Molecular Configurations and Persistence: Branched alkanes and additive energies

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- Background
  - Energy landscapes and branched alkanes
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  - Morse theory and sublevelset persistent homology
- Characterizing energy landscapes of branched alkanes
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  - Generalizing the process
- Future work
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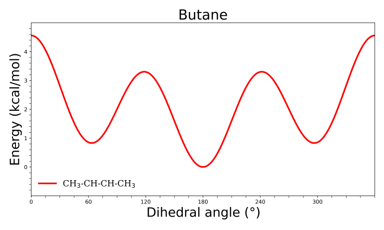
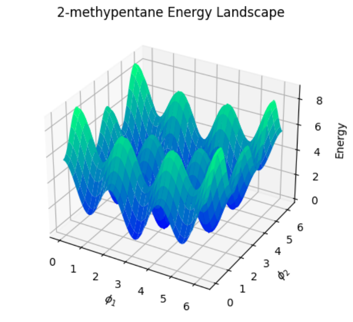
Motivation

Motivation

For any molecule, chemists want to understand the structure of its energy landscape.





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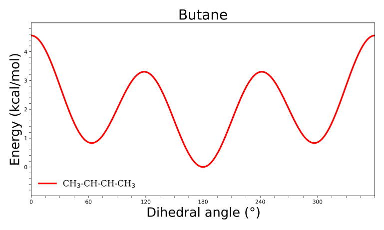
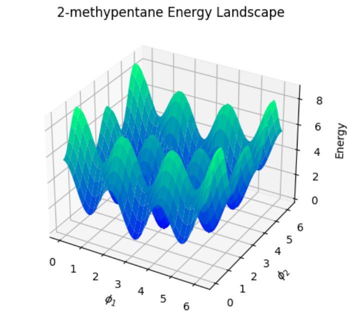
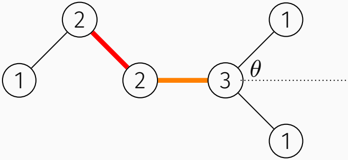
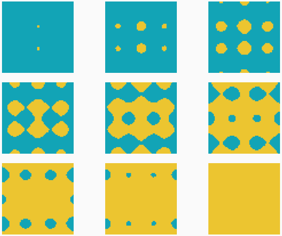


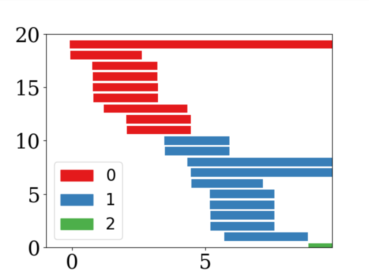


This quickly becomes rather difficult as the size of the molecule increases.

Goal: Use tools from topology to provide information about the structure of energy landscapes.

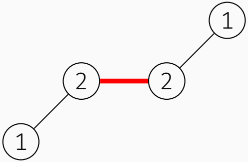


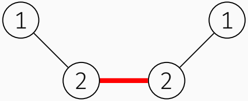




Background

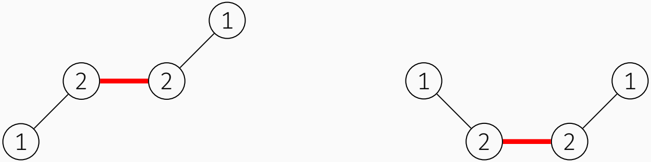
What is an Optimized Potentials for Liquid Simulations - United Atom (OPLS-UA) energy landscape?

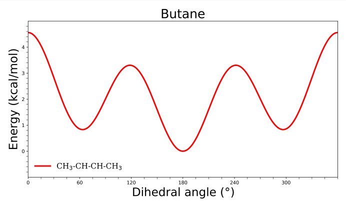




Energy landscapes

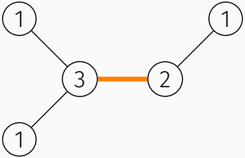
What is an Optimized Potentials for Liquid Simulations - United Atom (OPLS-UA) energy landscape?

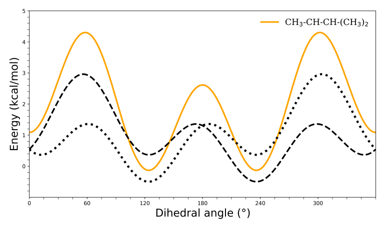




$$V_{\text{1-2-2-1}}(\phi_1) = c_0 + c_1[1 + \cos(\phi_1)] + c_2[1 - \cos(2\phi_1)] + c_3[1 + \cos(3\phi_1)]$$

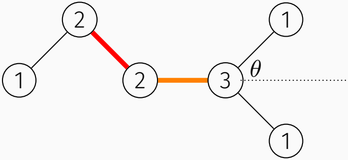
What is a branched alkane?

