javaPlex – persistent homology in Java

Andrew Tausz     Mikael Vejdemo-Johansson

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Persistent homology

In a large variety of areas we encounter the following fundamental problem:

**Problem**
Estimate topological features of a shape based on a family of sample points (*point clouds*).

**Applications**

- The space of natural $3 \times 3$ pixel patches is a Klein bottle.
- This Klein bottle yields new techniques for analyzing textures.
- Shape matching and shape databases.
- Filtering materials databases for high $CO_2$ adsorbitivity.
- Verifying sensor coverage for plane regions.
Persistent homology

Our favourite solution is due to Edelsbrunner, Letscher and Zomorodian.

Solution
Čech complexes, Vietoris-Rips complexes, $\alpha$-shapes and several other constructions capture by a filtered simplicial complex stemming from intersection relations of disks centered on the sample points.

Persistent homology tracks the changes in topological features, and picks out such features that remain present over a long time.
Persistent homology

Point cloud

Building complex
  Complexity: clique enumeration

Filtered simplicial complex

Compute homology
  Complexity: Worst case $O(n^3)$, typical $O(n)$

Betti barcode
Vietoris-Rips complex
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History of Plex

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1. Plex
2. JPlex
History of Plex

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1. Plex – C++, Matlab through MEX, memory hog
2. Jplex – Java, Matlab natively, BeanShell, highly optimized
Design properties for JAVAPLEX

JAVAPLEX grew out of dissatisfaction with both PLEX and JPlex.

Disadvantages

PLEX

- Dependent on exact Matlab version and MEX dialect
- Design carrying very many pointers: high memory consumption

JPlex

- Too highly optimized: no real capacity to extend or modify
- Not actually competitive enough to motivate this
Usage examples

This is joint work with David Eklund, Jonathan Hauenstein, Martina Scolamiero, and Chris Peterson.

**Application**

Consider as a linkage the configurations of cyclo-octane ($C_8H_{16}$). The carbon bonds in this have fixed length, and an angle of \( \arccos(-1/3) \approx 109.47 \). By fixing one carbon atom at the origin, and its closest neighbours at \((1, 0, 0)\) and \((-\frac{1}{3}, \frac{2}{3} \sqrt{2}, 0)\), we may study the distribution of the remaining atoms. The variety of possible configurations is a surface in \( \mathbb{R}^{15} \).

This variety was first described by *Martin, Thompson, Coutsias, and Watson* in *Topology of cyclo-octane energy landscape*. J. Chem. Phys. 132, 234115 (2010).
We sample, using \textsc{Bertini}, points on the real singular locus of the cyclo-octane variety. Using \textsc{Matlab} and \textsc{javaPlex}, we create a witness complex on 100 out of 1606 sampled points:
Cyclo-octane

```matlab
>> load Distances.out;
>> m_space = metric.impl.ExplicitMetricSpace(Distances);
>> diam = metric.utility.MetricUtility.estimateDiameter(m_space);
>> r_max = diam/2
ans = 3.1017
>> landmarks = api.Plex4.createMaxMinSelector(m_space,100);
>> stream = api.Plex4.createWitnessStream(landmarks,3,r_max/2);
>> stream.getSize()
ans = 11418
>> persistence = api.Plex4.getDefaultSimplicialAlgorithm(3);
>> fii = persistence.computeIntervals(stream);
>> fvi = stream.transform(fii);
>> api.Plex4.createBarcodePlot(fvi,'witness',r_max/2);
```
Cyclo-octane

From the Matlab code above, we acquire the Betti barcodes:

Which is strongly consistent with the structure of the singular set from Martin, Thompson, Coutsias, and Watson as a pair of disjoint circles.

The entire computation runs in 6 seconds. (mean running time for 10 runs, std.dev. 0.8s)
Cyclo-octane

- Computation with coefficients in $\mathbb{F}_2$ and $\mathbb{F}_3$ to look for torsion.
- Witness complex with 500 landmarks.
- Total complex 26M simplices.
- Computation time: 3 days.
- Severe memory issues.
- Surprising lack of difference between $\mathbb{F}_2$ and $\mathbb{F}_3$: torsion killed by particular intersection of sphere and Klein bottle.
Access to the package

Software package
Published on http://code.google.com/p/javaplex

JavaDoc documentation
Linked from software homepage.

Usage tutorial
Linked from software homepage. Thanks to Henry Adams for adapting the jPlex tutorial to javaPlex.

Questions or comments?