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SEMIDIFFERENTIAL TOPOLOGY AND THE ROPELENGTH PROBLEM

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1. INTRODUCTION

Part of the fascination of the ropelength problem is due to the mathematically nonstandard nature of the thickness constraint. This places the problem outside the domain of the classical calculus of variations, which might be described as the the method of Lagrange multipliers applied in an infinite-dimensional setting. The purpose of these notes is to describe a rather simple finite-dimensional analytic context that would supply a similar analogy for the ropelength problem, or more generally for any minimization problem for space curves with a thickness constraint.

The analogy is based on the observation, due to Gonzalez and Maddocks, that the thickness of a space curve may be expressed as the infimum of a suitably bounded family of smooth functions (the radii of circles passing through triples of points) on the space of curves. When this occurs in the finite-dimensional setting, -1 times such a function is **semiconvex** (see below for definitions). It turns out that such functions may be thought of as being essentially as smooth as C^2 functions, provided one is prepared to replace the linear algebra associated with tangent spaces and derivative maps with linear programming. (This is basically the idea of "convex analysis").

Before launching into the mathematics, here is a brief dictionary giving the correspondence between concepts in the smooth and semiconvex realms.

Smooth world	**Semiconvex world**
C^2 function	semiconvex function
C^2 submanifold	subset with locally positive reach
vector space	closed convex cone
linear function	sublinear function
gradient vector ∇f	closed convex set $\{\nabla\} f$ of subgradients
$\nabla f = 0$	$0 \in \{\nabla\} f$
level set $f^{-1}(0)$	sublevel set $f^{-1}(-\infty, 0]$
continuous vector field	upper semicontinuous field of closed convex sets
Lipschitz vector field	quasi-monotone field of closed convex sets
gradient flow (defined for all time)	gradient semiflow (defined for negative time)

2. BASIC DEFINITIONS

A set $S \subset \mathbb{R}^n$ is said to have **locally positive reach** if there exists a neighborhood U of S such that, whenever $x \in U$, there is a *unique* point $p \in S$ realizing the distance from x to S. In other words, $\overline{B}(x, \operatorname{dist}(x, S)) \cap S$ is a singleton for $x \in U$. Obviously a set with locally positive reach is locally closed. The most important

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examples are the closed convex sets, for which U can be taken to be the entire ambient space $\mathbb{R}^n$.

Associated to every point $x \in S$ are the **tangent cone**

$$(1)\quad \operatorname{Tan}_x S := \{v \in \mathbb{R}^n : v = \lim \frac{x_i - x}{|x_i - x|} \text{ for some sequence } S \ni x_1, x_2, \cdots \to x\}$$

and the **normal cone**

$$(2)\qquad \operatorname{Nor}_x S := (\operatorname{Tan}_x S)^* := \{w \in \mathbb{R}^n : w \cdot v \leq 0 \text{ for all } v \in \operatorname{Tan}_x S\}.$$

If S has locally positive reach, then $\operatorname{Tan}_x S$ is a closed convex cone. Thus by convex duality

$$(3)\qquad \operatorname{Tan}_x S = ((\operatorname{Tan}_x S)^*)^* = (\operatorname{Nor}_x S)^*.$$

In many respects such sets are geometrically just as nice as C^2 submanifolds or domains with C^2 boundary. Just as these more standard objects may be thought of as the geometric counterpart of the class of C^2 functions, the class of sets with locally positive reach has a certain class of functions as a natural counterpart. These are the **locally semiconvex** functions: a function $f : U \to \mathbb{R}$ is locally semiconvex if every point $x \in U$ admits a neighborhood $V_x \subset U$ such that the restriction $f|V_x$ may be decomposed as a sum $g + h$ of a smooth function g and a convex function h.

Such functions are very common. For instance, if $S \subset \mathbb{R}^n$ is closed and nonempty then the function $-\operatorname{dist}(S, \cdot)$ is semiconvex when restricted to the complement of S. More generally, if $\mathcal{F}$ is a family of $C^{1,1}$ functions on U such that

$$D^2 f|K \geq C_K, |Df||K \leq C_K, f|K \geq -C_K$$

for every compact set $K \subset U$ and every $f \in \mathcal{F}$, then $\sup_{\mathcal{F}} f$ is semiconvex. (To put the distance function in this context, let $\mathcal{F}$ be the family of distance functions from the points of S.) This is why we may think of the thickness of a knot as -1 times a semiconvex function on the space of $C^{1,1}$ knots.

