A. Discrete differential geometry of n-simplices (2008-09-27 by NM)

Because of convenience, we use monomials to represent coordinates of points. That is, point $(l_1, l_2, ..., l_n) \in \mathbb{R}^n$ is denoted by monomial ${x_1}^{l1}{x_2}^{l2} \cdots {x_n}^{ln}$ of n indeterminates.

A.1. **Space of n-simplices.** n-dimensional *standard lattice* L_n is the collection of all integer points of the n-dimensional Euclidean space $\mathbb{R}^n$:

$$L_n := \left\{ {x_1}^{l1}{x_2}^{l2} \cdots {x_n}^{ln} \mid l_i \in \mathbb{Z} \text{ for all } i \right\}.$$

And the collection S of all "slant" n-simplices is defined as follows:

$$S := \left\{ a \left[x_{\rho(1)} \cdots x_{\rho(n-1)} \right] \mid a \in L_n,\ \rho \in Sym_n \right\},$$

where Sym_n is the n-th symmetric group and $a \left[x_{\rho(1)} \cdots x_{\rho(n-1)} \right]$ denotes the convex hull of n points $a_0 = a$, $a_1 = a x_{\rho(1)}$, …, $a_{n-1} = a x_{\rho(1)} x_{\rho(2)} \cdots x_{\rho(n-1)}$ in $\mathbb{R}^n$, i.e.,

$$a \left[x_{\rho(1)} \cdots x_{\rho(n-1)} \right] := \left\{ \prod_{0 \le i < n} a_i^{\lambda_i} \mid 0 \le \lambda_i \in \mathbb{R} \text{ s.t. } \sum_{0 \le i < n} \lambda_i = 1 \right\}.$$

Then, the collection B of all "flat" n-simplices is defined as the quotient of S by "shift operator" σ on S (Fig.1(a)). That is, $B := S/\sigma$, where

$$\sigma \left(a \left[x_{\rho(1)} \cdots x_{\rho(n-1)} \right] \right) := a x_{\rho(1)} \left[x_{\rho(2)} \cdots x_{\rho(n)} \right].$$

On the other hand, n-dimensional *conjugate lattice* ${L_n}^*$ is define as follows:

$${L_n}^* := \left\{ (e/x_1)^{l1} (e/x_2)^{l2} \cdots (e/x_n)^{ln} \mid l_i \in \mathbb{Z} \text{ for all } i \right\},$$

where $e = x_1 x_2 \cdots x_n$.

A.2. **Differential structure on B.** "Tangent bundle" $T[B]$ on B is defined as the quotient of S by σ^n:

$$T[B] := S/\sigma^n,$$
$$\pi : T[B] \to B,\ \pi \left(s \mod \sigma^n \right) := s \mod \sigma.$$

We identify $T[B]$ with $B \times \{e/x_1, e/x_2, \ldots, e/x_n\}$ $(e = x_1 x_2 \cdots x_n)$ by one-to-one correspondence

$$T[B] \ni s \mod \sigma^n \sim (s \mod \sigma, Ds) \in B \times \{e/x_1, e/x_2, \ldots, e/x_n\},$$

where the "gradient" Ds of $s \in S$ is defined by

$$Da \left[x_{\rho(1)} \cdots x_{\rho(n-1)} \right] := x_{\rho(1)} \cdots x_{\rho(n-1)} = e/x_{\rho(n)}.$$

Let $s = a \left[x_{\rho(1)} \cdots x_{\rho(n-1)} \right] \in S$. Then $s \mod \sigma^n \in T[B]$ specifies "local trajectory" $\{s_U \mod \sigma, s \mod \sigma, s_D \mod \sigma\}$ at $s \mod \sigma \in B$ (Fig.1(b)), where

$$s_U := a \left[x_{\rho(1)} \cdots x_{\rho(n-2)} x_{\rho(n)} \right],$$
$$s_D := a x_{\rho(1)} \left[x_{\rho(2)} \cdots x_{\rho(n-1)} x_{\rho(1)} \right].$$

And we shall obtain a flow on B by patching these local trajectories together.