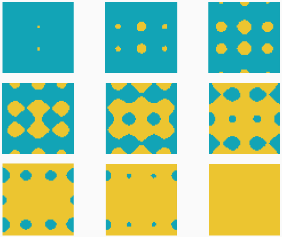


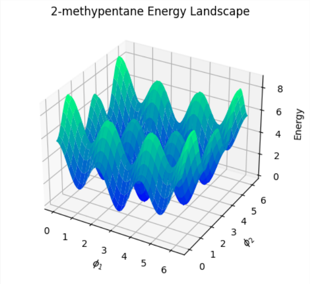


$$f(\phi_1) = \mathrm{V}_{\text{1-3-2-1}}(\phi_2 + \theta) + \mathrm{V}_{\text{1-3-2-1}}(\phi_2 - \theta)$$

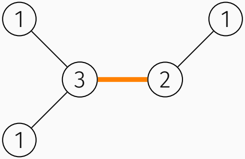
What does a bigger branched alkane energy landscape look like?

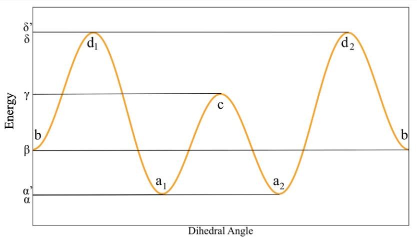


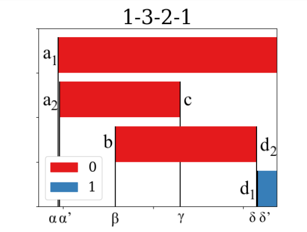




Goal: Calculate the sublevelset persistent homology of branched alkane energy landscapes.







Lemma 1

If $f : M \to \mathbb{R}$ is a Morse function, then the birth and non-infinite death times in the sublevelset persistent homology correspond to the critical points of f. Each k-dimensional bar has birth time corresponding to a critical point of index k, and death time either equal to infinity or otherwise corresponding to a critical point of index $k+1$. Furthermore, the number of semi-infinite bars in dimension k is given by the k-dimensional homology of M.

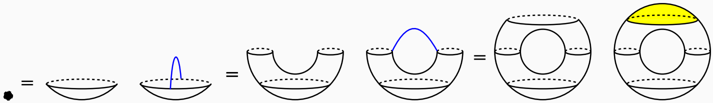
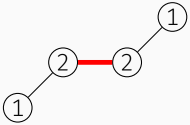


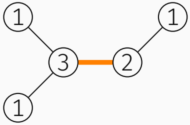
Figure: Nudged elastic band in topological data analysis. Henry Adams, Atanas Atanasov, and Gunnar Carlsson. Topological Methods in Nonlinear Analysis 45 (2015), 247-272.

Definition 2

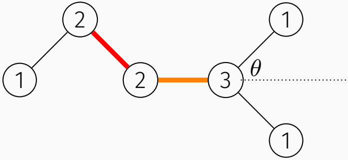
If $g_i : X_i \to \mathbb{R}$ is a collection of functions for $i = 1, \ldots, n$, then one can define their sum f on the product space by $f \colon X_1 \times \ldots \times X_n \to \mathbb{R}$ given by $f(x_1, \ldots, x_n) = g_1(x_1) + \ldots + g_n(x_n)$.



$g_1 : S^1 \to \mathbb{R}$

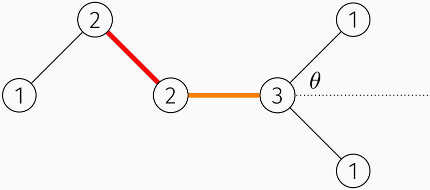


$g_2 : S^1 \to \mathbb{R}$



$f \colon (S^1)^2 \to \mathbb{R}$

$f(\phi_1, \phi_2) = g_1(\phi_1) + g_2(\phi_2)$



$$f(\phi_1, \phi_2) = \mathrm{V}_{1\text{-}2\text{-}2\text{-}1}(\phi_1) + [\mathrm{V}_{1\text{-}3\text{-}2\text{-}1}(\phi_2 + \theta) + \mathrm{V}_{1\text{-}3\text{-}2\text{-}1}(\phi_2 - \theta)]$$

Additionally, we know that the critical points of the component functions make up the critical points of the additive function.

Lemma 3

Let $X_1, \dots X_n$ be manifolds, let $f_i \colon X_i \to \mathbb{R}$ be Morse functions, and let $f \colon X_1 \times \cdots \times X_n \to \mathbb{R}$ be the additive function over a product space defined by $f(x_1, \dots, x_n) = \sum_{i=1}^{n} f_i(x_i)$. Then f is a Morse function. Further, the point $(x_1, x_2, \dots, x_n)$ is a critical point of f if and only if each coordinate x_i is a critical point of f_i. Finally, the index of a critical point $(x_1, x_2, \dots, x_n)$, denoted by $\mu_f(x_1, x_2, \dots, x_n)$, is equal to the sum of all indices of the component functions,

$$\mu_f(x_1, x_2, \dots, x_n) = \sum_{i=1}^{n} \mu_{f_i}(x_i).$$

Theorem 4 (Persistent Künneth Formula [GP19])

