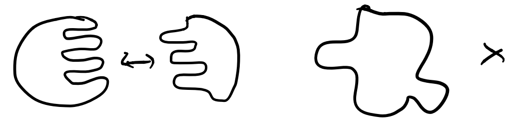
Elevation

Motivation: Protein molecules interact with each other via cavities and protrusions of the surface.

(E.g. The specificity of enzymes)



Thus, we would like a function on a surface characterizing the cavity and protrustion. In the earth (sphere), we could define the "height" of a place as its "mean sea level". This makes much sense because of the (relative) uniform geometric shape of the earth. The mass of the earth distribute uniformly among the center of mass in all directions. This article introduce a function defined for general surfaces with genus g, which is an analogue of the height function on earth, called the elevation function.

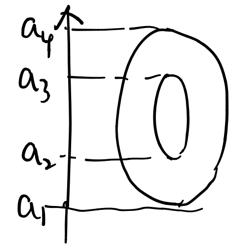
The maxima of the function give us information about the taller places on the surface. Using this, we could do prediction about how protein molecules interact with each other once their geometric shape is given.

I. Definition of the Elevation Function

During this notes, M denote a smooth closed 2-manifold $\subseteq \mathbb{R}^3$.

Recall: A smooth function $f: M \to \mathbb{R}$ is called Morse if its critical pts all have different values and non-degenerate.

E.g. The height function on a torus.



Choose $b_0 < a_1 < b_1 < a_2 < b_2 < a_3 < b_3 < a_4 < b_4$.

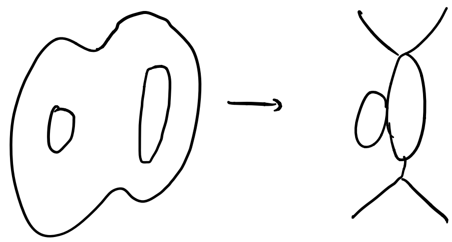
let $M_i = f^{-1}(-\infty, b_i]$, $M^i = f^{-1}[b_i, \infty)$, we get a filtration $\phi = M_0 \subseteq M_1 \subseteq \cdots \subseteq M_4 = (M, \phi) \subseteq (M, M^3) \subseteq \cdots \subseteq (M, M^0 = M)$.

So we get persistence vector spaces

$$0 = H_p(M_0) \to H_p(M_1) \to \cdots \to H_p(M) \to H_p(M, M^3) \to \cdots \to H_p(M, M) = 0$$

Started & ended with 0, everything gets born eventually dies. So the persistence diagrams contain only finite points and every critical pt is paired to another.

Actually, for a genus g surface, one can draw its Reeb graph, which maps each component of each level set to a point. The Reeb graph is generated by g cycles such that each cycle is a linear combination (mod 2) of the generators. Each cycle has a unique lowest and highest point, denoted lo-pt, hi-pt.



We can choose a basis such that each lo-pt and hi-pt are different. Then the pairs in the extended persistence are the (lo-pt, hi-pt) pairs. Finally, we pair the minimum with the maximum.

By the persistence symmetry theorem, f and $-f$ have the same critical pts and (x, y) is paired by $f \Leftrightarrow$ it is paired by $-f$.

Now we can consider defining the height in other directions. For every $u \in S^2$, $x \in M$, call $f_u(x) := \langle x, u \rangle$ the height of x in the direction u. Get a 2-parameter height function $\text{Height}: M \times S^2 \to \mathbb{R}$, $(x, u) \mapsto f_u(x)$. Clearly $f_{-u}(x) = -f_u(x)$.

Let n_x denote the outer normal direction of $x \in M$.

Then clearly x is a critical pt of $u \Leftrightarrow u \perp \pm n_x$.

It would be too idealistic to expect all f_u to be Morse.

For some u, f_u may have a

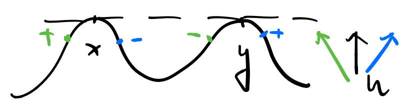
① flat point: M has a geodesic through x, restricted to which f_u has an inflection point.

In this case, f_u has a degenerate critical point.