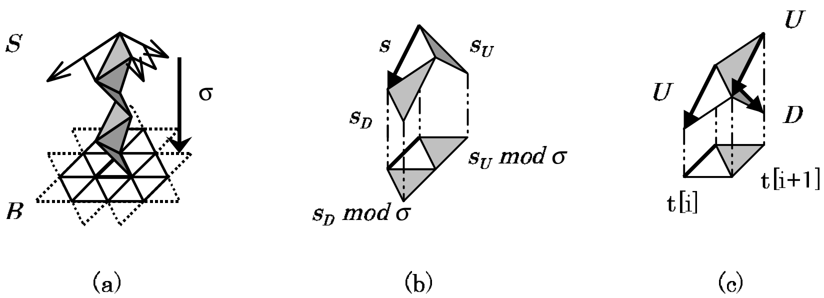

FIGURE 1. Differential geometry of 3-simplices. (a): Fiber of S over a point of B. (b): The local trajectory specified by $s \in S$. (c): The second derivative along orbit $\{t[i]\}$.

A.3. **Tangent cone and cotangent cone.** For $A \subset L_n$, *tangent cone* $ConeA$ of L_n is defined as follows:

$$ConeA := \left\{ p{x_1}^{l1}{x_2}^{l2} \cdots {x_n}^{ln} \in L_n \mid p \in A \text{ and } 0 \leq l_i \in \mathbb{Z} \text{ for all } i \right\}.$$

Then, the "boundary surfaces" $d_S w$ of $w = ConeA$ is given by

$$d_S w := \left\{ a \left[x_{\rho(1)} \cdots x_{\rho(n-1)} \right] \in S \mid l_w(a_i) = 0 \text{ for all } i \right\},$$

where $a_0 = a$, $a_1 = ax_{\rho(1)}$, …, $a_{n-1} = ax_{\rho(1)}x_{\rho(2)} \cdots x_{\rho(n-1)}$ and

$$l_w(z) := \max_{p \in w} \left\{ \min_{1 \leq i \leq n} \left\{ l_i \in \mathbb{Z} \mid \prod_{1 \leq i \leq n} {x_i}^{li} = z/p \right\} \right\}$$

for $z \in L_n$. Note that the boundary surfaces of a tangent cone induce a vector field on B.

In the same way, we define *cotangent cone* $Cone^*A$ ($A \subset L_n$) as follows:

$$Cone^*A := \left\{ p(e/x_1)^{l1}(e/x_2)^{l2} \cdots (e/x_n)^{ln} \in L_n \mid p \in A \text{ and } 0 \leq l_i \in \mathbb{Z} \text{ for all } i \right\}.$$

A.4. **Vector field on B.** Let $w = ConeA$ be a tangent cone. Then $d_S w$ specifies an n-simplex $s \in d_S w$ uniquely over each $t \in B$, which we denote by $\Gamma_w(t)$:

$$\Gamma_w(t) := \text{ the unique } n\text{-simplex } s \in d_S w \text{ s.t. } t = s \mod \sigma.$$

That is, Γ_w induces "vector field" X_w over B:

$$X_w(s \mod \sigma) := D\Gamma_w(s \mod \sigma).$$

Let $\{t[i]\} \subset B$ be a trajectory defined by vector field X_w. And we define the "second derivative" $D^2\Gamma_w(t[i])$ of Γ_w along $\{t[i]\}$ as a $\{U, D\}$-valued function:

$$D^2\Gamma_w(t[i+1]) := \begin{cases} D^2\Gamma_w(t[i]) & \text{if } X_w(t[i+1]) = X_w(t[i]), \\ -D^2\Gamma_w(t[i]) & \text{else,} \end{cases}$$

where $-D := U$ and $-U := D$ (Fig.1(c)). Then, we could encode the conformation of a trajectory by the second derivative along the trajectory.