There is a natural short exact sequence of graded modules

$$0 \to \bigoplus_{i+j=n} (PH_i(X) \otimes PH_j(Y)) \to PH_n(X \otimes_f Y) \to \bigoplus_{i+j=n} \mathrm{Tor}(PH_i(X), PH_{j-1}(Y)) \to 0.$$

If $H_i(X)$ and $H_j(Y)$ are point-wise finite, then

$$\begin{aligned} &\mathrm{bcd}_n(X \otimes_f Y) \\ = &\bigsqcup_{i+j=n} \left\{ (\ell_J + I) \cap (\ell_I + J) \mid I \in \mathrm{bcd}_i(X), J \in \mathrm{bcd}_j(Y) \right\} \\ &\sqcup \bigsqcup_{i+j=n} \left\{ (r_J + I) \cap (r_I + J) \mid I \in \mathrm{bcd}_i(X), J \in \mathrm{bcd}_{j-1}(Y) \right\} \\ = &\bigsqcup_{i+j=n} \left\{ [\ell_I + \ell_J, \min(\ell_J + r_I, \ell_I + r_J)) \mid I \in \mathrm{bcd}_i(X), J \in \mathrm{bcd}_j(Y) \right\} \\ &\sqcup \bigsqcup_{i+j=n} \left\{ [\max(\ell_I + r_J, \ell_J + r_I), r_I + r_J) \mid I \in \mathrm{bcd}_i(X), J \in \mathrm{bcd}_{j-1}(Y) \right\}. \end{aligned}$$

Here ℓ and r are the left and right endpoints of the interval.

The Process

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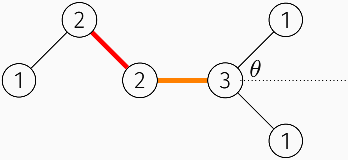

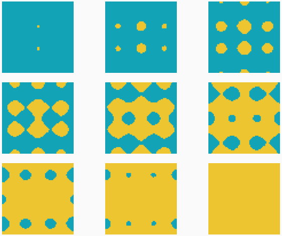

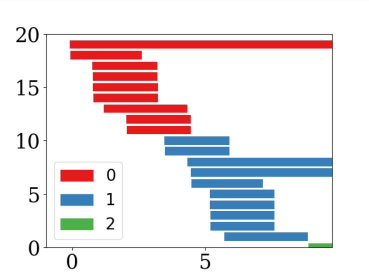

The Process via GUDHI

- ◇ Calculate good approximations for each base bond energy landscape
- ◇ Use GUDHI to calculate the persistence diagrams
  - **Input:** Number of each type of bond
  - **Internal process:** Construct mesh, construct energy function, evaluate function over the mesh, compute the cubical complex, compute sublevelset persistence
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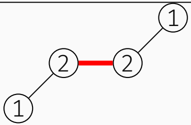
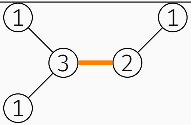
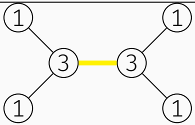
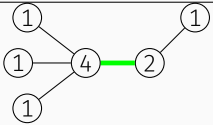
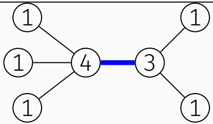
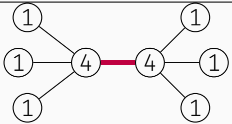
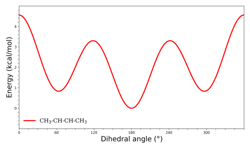
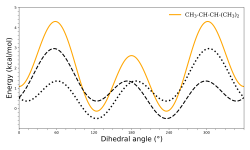
- Limitations: 9 internal bonds max (takes hours, will address), very idealized (1-x-y-1, non-bonded atom interactions, will not address)
- **Goal:** Characterize the energy landscapes without having to go through this process

1-2-2-1: butane	1-3-2-1: isopentane
	
1-3-3-1: 2,3-dimethylbutane	1-4-2-1: 2,2-dimethylbutane
	
1-4-3-1: triptane	1-4-4-1: tetramethylbutane
	

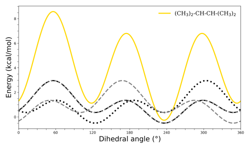
1-2-2-1

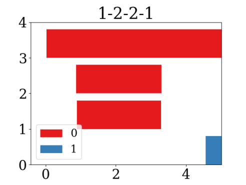


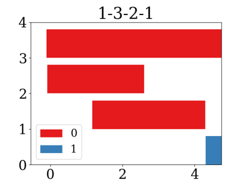
1-3-2-1

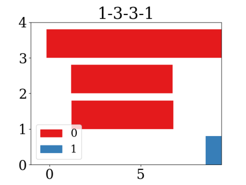


1-3-3-1



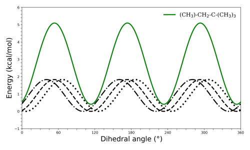


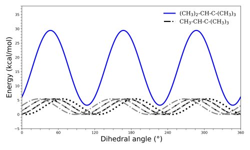


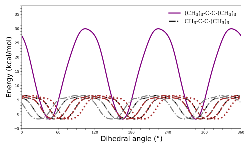


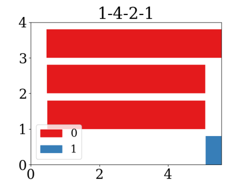
EL's and sublevelset persistence of base bonds