3. CALCULUS OF SEMI-CONVEX FUNCTIONS

Just as differentiable manifolds and functions are locally modelled on vector spaces and linear maps, the sets and functions above are locally modelled on closed convex sets and **sublinear** functions, i.e. convex functions $\alpha : \mathbb{R}^n \to \mathbb{R}$ that are positively homogeneous of degree 1:

$$\begin{aligned} (4)\qquad \alpha(tx) &= t\alpha(x) \text{ for } t \geq 0 \\ (5)\qquad \alpha(tx + (1-t)y) &\geq t\alpha(x) + (1-t)\alpha(y) \text{ for } 0 \leq t \leq 1. \end{aligned}$$

Note that if α is such a function then

$$(6)\qquad K_\alpha := \{v : v \cdot x \leq \alpha(x) \text{ for all } x \in \mathbb{R}^n\}$$

is closed and convex, and

$$(7)\qquad \alpha(x) = \sup\{v \cdot x : v \in K_\alpha\}.$$

Let $f : U \to \mathbb{R}$ be a semiconvex function. For every point $x \in U$ and every vector $v \in \mathbb{R}^n$, the directional derivative

$$D_x f(v) := \lim_{t \downarrow 0} t^{-1}(f(x + tv) - f(x))$$

exists. In fact the map $D_x f$ is sublinear. The closed convex set $\{\nabla\}_x f := K_{D_x f}$, defined as in (6), is called the **subgradient** of f. The relation (7) translates into the important formula

$$D_x f(v) = \sup\{v \cdot x : v \in \{\nabla\}_x f\} \tag{8}$$

The subgradient field has the following properties:

- It is **upper semicontinuous**, i.e. if $x_1, x_2, \cdots \to x_0$ and $v_i \in \{\nabla\}_{x_i} f$, with $v_i \to v_0$, then $v_0 \in \{\nabla\}_{x_0} f$
- It is **quasi-monotone**, i.e. if $V \subset U$ is convex then there is a constant $C = C_V < \infty$ such that if $x_0, x_1 \in V$ and $v_i \in \{\nabla\}_{x_i} f$, then

$$(v_0 - v_1) \cdot (x_0 - x_1) \geq -C|x_0 - x_1|^2. \tag{9}$$

Furthermore, the addition formula for derivatives holds: if f, g are semiconvex, then so is $f + g$, and

$$\{\nabla\}_x (f + g) = \{\nabla\}_x f + \{\nabla\}_x g. \tag{10}$$

Here the + on the right-hand side denotes Minkowski addition: for $A, B \subset \mathbb{R}^n$,

$$A + B := \{x + y : x \in A, y \in B\}. \tag{11}$$

A point $x \in U$ is a **critical point** of f if $0 \in \{\nabla\}_x f$; otherwise x is a **regular point**. Note that x is regular iff there exists a vector v such that $D_x f(v) > 0$. Critical and regular values of f are now defined in the usual way. With these definitions, the implicit function theorem holds: if x is a regular point of f, then there is a neighborhood W of x and a map $\phi : W \to \mathbb{R}^{n-1}$ such that $x' \mapsto (\phi(x'), f(x'))$ is a biLipschitz homeomorphism between W and some open subset of $\mathbb{R}^n$.

We can also define critical and regular values for the restriction of a semiconvex function f to a set S with locally positive reach: we say that $x \in S$ is a critical point of $f|S$ if

$$D_x f | \operatorname{Tan}_x S \geq 0. \tag{12}$$

Thus a local minimum of $f|S$ is necessarily a critical point, but a local maximum need not be. By (8), condition (12) is equivalent to: *for all* $w \in \operatorname{Tan}_x S$, *there exists* $v \in \{\nabla\}_x f$ *such that* $v \cdot w \geq 0$. In the important special case where f is everywhere differentiable, this is in turn equivalent to

$$-\nabla_x f \in \operatorname{Nor}_x S. \tag{13}$$

Suppose $c \in \mathbb{R}$ has the following property: if $x_1, x_2, \cdots \to x \in U$, with $v_i \in \{\nabla\}_{x_i} f$, $f(x) = c$ and $f(x_i) > c$, then $v_i \not\to 0$. Then we say that c is a **weakly regular** value of f. Since the subgradient field is upper semicontinuous, a regular value of f is weakly regular.

