\nabla\cdot\left(\frac{\nabla h}{\sqrt{1+|\nabla h|^2}}\right) = -2H(h)}$

$$\cancel{= -\int_\Gamma \nabla\cdot\left(\frac{\nabla h}{\sqrt{1+|\nabla h|^2}}\right)\frac{1}{\sqrt{1+|\nabla h|^2}}\varphi\, dS}$$

$$\delta E[h] = -2H(h).$$

Let $\hat{E}[h] = \int_{\Gamma} H\, dS = \int_{D} \frac{1}{2} \nabla \cdot \left(\frac{\nabla h}{\sqrt{1+|\nabla h|^2}} \right) \sqrt{1+|\nabla h|^2}\, dx dy$.

$\forall \varphi \in C_c^\infty(D)$.

$$\delta \hat{E}[h][\varphi] \equiv \frac{d}{dt}\Big|_{t=0} \hat{E}[h+t\varphi]$$

$$= \frac{d}{dt}\Big|_{t=0} \int_{D} \frac{1}{2} \nabla \cdot \left(\frac{\nabla h + t\nabla \varphi}{\sqrt{1+|\nabla h + t\nabla\varphi|^2}} \right) \sqrt{1+|\nabla h + t\nabla \varphi|^2}\, dx dy$$

This calculation is more tedious. There will be more than 100 terms. One can use Matlab or Mathematica (symbolic computation) to carry out this calculation. The result is

$$\delta \hat{E}[h][\varphi] = -\int_{D} \frac{u_{xx}u_{yy} - u_{xy}^2}{(1+h_x^2+h_y^2)^{5/2}} \varphi\, dx dy$$

$$= -\int_{\Gamma} K \varphi\, dS.$$

Hence, $\delta \int_{\Gamma} H\, dS = -K$ on Γ.

We can obtain the same result for general cases where surface is not necessary represented by a graph of a function.

The notes on general cases will not be presented now – due to the lack of time to prepare and write them. I will try to add them later. Just one remark: for second variations, different perturbations may lead to different results. So, be careful when reading a paper about these.

Consider now

$$\hat{E}[h] = \int_\Gamma H\,dS = \int_D \frac{1}{2}\nabla\cdot\left(\frac{\nabla h}{\sqrt{1+|\nabla h|^2}}\right)\sqrt{1+|\nabla h|^2}\,dx\,dy.$$

$\forall \varphi \in C_c^\infty(D)$:

$$\delta\hat{E}[h][\varphi] = \frac{d}{dt}\Big|_{t=0} \hat{E}[h+t\varphi]$$

$$= \frac{d}{dt}\Big|_{t=0} \int_D \frac{1}{2}\nabla\cdot\left(\frac{\nabla h + t\nabla\varphi}{\sqrt{1+|\nabla h + t\nabla\varphi|^2}}\right)\sqrt{1+|\nabla h + t\nabla\varphi|^2}\,dx\,dy$$

Taylor expand the integrand w.r.t. t.

$$= \frac{1}{2}\nabla\cdot\left[(\nabla h + t\nabla\varphi)(1+|\nabla h|^2 + 2t\,\nabla h\cdot\nabla\varphi)^{-\frac{1}{2}}\right]\cdot(1+|\nabla h|^2 + 2t\,\nabla h\cdot\nabla\varphi)^{\frac{1}{2}} + O(t^2)$$

$$= \frac{1}{2}\nabla\cdot\left[\frac{\nabla h + t\nabla\varphi}{\sqrt{1+|\nabla h|^2}}\left(1+\frac{2t\,\nabla h\cdot\nabla\varphi}{1+|\nabla h|^2}\right)^{-\frac{1}{2}}\right]\cdot\sqrt{1+|\nabla h|^2}\left(1+\frac{2t\,\nabla h\cdot\nabla\varphi}{1+|\nabla h|^2}\right)^{\frac{1}{2}} + O(t^2)$$

$$= \frac{1}{2}\nabla\cdot\left[\frac{\nabla h + t\nabla\varphi}{\sqrt{1+|\nabla h|^2}}\left(1 - t\frac{\nabla h\cdot\nabla\varphi}{1+|\nabla h|^2}\right)\right]\cdot\sqrt{1+|\nabla h|^2}\left(1 + t\frac{\nabla h\cdot\nabla\varphi}{1+|\nabla h|^2}\right) + O(t^2)$$

$$= \frac{1}{2}\nabla\cdot\left[\frac{\nabla h + t\nabla\varphi}{\sqrt{1+|\nabla h|^2}} - \frac{(\nabla h\cdot\nabla\varphi)\nabla h}{\sqrt{1+|\nabla h|^2}^{\,3}}\right]\cdot\left(\sqrt{1+|\nabla h|^2} + t\frac{\nabla h\cdot\nabla\varphi}{\sqrt{1+|\nabla h|^2}}\right) + O(t^2)$$

$$= \frac{1}{2}\left[\nabla\cdot\left(\frac{\nabla h}{\sqrt{1+|\nabla h|^2}}\right) + t\,\nabla\cdot\left(\frac{\nabla\varphi}{\sqrt{1+|\nabla h|^2}}\right) - \nabla\cdot\frac{(\nabla h\cdot\nabla\varphi)\nabla h}{(1+|\nabla h|^2)^{3/2}}\right]\cdot\left(\sqrt{1+|\nabla h|^2} + t\frac{\nabla h\cdot\nabla\varphi}{\sqrt{1+|\nabla h|^2}}\right) + O(t^2)$$

$$= \frac{1}{2}[\cdots]t^0 + \frac{1}{2}[\cdots]t + O(t^2).$$

only need this term

$$= \frac{1}{2}t\left[\nabla\cdot\left(\frac{\nabla h}{\sqrt{1+|\nabla h|^2}}\right)\cdot\frac{\nabla h\cdot\nabla\varphi}{\sqrt{1+|\nabla h|^2}} + \nabla\cdot\left(\frac{\nabla\varphi}{\sqrt{1+|\nabla h|^2}}\right)\sqrt{1+|\nabla h|^2}\right.$$