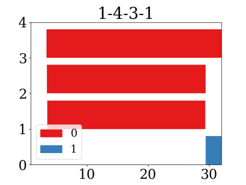
1-4-2-1	1-4-3-1	1-4-4-1

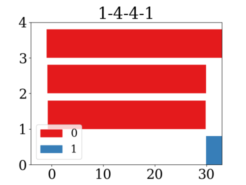




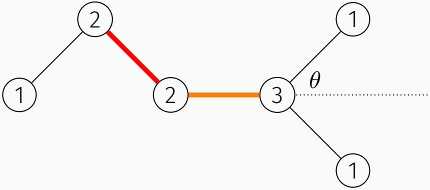




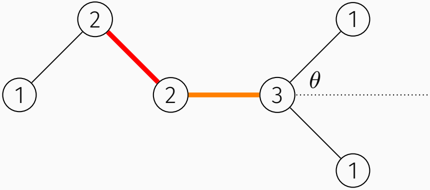


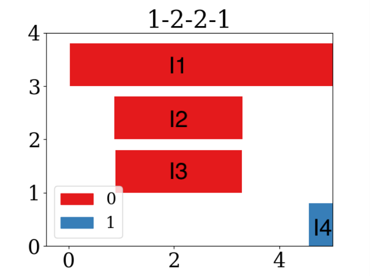


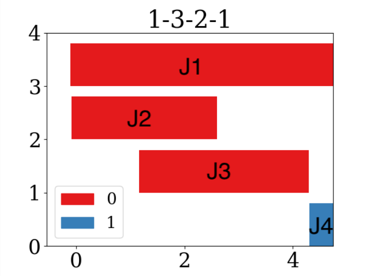
2,2-METHYLPENTANE



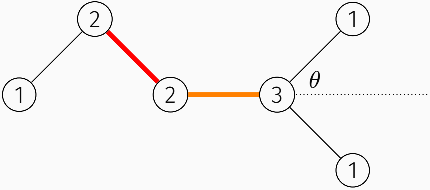
2,2-methylpentane

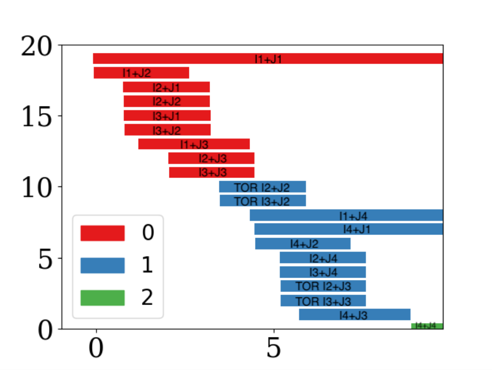


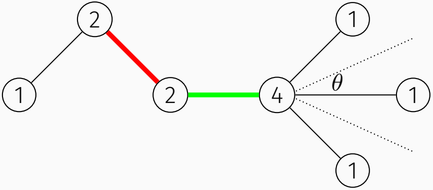




2,2-METHYLPENTANE






2
1
2
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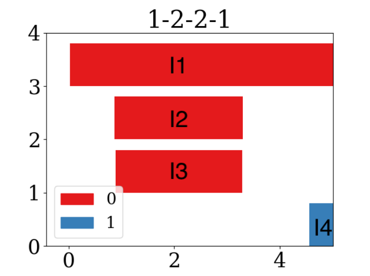
1
1


1-2-2-1
I1
I2
I3
I4
0
1
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2
3
4
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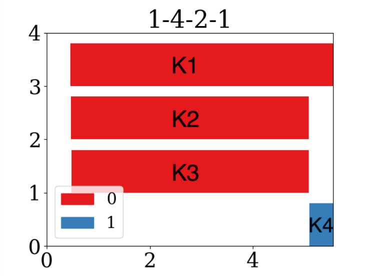
2
4