Theorem 3.1. *(Bangert? Kohlmann?) A set* $S \subset U$ *has locally positive reach if and only if there exists a semiconvex function* $g : U \to \mathbb{R}$ *such that* 0 *is a weakly regular value of* f *and*

$$S = g^{-1}(-\infty, 0]. \tag{14}$$

If in fact 0 is a *regular* value of g then

$$\operatorname{Nor}_x S = \operatorname{cone}\{\nabla\}_x g. \tag{15}$$

In particular, condition (12) may be written: *if* $D_x f(v) < 0$ *then* $D_x g(v) > 0$. Thinking of thickness as $-g$ and length as f, this is the starting point for the balance criterion for critical points for ropelength.

Every semiconvex function f may be represented locally as a **max function**, i.e.

$$f = \max_{\phi \in \mathcal{G}} \phi \tag{16}$$

for some family $\mathcal{G}$ of smooth functions, locally bounded in the C^2 norm. This follows at once from the definition of semiconvex functions and the fact that a convex function is the maximum of a family of *linear* functions. Conversely, if the Hessians $D^2\phi, \phi \in \mathcal{G}$ are uniformly bounded as quadratic forms, then any f as above is semiconvex.

The representation (16) is helpful because of **Clarke's differentiation theorem for max functions:**

Theorem 3.2. *Suppose $f : U \to \mathbb{R}$ is given by (16), where $\mathcal{G} \subset C^1$. Then for all $x \in U$ the directional derivative function $v \mapsto D_x f(v)$ is sublinear, and is given by*

$$D_x f(v) = \max\{\nabla_x \phi \cdot v : \phi \in \mathcal{G}, \phi(x) = f(x)\}. \tag{17}$$

Corollary 3.3. *Suppose $f, g : U \to \mathbb{R}$ are semiconvex functions. Then $h := \max\{f, g\}$ is semiconvex. If $x \in U$ is a point such that $h(x) = f(x) = g(x)$, then*

$$\{\nabla\}_x h = \text{convexhull}(\{\nabla\}_x f \cup \{\nabla\}_x g). \tag{18}$$

4. FLOWS

If $f : U \to \mathbb{R}$ is a C^2 function, then the vector field ∇f is C^1 and the gradient flow is well-defined and continuous. In fact, since the standard existence and uniqueness theorem for ODE works for Lipschitz vector fields, this is also true for $C^{1,1}$ functions. Likewise, if $M \subset U$ is a C^2 (or $C^{1,1}$) submanifold then the gradient flow of $f|M$ exists. Of course this is really just another instance of the first flow.

It turns out that the same constructions may be carried out if f is merely semiconvex and M is a set with positive reach. However, trajectories of the flow may bifurcate in forward time, so strictly speaking the flow is only defined for negative time. Again the flow of $f|M$ may be viewed as a special case of the unrestricted flow, but in a different sense than in the smooth theory.

For f semiconvex, put $\nabla_x^\circ f$ to be the unique element of $\{\nabla\}_x f$ of smallest length. We refer to this vector as the **principal gradient** of f at x.

Theorem 4.1. *(Brézis) Let $f : U \to \mathbb{R}$ be a semiconvex function and $x \in U$. Then there exists a unique maximal locally Lipschitz curve $\Gamma(x, \cdot) : (-c_x, 0] \to U$, $0 < c_x \leq \infty$, such that*

- *$\Gamma(x, 0) = x$ and*
- *for a.e. $t \in (-c_x, 0]$,*

$$\frac{d\Gamma(x,t)}{dt} \in \{\nabla\}_{\Gamma(x,t)} f. \tag{19}$$

Furthermore the resulting function Γ has the following properties:

- *the domain of Γ is open in $U \times (-\infty, 0]$,*
- *Γ is locally Lipschitz,*