In the above picture, if we pertube u to the left slightly to u', we get to paired critical points near x.

As u' move to u, the two paired pts converge to x and then vanish. We call the pt x a birth-death pt.

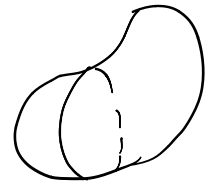
② Shared tangent line: Two pts $x, y \in M$ have the same or antipodal normal direction: $n_x = \pm n_y$ and share the same tangent line.



In this case, f_u has two critical pts with the same function value.

If we pertube u slightly to the left (green), we get a paired critical pts near x and y. As $\nwarrow$ turn to u, the two pts converge to x, y respectively, with the same height. As u turn to right $\nearrow$, we get another paired critical pts near x and y, but change their positions in the order of height. In this case, we call x, y points of interchange.

For both ①, ②, we choose an one-parameter curve on M through the critical pts and let u move along the one-parameter direction to talk about the birth-death and interchange property. If u move along the other degree of freedom, we get a curve of singularities. The intersection pts of curves of singularities are called codimension-2 singularities, formed by two bd-pts, two interchanges or an interchange and a bd-pt. Singularities that are not at the intersection pts are called codimension-1 singularity.



We make <u>the first genericity assumption</u> on M:

The height function $H: M \times S^2 \to \mathbb{R}$ has only codimension-1 or 2 singularity.

Now we can define the elevation function on M.

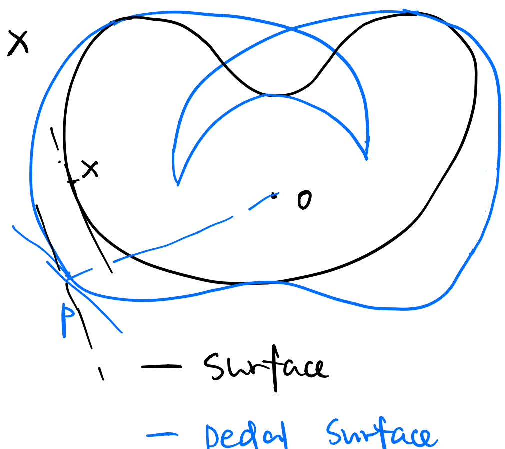
Each $x \in M$ has a unique normal direction n_x, thus a unique (up to a sign) direction u at which x is critical. x is paired by f_u another pt $y \in M$. We define $\text{pers}(x) = \text{pers}(y) = |f_u(x) - f_u(y)|$. By the symmetry thm. this is well-defined whenever f_u is Morse. Then we define $\text{elevation}(x) = \text{pers}(x)$. If f_u is not Morse, we take the limit along a regular curve through x. Here "regular" means on which the height function is Morse.

We get Elevation: $M \to \mathbb{R}$. This is the analogue of height on earth. Clearly, the elevation is invariant under rigid motions of M. It is the height difference between a pt on M and another canonically defined pt on M.

II. Pedal Surface

There is a 1-1 correspondence between a surface in $\mathbb{R}^3$ and its pedal surface. Pedal surface is useful in studying the properties of the height function and elevation function.

Let $M \subseteq \mathbb{R}^3$. $0 \in \mathbb{R}^3$ be the origin. $\forall x \in M$, it has a tangent plane T_x. pedal: $M \to \mathbb{R}^3$. $x \mapsto$ the orthogonal projection of 0 onto T_x. Let $P = \text{pedal}(M)$, called the pedal surface of M.

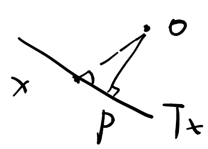


Observe that: ① If $x \perp T_x$, then $\text{pedal}(x) = x$

② $n_x = \pm n_y \iff \text{pedal}(x)$, $\text{pedal}(y)$ and 0 colinear ; $T_x = T_y \iff \text{pedal}(x) = \text{pedal}(y)$.