1-4-2-1
K1
K2
K3
K4
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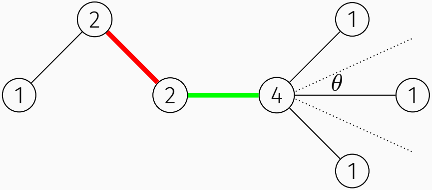
4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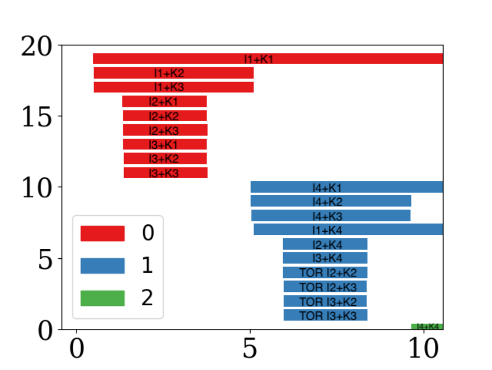
I1+K1
I1+K2
I1+K3
I2+K1
I2+K2
I2+K3
I3+K1
I3+K2
I3+K3
I4+K1
I4+K2
I4+K3
I1+K4
I2+K4
I3+K4
TOR I2+K2
TOR I2+K3
TOR I3+K2
TOR I3+K3
I4+K4
0
1
2
20
15
10
5
0
0
5
10

General Results

Remark 1

The energy landscape for any branched alkane, $f : (S^1)^n \to \mathbb{R}$ *has* $\binom{n}{k}$ *semi-infinite bars in dimension* k*.*

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Theorem 5 (S.)

The energy function of any branched alkane, $f : (S^1)^n \to \mathbb{R}$ can be decomposed into functions on each bond x-y where each function consists of dihedral types w-x-y-z. Thus, if c_i is the number of critical points for each bond, we have

$$2^n \text{ semi-infinite bars} + \frac{\prod_{i=1}^{n} c_i - 2^n}{2} \text{ finite bars.}$$

Theorem 6 (S.)

The sublevelset persistent homology on any analytical branched alkane with n internal bonds with potential energy landscape $f\colon (S^1)^n \mapsto \mathbb{R}$ *has* $\binom{n}{k} + (3^n - 1)\binom{n-1}{k}$ *persistent homology bars in dimension k.*

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The sublevelset persistent homology on any analytical branched alkane with n internal bonds with potential energy landscape $f\colon (S^1)^n \mapsto \mathbb{R}$ has $\binom{n}{k} + (3^n - 1)\binom{n-1}{k}$ persistent homology bars in dimension k.

Theorem 7 (S.)

Let $X_1, \ldots, X_n$ be a set of energy landscapes. Let $\{bcd(X_q)\}_{q=1}^{n}$ be the corresponding set of barcodes with bar lengths $\{\ell_r\}_{r=0}^{m}$, where $\ell_0 = \infty$ and all other lengths are ordered greatest to least (i.e. $\ell_r > \ell_{r+1}$). Let $x_{q,r}$ be the number of bars in $bcd(X_q)$ with length ℓ_r. Then, the number of bars of length ℓ_r in $bcd(X_1) \otimes_f \cdots \otimes_f bcd(X_q)$ is

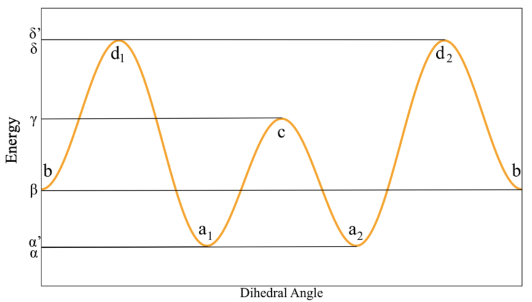
$$\mathrm{count}_n(r,0) - \mathrm{count}_n(r-1,0) + \mathrm{count}_n(r,1) - \mathrm{count}_n(r-1,1).$$

An example of sublevelset persistence characterization

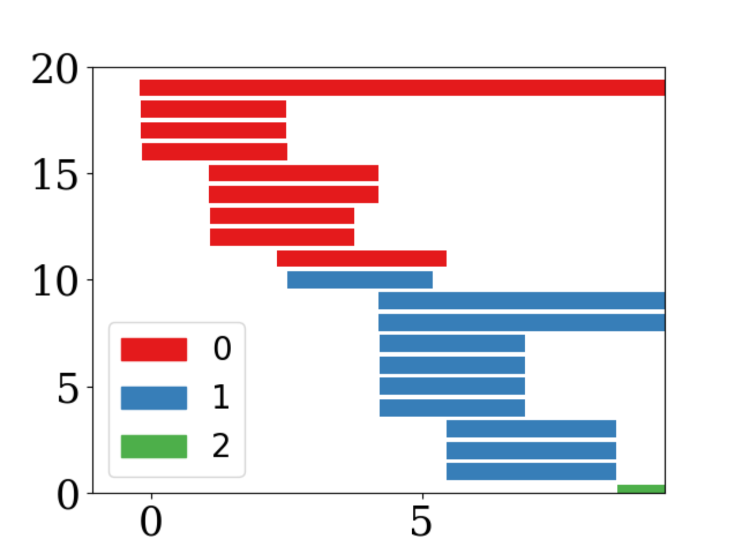
Goal: Completely characterize the sublevelset persistent homology of all branched alkanes consisting exclusively of 3-2 internal bonds

Original motivation: Polypropylene and Polybutylene (Plastics)

Internal bond 3-2



Example: Two 3-2 internal bond



Definition 8
Let $f\colon (S^1)^n \to \mathbb{R}$ be the branched alkane energy function with n internal 3-2 bonds, and let $k \leq n$ be the index of a critical point. Let $i_1 + i_2 \leq k$ and let $j_1 + j_2 \leq n - k$. We say that an index k critical point $(\phi_1, \ldots, \phi_n)$ of f is of $\mathrm{class}(n, k, i_1, i_2, j_1, j_2)$ if the list of points, $(\phi_1, \ldots, \phi_n)$, consists of the breakdown of critical points of the 3-2 bond, outlined below.