- $\Gamma(x, -t-s) = \Gamma(\Gamma(x,-t), -s))$ *for all* $t, s \geq 0$, *and*
- $\Gamma(x, \cdot)$ *is differentiable from the left everywhere in* $(-c_x, 0]$, *with*

$$\frac{d\Gamma(x,t)}{dt-} = \nabla^\circ_{\Gamma(x,t)} f. \tag{20}$$

Note that the uniqueness of the flow Γ, and the locally Lipschitz dependence on initial conditions, both follow at once from the quasi-monotonicity of $\{\nabla\}f$: if V, C and x_0, x_1 are as in (9), then for a.e. $t \geq 0$ such that $\Gamma(\{x_i\} \times [0, -t]) \subset V$, we have

$$\begin{aligned} \frac{d}{dt} |\Gamma(x_0, -t) - \Gamma(x_1, -t)|^2 &= 2\left(\frac{d\Gamma(x_0,-t)}{dt} - \frac{d\Gamma(x_1,-t)}{dt} \right) \cdot (\Gamma(x_0,-t) - \Gamma(x_1,-t)) \\ &\leq 2C\, |\Gamma(x_0,-t) - \Gamma(x_1,-t)|^2, \end{aligned}$$

and therefore

$$|\Gamma(x_0,-t) - \Gamma(x_1,-t)| \leq e^{Ct} |x_0 - x_1|. \tag{21}$$

Of course Γ may be viewed as the descent flow for f. Observe that the last conclusion of Theorem 4.2 implies that x is a critical point of f iff $\Gamma(x, -t) = x$ for all $t \geq 0$.

Now let $S \subset U$ be a set with locally positive reach and $f : U \to \mathbb{R}$ a semiconvex function. For simplicity we will also assume that S is compact. We now construct a descent flow for the restriction of f to S; more precisely, a locally Lipschitz flow Γ on S, defined for negative time, with the property that the left-side derivative always exists and is given by

$$\frac{d}{dt-}\Gamma(x,t) = \left(\mathrm{proj}_{(-\,\mathrm{Tan}_{\Gamma(x,t)} S)} (\{\nabla\}_{\Gamma(x,t)} f) \right)^\circ . \tag{22}$$

Here proj_C denotes the nearest point projection to the closed convex set C, and C° denotes the element of smallest length in C.

In fact this flow is realizable as the restriction to S of the descent flow of a certain semiconvex function. For simplicity let us assume that there exists a semiconvex function $g : U \to \mathbb{R}$ such that $S = g^{-1}(-\infty, 0]$, and such that 0 is *regular* value of g. Put

$$R := 2 \sup \left\{ \frac{|v|}{|\nabla^\circ_x g|} : v \in \{\nabla\}_x f, x \in S \right\} \tag{23}$$

and

$$\bar{g}_f := R \max\{0, g\} + f. \tag{24}$$

Theorem 4.2. *If* $x \in S$ *then the principal gradient of* $\bar{g}_f$ *is*

$$\nabla^\circ_x \bar{g}_f = \left[\mathrm{proj}_{(-Tan(S,x))} (\{\nabla\}_x f) \right]^\circ . \tag{25}$$

For the present we will prove this in the special case where f is C^1. In the analogy with the rope-shortening flow, f is the length function and $-g$ is the thickness.

Lemma 4.3. *Let* $C \subset \mathbb{R}^n$ *be a closed convex cone and* $v \in \mathbb{R}^n$. *Then*

$$v = \mathrm{proj}_C(v) + \mathrm{proj}_{C^*}(v). \tag{26}$$

and

$$\mathrm{proj}_C(v) \cdot \mathrm{proj}_{C^*}(v) = 0. \tag{27}$$

Moreover, (26) is the unique decomposition of v as a sum of a pair of orthogonal vectors from C and C^*.

Proof. Observe first that

$$(v - \operatorname{proj}_C(v)) \cdot \operatorname{proj}_C(v) = 0, \tag{28}$$

for otherwise

$$\begin{aligned} |v - (1+t)\operatorname{proj}_C(v)|^2 &= |v - \operatorname{proj}_C(v)|^2 - 2t(v - \operatorname{proj}_C(v)) \cdot \operatorname{proj}_C(v) \\ &\quad + t^2|\operatorname{proj}_C(v)|^2 \\ &< |v - \operatorname{proj}_C(v)|^2 \end{aligned}$$

for an appropriate choice of $t > -1$. Furthermore,

$$v - \operatorname{proj}_C(v) \in C^*, \tag{29}$$

since otherwise there exists $w \in C$ such that $w \cdot (v - \operatorname{proj}_C(v)) > 0$ and

$$\begin{aligned} |v - (\operatorname{proj}_C(v) + tw)|^2 &= |v - \operatorname{proj}_C(v)|^2 - 2t(v - \operatorname{proj}_C(v)) \cdot w \\ &\quad + t^2|w|^2 \\ &\le |v - \operatorname{proj}_C(v)|^2 \end{aligned}$$

for small $t > 0$.