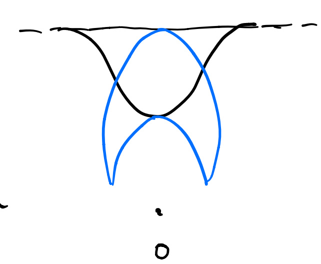
③ If $u = n_x$, then $\langle x, u \rangle = \langle \text{pedal}(x), u \rangle$, i.e. x and $\text{pedal}(x)$ have the same height in the direction of n_x.

④ The diameter sphere $0x$ with center $\frac{x}{2}$ intersects T_x at the diameter circle of x and p. We can use this to recover M from P: let θ be the angle between $p \in P$ and T_p of p. Then θ is also the angle between x and T_x. Then $|0x| = 2\frac{|0p|}{\sin\theta}$. $\langle ox, op \rangle = \frac{\pi}{2} - \theta$.



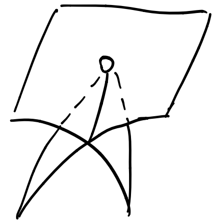
Singularities in pedal:

1. The birth-death pt correspond to a cusp (尖点) in pedal surface: since the tangent plane reverse its direction across the inflection pt.

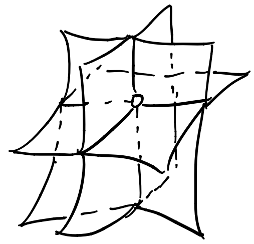


2. By ② above, a shared tangent line causes a self-intersection of the pedal surface.

3. On M, two flat pts share a tangent line; on P, two cusps and a self-intersection curve end at a dovetail point. (燕尾点)

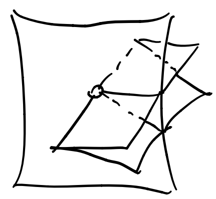


4. On M, three points share a tangent line and two concurrent interchanges share a critical pt. This forces the interchange of the remaining two critical pts. On P, three self-intersection curves intersect at a "triple point".



5. On M, a concurrent birth-death point and an interchange share a critical pt.

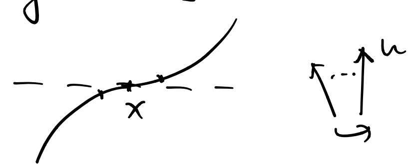
   On P, a cusp curve and a self-intersection curve intersect at a "cusp intersection".



III. Continuity and Smoothness of the Elevation

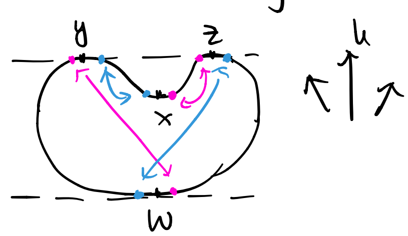
I told a lie when defining the elevation function at singular directions: when f_u is not Morse, the limit of the height function in a neighborhood of $u \in S^2$ may not exist. Let's analyze the two kind of singularities.

① Flat point: As u reaching the singular



direction, the pair of critical points get closer and the elevation converge to 0. In this case, the limit exist and we define the elevation of x to be 0. Continuity ✓

② Interchange point: Consider the elevation near y and z. From left to right.

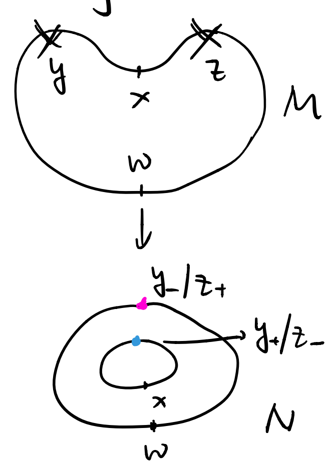


points (pink) near y are paired with points near w and the elevation converges to the vertical distance between y, w. From right to left, points (blue) near y are paired to points near x and the elevation converges to the vertical distance between y, x. So the left and right limits at y are different. Same circumstance occur at z, along the singular curve of interchange.

Note that although the pairing near x change from y to z from left to right, the elevation near x is cts since y, z have the same height in the vertical direction. Note also that not all interchanges cause such discontinuity.