Type 1-3-2-1		
Critical Point	Feature Type	Number of copies
d_1	Local Max*	i_1
d_2	Global Max	i_2
c	Local Max	$k - i_1 - i_2$
a_1	Global Min	j_1
a_2	Local Min*	j_2
b	Local Min	$n - k - j_1 - j_2$

Note, the * denotes that the critical point has been shifted by ε, and hence, has switched from global to local.

Lemma 9 (S.)

The number of critical points of f *in each* $\mathrm{class}(n, k, i_1, i_2, j_1, j_2)$ *is*

$$\binom{n}{j_1, j_2, n-k-j_1-j_2, i_1, i_2, k-i_1-i_2}.$$

Lemma 9 (S.)
The number of critical points of f in each $\mathrm{class}(n, k, i_1, i_2, j_1, j_2)$ *is*

$$\binom{n}{j_1, j_2, n-k-j_1-j_2, i_1, i_2, k-i_1-i_2}.$$

Lemma 10 (S.)
For $f\colon (S^1)^n \to \mathbb{R}$ *where* $f(\phi_1, \ldots, \phi_n) = \sum_{i=1}^{n} f_{1\text{-}3\text{-}2\text{-}1}(\phi_i)$*, all critical points of* $\mathrm{class}(n, k, i_1, i_2, j_1, j_2)$ *have energy value*

$$E(n, k, i_1, i_2, j_1, j_2) = (j_1)\alpha + (j_2)\alpha' + (n-k-j_1-j_2)\beta + (k-i_1-i_2)\gamma + (i_1)\delta + (i_2)\delta'.$$

Theorem 11 (S.)

For any branched alkane consisting of n 3-2 internal bonds, consider the k-dimensional sublevelset persistent homology barcodes of the branched alkane energy landscape, $f_n : (S^1)^n \to \mathbb{R}$. Let $k \leq n$, $i_1 + i_2 \leq k$, and $j_1 + j_2 \leq n - k$. Hence, for any class$(n, k, i_1, i_2, j_1, j_2)$, the birth time of any k-dimensional bars in that class is

$$E(n, k, i_1, i_2, j_1, j_2) = (j_1)\alpha + (j_2)\overline{\alpha} + (n-k-j_1-j_2)\beta + (k-i_1-i_2)\gamma + (i_1)\delta + (i_2)\overline{\delta},$$

where the number of bars in that class is given below by:

- $i_1 = 0$, $i_2 = k$, $j_1 = n - k$, $j_2 = 0$ *gives*

$$\binom{n}{j_1, j_2, n-k-j_1-j_2, i_1, i_2, k-i_1-i_2}$$

semi-infinite bars,

Theorem 11 (S. – continued)

- $i_1 + i_2 = k$, $j_2 = 0$, $n - k < j_1$ *gives*

$$\sum_{\ell=0}^{i_1} (-1)^\ell \binom{n}{j_1, j_2, n-k-j_1-j_2+\ell, i_1-\ell, i_2, k-i_1-i_2}$$

  bars of length $\delta - \beta$,

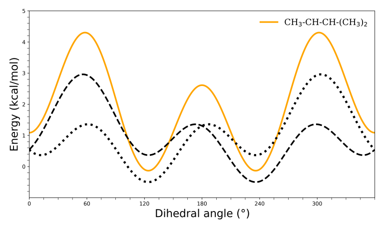
- $j_2 \neq 0$ *gives*

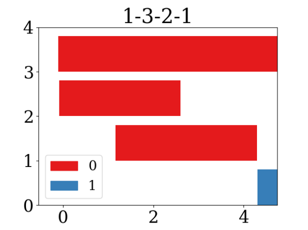
$$\sum_{\ell=0}^{k-i_1-i_2} (-1)^\ell \binom{n}{j_1, j_2+\ell, n-k-j_1-j_2, i_1, i_2, k-i_1-i_2-\ell}$$

  bars of length $\gamma - \alpha$, *and*

- *0 bars born for any other type of critical point.*

- Split critical points into appropriate classes
  - Introduce perturbation by ε
- Identify which classes correspond to which bar lengths
  - For example, $j_2 \neq 0$ gives classes that correspond to bars of length $\gamma - \alpha$
- Figure out which classes results in the death of bars from other classes
  - For $\gamma - \alpha$ length bars, class$(n, k, i_1, i_2, j_1, j_2)$ kills bars from class$(n, k-1, i_1, i_2, j_1, j_2+1)$
- Count via induction on number of internal bonds