Thus $v = \operatorname{proj}_C(v) + (v - \operatorname{proj}_C(v))$ is an orthogonal decomposition as a sum of vectors from C and C^*. By the same token, $v = \operatorname{proj}_{C^*}(v) + (v - \operatorname{proj}_{C^*}(v))$ is another such decomposition. But if $v = u + w = u' + w'$, where $u, u' \in C$ and $w, w' \in C^*$ then

$$\begin{aligned} |v|^2 &= (u+w) \cdot (u'+w') \\ &= u \cdot u' + u \cdot w' + u' \cdot w + w \cdot w' \\ &\le u \cdot u' + w \cdot w' \\ &\le |u||u'| + |w||w'| \qquad \text{(with equality iff } u = u', w = w') \\ &\le (|u|^2 + |w|^2)^{\frac{1}{2}}(|u'|^2 + |w'|^2)^{\frac{1}{2}} \\ &= |v|^2. \end{aligned}$$

Hence equality holds throughout, so $u = u'$ and $w = w'$. □

Another formulation of this fact is useful:

Corollary 4.4. *Let $C \subset \mathbb{R}^n$ be a closed convex cone and $v \in \mathbb{R}^n$. Then*

$$(v + C)^\circ = \operatorname{proj}_{(-C^*)}(v) \tag{30}$$

Proof. Since $(v + C)^\circ$ is the nearest point projection of 0 to $v + C$,

$$\begin{aligned} (v+C)^\circ &= v + \operatorname{proj}_C(-v) \\ &= v - \operatorname{proj}_{(-C)}(v) \\ &= \operatorname{proj}_{(-C^*)}(v) \end{aligned}$$

by Lemma 4.3. □

Now we can prove Theorem 4.2. By Corollary 3.3, $\{\nabla\}_x \bar{g}_f$ is the singleton $\{\nabla_x f\}$ for x in the interior of S; on the other hand $\operatorname{Tan}_x S = \mathbb{R}^n$ for such x. Therefore it is enough to check (25) for x lying in the boundary of S. For such x, we claim that

$$\{\nabla\}_x \bar{g}_f \cap B(0, |\nabla_x f|) = (\nabla_x f + \operatorname{cone}(\{\nabla\}_x g)) \cap B(0, |\nabla_x f|). \tag{31}$$

Since

$$\{\nabla\}_x\bar{g}_f = \nabla_x f + \text{convexhull}(\{0\} \cup R\{\nabla\}_x g), \tag{32}$$

the inclusion $\subset$ is obvious. To prove the opposite inclusion, let

$$v \in (\nabla_x f + \text{cone}(\{\nabla\}_x g)) \cap B(0, |\nabla_x f|).$$

Thus

$$v = \nabla_x f + tw,$$

where $w \in (\{\nabla\}_x g)$ and $t \geq 0$, and furthermore $|v| < |\nabla_x f|$, which implies

$$\begin{aligned} |\nabla_x f|^2 &> |\nabla_x f + tw|^2 \\ &= |\nabla_x f|^2 + 2t\nabla_x f \cdot w + t^2|w|^2, \end{aligned}$$

so

$$|w||\nabla_x f| \geq -\nabla_x f \cdot w > \frac{t}{2}|w|^2, \tag{33}$$

whence

$$t < \frac{2|\nabla_x f|}{|w|} \leq R. \tag{34}$$

This proves (31).

Now we apply Corollary 4.4 with $v = \nabla_x f$ and $C = \text{cone}(\{\nabla\}_x g) = \text{Nor}_x S$ to obtain

$$(\nabla_x f + \text{Nor}_x S)^\circ = \text{proj}_{(-\text{Tan}_x S)}(\nabla_x f). \tag{35}$$

Since this is an orthogonal summand of $\nabla_x f$, its length is $\leq |\nabla_x f|$, and it follows from (31) that it lies in $\{\nabla\}_x\bar{g}_f \cap B(0, |\nabla_x f|)$. In fact it must be the element of smallest length in this set, and therefore it is $\nabla^\circ_x \bar{g}_f$, as claimed. □