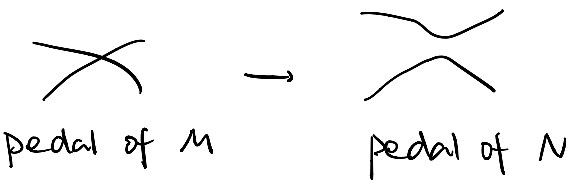
<u>Surgery</u>. We need the continuity of the elevation through our discussion. Therefore, we do a reversable surgery on M to get another manifold N, on which the elevation function is cts. Specifically, we first cut M along the curves where the elevation not cts and get a manifold B with boundary, then glue the boundary of B by identifying points with same limits.

In the example above, we cut at y, z, glue the left end of y to the right end of z and glue the right end of y to the left end of z. The resulting manifold N is not



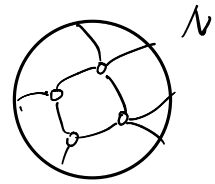
Connected, but with cts elevation function on it.

The self-intersection of the pedal surface is also solved.



We do the surgery for all interchanges causing discontinuity, including triple points, dovetail points... and so on.

Now talk about smoothness. The elevation function on N is smooth on all nonsingular points on M, but not necessarily on the gluing part. To describe this, define an antipodal map $N \to N$, mapping x to its paired pt $y = \text{antipodal}(x)$. We have $\text{antipodal}^2 = id$. Let B be the intermediate manifold with boundary and identify $Bd(B)$ with its image on N. Let $S = Bd(B) \cup \text{antipodal}(Bd\,B) \subseteq N$. I.e. the preimage of S on M contain the points where the elevation is discts and their antipodal pts. By the genericity assumption A, S is a one-dimensional graph, whose vertices are of degree 3 or 4.



Each degree 3 node corresponds to a triple point. (gluing three singular curves at a common point)

Each degree 4 node is the intersection between an arc in $Bd(B)$ and an arc in its antipodal image.

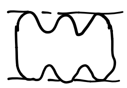
By S we define the <u>stratification</u> of N, consisting of <u>stratas</u>, that is: ① The open connected region in $N - S$

② The open arcs in $S - S_0$ ($S_0 :=$ nodes of S)

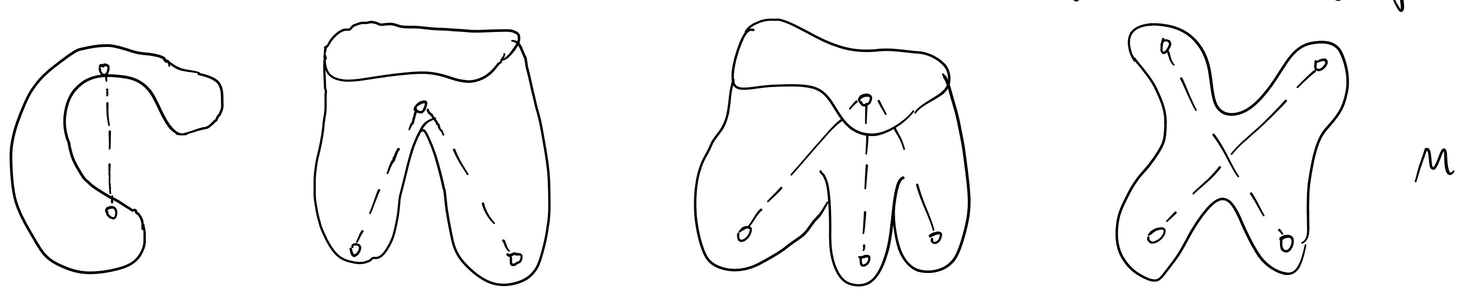
③ The nodes S_0 of S. By this stratification, we make our second genericity assumption, characterizing the smoothness of the elevation function in N: The elevation restricted to every strata is a Morse function.

IV. Elevation Maxima

As discussed before, the elevation maxima is what we are interested in. By "maximum" we mean the local maximum of the elevation function.