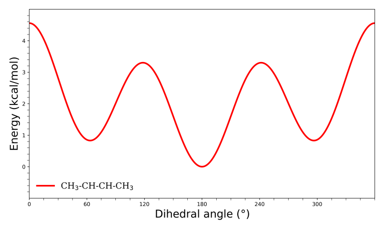


Another example of sublevelset persistence characterization

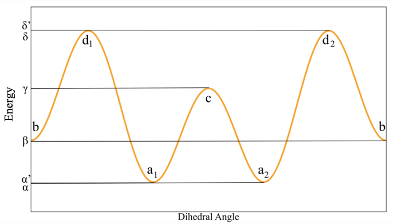
Goal: Completely characterize the sublevelset persistent homology of all branched alkanes consisting exclusively of 2-2 and 3-2 internal bonds

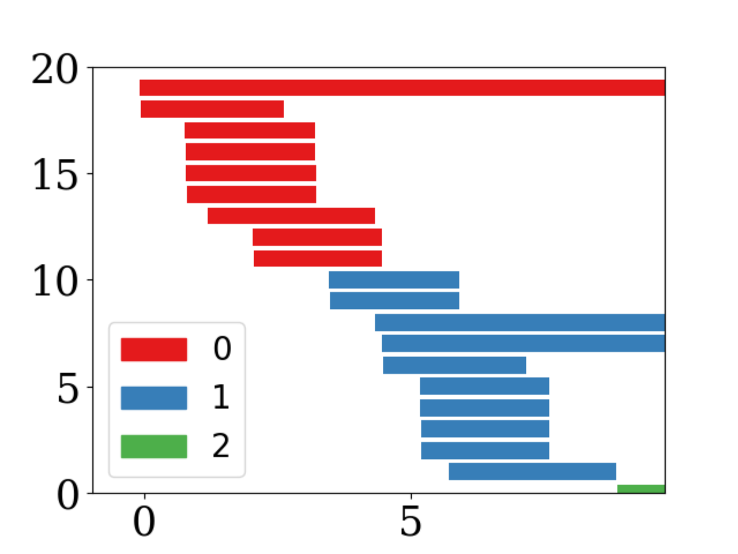
Motivation: Show how we can characterize for two different internal types. This will allow us to describe the characterization process.

Internal bond 2-2



Internal bond 3-2




20
15
10
5
0
0
5
0
1
2

Just like last time, we define a class of critical points:

$$class\left(\begin{bmatrix} n_1 & k_1 & i_{11} & 0 & j_{11} & 0 \\ n_2 & k_2 & i_{21} & i_{22} & j_{21} & j_{22} \end{bmatrix}\right).$$

We count the number of points in each class,

$$\left|class\left(\begin{bmatrix} n_1 & k_1 & i_{11} & 0 & j_{11} & 0 \\ n_2 & k_2 & i_{21} & i_{22} & j_{21} & j_{22} \end{bmatrix}\right)\right| =$$

$$2^{n_1-i_{11}-j_{11}}\binom{n_1}{i_{11}, k_1-i_{11}, j_{11}, n_1-k_1-j_{11}}\binom{n_2}{i_{21}, i_{22}, k_2-i_{21}-i_{22}, j_{21}, j_{22}, n_2-k_2-j_{21}-j_{22}}$$

We also find the energy value associated to each class:

$$E\left(class\left(\begin{bmatrix} n_1 & k_1 & i_{11} & 0 & j_{11} & 0 \\ n_2 & k_2 & i_{21} & i_{22} & j_{21} & j_{22} \end{bmatrix}\right)\right) =$$
$$(j_{11})\alpha_1 + (n_{11}-k_{11}-j_{11})\beta_1 + (k_1-i_{11})\gamma_1 + (i_{11})\delta_1$$
$$+ (j_{21})\alpha_2 + (j_{22})\alpha_2' + (n_2-k_2-j_{21}-j_{22})\beta_2 + (k_2-i_{21}-i_{22})\gamma_2 + (i_{21})\delta_2 + (i_{22})\delta_2'.$$

Theorem 12 (S.)

For any branched alkane consisting of n_1 internal bonds of type 2-2 and n_2 internal bonds of type 3-2, consider the k-dimensional sublevelset persistent homology barcodes of the branched alkane energy landscape, $f\colon (S^1)^n \to \mathbb{R}$. Let $k = k_1 + k_2$, $k_1 + k_2 \leq n_1 + n_2$, $i_{11} + i_{21} + i_{22} \leq k_1 + k_2$, $i_{11} \leq k_1$, $i_{21} + i_{22} \leq k_2$, $j_{11} + j_{21} + j_{22} \leq n_1 + n_2 - k_1 - k_2$, $j_{21} + j_{22} \leq n_2 - k_2$, and $j_{11} \leq n_1 - k_1$. Hence, for any class $\left(\begin{bmatrix} n_1 & k_1 & i_{11} & 0 & j_{11} & 0 \\ n_2 & k_2 & i_{21} & i_{22} & j_{21} & j_{22} \end{bmatrix}\right)$, the birth time of any k-dimensional bars in that class is

