Extended Persistence

(Edelsbrunner and Harer, 2010, VII.3)
Extended filtration

- \( f : \mathbb{M} \to \mathbb{R} \)
- \( a_1 < a_2 < \cdots < a_n \): homological critical values of \( f \)
- Find interleaved values \( b_i \):
  \[
  b_0 < a_1 < b_1 < \cdots < a_n < b_n
  \]
- **Sublevel sets** \( \mathbb{M}_{b_i} = f^{-1}(-\infty, b_i] \), 2-manifolds with boundary
- **Superlevel sets** \( \mathbb{M}^{b_i} = [b_i, \infty) \)
- Fix dimension \( p \), sequence of homology groups:
  \[
  0 = H_p(\mathbb{M}_{b_0}) \to H_p(\mathbb{M}_{b_1}) \to \cdots \to H_p(\mathbb{M}_{b_n})
  = H_p(\mathbb{M}, \mathbb{M}^{b_n}) \to H_p(\mathbb{M}, \mathbb{M}^{b_{n-1}}) \to \cdots \to H_p(\mathbb{M}, \mathbb{M}^{b_0}) = 0
  \]
- Absolute homology, e.g. \( H_p(\mathbb{M}_b) \)
- Relative homology, e.g. \( H_p(\mathbb{M}, \mathbb{M}_b) \)
Extended persistence on 2-manifold

- **(dim 0)** \([a_2, a_3], [a_1, a_{10}]\);
- **(dim 1)** \([a_4, a_7], [a_5, a_6], [a_6, a_5], [a_7, a_4], [a_8, a_9], [a_9, a_8]\);
- **(dim 2)** \([a_{10}, a_1], [a_3, a_2]\).
Elevation Functions and Protein Docking
Agarwal et al. (2006); Wang et al. (2011, 2005)
Motivation

- Identify cavities and protrusions of macromolecules for the purpose of protein docking.
- Goal: compute elevation maxima faster in practice!
**Persistence**

- Persistence for a single variable function $f : \mathbb{R} \to \mathbb{R}$
- $f$ can be extended to $f : \mathbb{M} \to \mathbb{R}$
- Connectivity of sub level set changes at a critical value
- Topological feature has persistence at $f(y) - f(x)$.
Stability of persistence diagrams

- Given $f, g : X \to \mathbb{R}$, define $\|f - g\|_{\infty} = \sup_{x \in X} |f(x) - g(x)|$, and $d_B(Dgm f, Dgm g) = \inf_{\gamma} \sup_{x} \|x - \gamma(x)\|_{\infty}$, then we have

$$d_B(Dgm f, Dgm g) \leq \|f - g\|_{\infty}.$$
For $u \in S^1$, $p(x) = p(y) = |h_u(x) - h_u(y)|$

$E : M \to \mathbb{R}$, s.t. $E(x) = p(x)$. 

$h_u : M \to \mathbb{R}$
Critical points and elevation maxima

- Top: critical points.
- Bottom: elevation local maxima are sets of critical points that are paired by the persistence algorithm in a given height direction.
Elevation on 2-manifold

- For $u \in S^2$, $p(x) = p(y) = |h_u(x) - h_u(y)|$.
- $E : \mathbb{M} \to \mathbb{R}$, s.t., $E(x) = p(x)$
Smooth case, a vertex is critical in two directions, \( u \) and \( -u \)

PL approximation, a vertex is generally critical for an entire region of directions

The critical region of a vertex is the closure of the set of directions along which it is critical
Protein surfaces
Examples of critical regions
Generate rigid motions from feature sets $\phi_A$ and $\phi_B$ obtained by analyzing the shapes of two proteins $A$ and $B$.

A feature consists of two points $u$ and its partner $v$ with common surface normals $n_v = n_u$ and common elevation $E(v) = E(u)$.

Its length is the Euclidean distance between them $||u - v||$.

Each maximum of the elevation function is defined by $k = \{2, 3, 4\}$ points and give rise to $\binom{k}{2}$ features.

\[
\text{for every } \alpha \in \Phi_A \text{ and every } \beta \in \Phi_B \text{ do} \\
\text{if } \alpha, \beta \text{ form a plausible alignment then} \\
\quad \mu = \text{Align}(\alpha, \beta); \\
\quad \text{compute the contact and collision numbers for } (A, \mu(B)); \\
\quad \text{if } (A, \mu(B)) \text{ is valid then add } \mu \text{ to } \Gamma \text{ endif} \\
\text{endif} \\
\text{endfor}; \text{ sort } \Gamma \text{ by contact number.}
\]

Wang et al. (2005)