For $x \in N$, let $\mu(x)$ denote the # of preimages of x on M, called the multiplicity of x. Suppose the pair (x, y) gives an elevation maximum on N. Then neither x nor y is a flat point, since otherwise it has 0 elevation. We further assume that points of multiplicity 3 can only be paired with points of multiplicity 1. (no  or )

Then we call the maximum (x, y)
- one-legged, if $\mu(x) = \mu(y) = 1$
- two-legged, if $\mu(x) = 1$, $\mu(y) = 2$
- three-legged, if $\mu(x) = 1$, $\mu(y) = 3$
- four-legged, if $\mu(x) = \mu(y) = 2$.



one-legged   two-legged   three-legged   four-legged

One can see from the figures that the four kind of maxima correspond to different geometric pictures of the original manifold M.

If a pair (x, y) gives a local maximum on N, we want to set more restrictions to the meaning of being a local maximum on M. For example,  it would not make much sense to call this a two-legged maximum. Therefore, we give necessary conditions for a pair (x, y) to give a local elevation maximum on M. Let $x_1, \dots, x_n$ be the preimages of x on M, where $n = \mu(x)$. Similarly $y_1, \dots, y_m$ for y.

Necessary conditions for a maximum

① (x, y) is a one-legged maximum only if $n_x = \pm y - x$

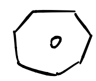
② (x, y) is a two-legged maximum only if n_x, $y_1 - x$ and $y_2 - x$ are linearly dependent and the orthogonal projection of x onto the line $\overline{y_1 y_2}$ lies between y_1 and y_2.

③ (x, y) is a three-legged maximum only if the orthogonel projection of x onto the plane $\overline{y_1 y_2 y_3}$ lies inside the triangle $\Delta y_1 y_2 y_3$.

④ (x, y) is a four-legged maximum only if the orthogonal projections of the segments $x_1 x_2$ and $y_1 y_2$ onto a plane parallel to both intersect.

V. Algorithm

In calculation, we trianglize the manifold to a 2-dimensional simplicial complex K. The genericity assumption of K is that its vertices are in general position. (i.e. no four pts are coplanar) First we need to decide the critical pts in K for a given direction $u \in S^2$. This is easy for an interior point of a 2-simplex, since we can simply determine whether u is orthogonal to the plane containing the simplex. But for pts on edges and vertices, there are many orthogonal directions because of the non-smoothness. Recall what we learned in the section 3 & 4 of chapter VI, Morse function:

The lower link for a regular vertex is , for a local minimum is ϕ, for a local maximum is  and for a saddle is . Motivated by this, we say a point x in the interior of a simplex σ is critical at direction u, if (i) $\langle u, z-x \rangle = 0$, $\forall z \in \sigma$. (ii) The lower link of x w.r.t. the function f_u is not contractible to a point.

Let $N(x) \subseteq S^2$ be the directions in which x is critical.

$N(x, y) = N(x) \cap N(y)$ and so on. Then the necessary conditions in the previous section translate to

① (x, y) is a one-legged maximum only if $\frac{x-y}{\|x-y\|} \in N(x, y)$

② (x, y) is a two-legged maximum only if the orthogonal projection z of x onto $\overline{y_1 y_2}$ lies between y_1 and y_2, and $\frac{z-x}{\|z-x\|} \in N(x, y_1, y_2)$.

③ (x, y) is a three-legged maximum only if the orthogonal projection z of x onto plane $\overline{y_1 y_2 y_3}$ lies in $\Delta y_1 y_2 y_3$ and $\frac{z-x}{\|z-x\|} \in N(x, y_1, y_2, y_3)$

④ (x, y) is a four-legged maximum only if the shortest line segment containing the lines $\overline{x_1x_2}$, $\overline{y_1y_2}$ touches both line segments x_1x_2 and y_1y_2, and $\frac{z-w}{\|z-w\|} \in N(x_1, x_2, y_1, y_2)$.

The pairs (x, y) satisfying one of the conditions are candidates for local maxima. It remains to check that (x, y) is paired at the direction $N(x, y)$. This can be done using extended persistence algorithm.

VI. Experiment

See the article.