$$E\left(class\left(\begin{bmatrix} n_1 & k_1 & i_{11} & 0 & j_{11} & 0 \\ n_2 & k_2 & i_{21} & i_{22} & j_{21} & j_{22} \end{bmatrix}\right)\right) =$$

$$\begin{aligned} &(j_{11})\alpha_1 + (n_{11} - k_{11} - j_{11})\beta_1 + (k_1 - i_{11})\gamma_1 + (i_{11})\delta_1 \\ &+ (j_{21})\alpha_2 + (j_{22})\alpha_2' + (n_2 - k_2 - j_{21} - j_{22})\beta_2 + (k_2 - i_{21} - i_{22})\gamma_2 + (i_{21})\delta_2 + (i_{22})\delta_2'. \end{aligned}$$

where the number of bars born in that class is given below by:

Theorem 12 (S. – Continued)

1. $i_{11}+i_{22}=k_1+k_2$, $i_{21}=0$, $j_{22}=0$, $(n_1+n_2)-(k_1+k_2)=j_{11}+j_{21}$ *gives*

$$\left|class\left(\begin{bmatrix} n_1 & k_1 & i_{11} & 0 & j_{11} & 0 \\ n_2 & k_2 & i_{21} & i_{22} & j_{21} & j_{22} \end{bmatrix}\right)\right|$$

semi-infinite bars,

2. $i_{11}+i_{22}=k_1+k_2$, $j_{22}=0$, $n_1-k_1-j_{11}=0$, *and* $(n_1+n_2)-(k_1+k_2)>j_{11}+j_{21}$ *gives*

$$\sum_{\ell'=0}^{i_{21}}(-1)^{\ell}\left[\binom{n_1}{i_{11},k_1-i_{11},j_{11},n_1-k_1-j_{11}}\binom{n_2}{i_{21}-\ell,i_{22},k_2-i_{21}-i_{22},j_{21},j_{22},n_2-k_2-j_{21}-j_{22}+\ell}\right]$$

bars of length $\delta_2-\beta_2$,

Theorem 12 (S. – Continued)

3. *$j_{22} > 0$ and $i_{11} + j_{11} > 0$ gives*

$$\sum_{\ell=0}^{k_2-i_{21}-i_{22}} (-1)^\ell \left[\binom{n_1}{i_{11}, k_1 - i_{11}, j_{11}, n_1 - k_1 - j_{11}} \binom{n_2}{i_{21}, i_{22}, k_2 - i_{21} - i_{22} - \ell, j_{21}, j_{22} + \ell, n_2 - k_2 - j_{21} - j_{22})!} \right]$$

bars of length $\gamma_2 - \alpha_2$, and

4. *$n_1 - k_1 - j_{11} > 0$ gives*

$$2^{n_1-i_{11}-j_{11}} \sum_{\ell=0}^{k_1-i_{11}} (-1)^\ell \left[\binom{n_1}{i_{11}, k_1 - i_{11} - \ell, j_{11}, n_1 - k_1 - j_{11} + \ell} \binom{n_2}{i_{21}, i_{22}, k_2 - i_{21} - i_{22}, j_{21}, j_{22}, n_2 - k_2 - j_{21} - j_{22}} \right]$$

bars of length $\gamma_1 - \beta_1$, and

5. *0 bars born for any other type of critical point.*

Let f be an energy landscape such that $f\colon (S^1)^n \to \mathbb{R}$ where $f(\phi_1, \ldots, \phi_n) = g_1(\phi_1) + \ldots + g_n(\phi_n)$. To characterize the sublevelset persistence,

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1. Identify the different bar lengths in all component functions. These lengths will be used to partition the classes.
   –For the 3-2/2-2 case, we had 4; semi-infinite, $\delta_2 - \beta_2$, $\gamma_2 - \alpha_2$, and $\gamma_1 - \beta_1$

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2. Construct the class matrix.
   –$class\left(\begin{bmatrix} n_1 & k_1 & i_{11} & 0 & j_{11} & 0 \\ n_2 & k_2 & i_{21} & i_{22} & j_{21} & j_{22} \end{bmatrix}\right)$

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3. Determine the number of points in each class.
   –Start with the multinomial coefficient and adjust as needed ($2^{n_1 - i_{11} - j_{11}}$)

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4. Identify which classes correspond to which bar length and energy value.
   –These are the restrictions on j_{22}, j_{11}, etc.
5. Count the number of bars created by each class.
   –The alternating sums in both theorems, birth classes will pair with death classes and each pair is dependent on bar length

Future work

- Applications to polymers and plastics – in progress with Adams, Clark, and Sadhu
- Change generalization of 1-x-y-1 to w-x-y-z
- Look at other inputs: bond length, type of bond, etc.
- Other structures: alkenes, alkynes, cyclo-alkanes, etc.
- Non-organic compounds

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Questions?