

# CS 6170: Computational Topology, Spring 2019

## Lecture 21

Topological Data Analysis for Data Scientists

Dr. Bei Wang

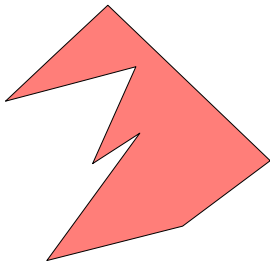
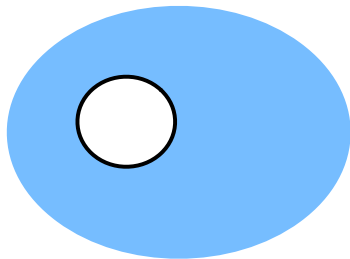
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March 26, 2019

## Simply Connectedness

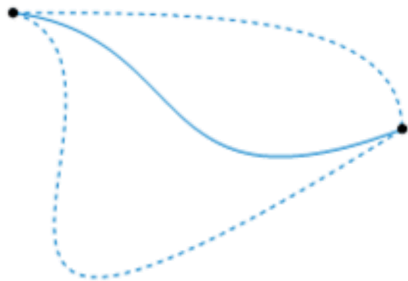
## Simply connected topological space

- A topological space is simply connected if it is path-connected and every path between two points can be *continuously* transformed into any other such path while preserving the endpoints.



# Homotopy

- A *homotopy* between two continuous functions  $f, g : \mathbb{X} \rightarrow \mathbb{Y}$  is defined to be a *continuous* function  $H : \mathbb{X} \times [0, 1] \rightarrow \mathbb{Y}$  such that, if  $x \in \mathbb{X}$  then  $H(x, 0) = f(x)$ , and  $H(x, 1) = g(x)$ .
- A *homotopy* between two continuous functions  $f, g : \mathbb{X} \rightarrow \mathbb{Y}$  is a family of continuous functions  $h_t : \mathbb{X} \rightarrow \mathbb{Y}$  for  $t \in [0, 1]$  such that  $h_0 = f$  and  $h_1 = g$ , and the map  $(x, t) \mapsto h_t(x)$  is *continuous* from  $\mathbb{X} \times [0, 1]$  to  $\mathbb{Y}$ .
- The two versions coincide by setting  $h_t(x) = H(x, t)$ .



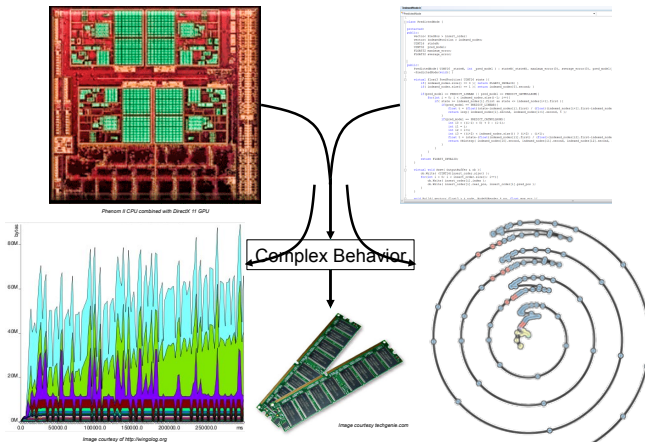
## Simply connected topological space

- A topological space  $\mathbb{X}$  is *simply connected* if it is path-connected and any loop in  $\mathbb{X}$  defined by  $f : \mathbb{S}^1 \rightarrow \mathbb{X}$  can be contracted to a point.
- $\mathbb{X}$  is *simply connected* if and only if it is *path-connected*, and whenever  $p : [0, 1] \rightarrow \mathbb{X}$  and  $q : [0, 1] \rightarrow \mathbb{X}$  are two paths (i.e.: continuous maps) with the same start and endpoint  $p(0) = q(0)$  and  $p(1) = q(1)$ , then  $p$  can be continuously deformed into  $q$  while keeping both endpoints fixed.
- Explicitly, there exists a continuous homotopy  $F : [0, 1] \times [0, 1] \rightarrow \mathbb{X}$  such that  $F(x, 0) = p(x)$  and  $F(x, 1) = q(x)$ .
- $\mathbb{X}$  is *path-connected* if there is a path joining any two points in  $\mathbb{X}$ .

TDA: Relation to Time Series Analysis  
Choudhury et al. (2012)

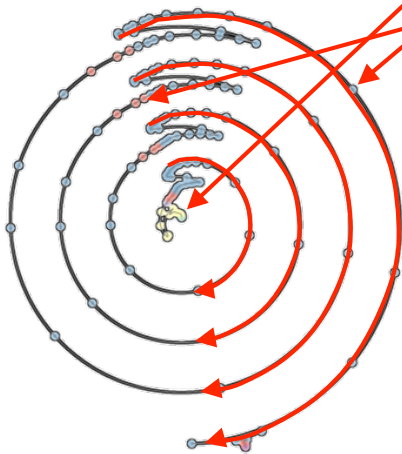
# A story from software visualization

- Detecting circular structures in memory reference traces
- Takens embedding
- Capture recurrent nature of the program

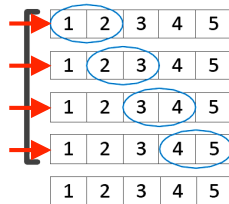


# Example

Visualize circular structures in memory access patterns

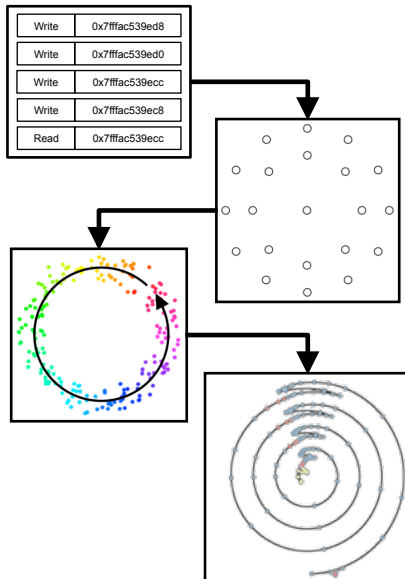


```
File: sort.cpp
1: void bubblesort(std::vector<double>& v){
2:   for(unsigned end=v.size()-1; end >= 0; end--){
3:     bool swapped = false;
4:     for(unsigned i=0; i<end; i++){
5:       if(v[i] > v[i+1]){
6:         std::swap(v[i], v[i+1]);
7:         swapped = true;
8:       }
9:     }
10:    if(!swapped) break;
11:  }
12: }
```





# System pipeline



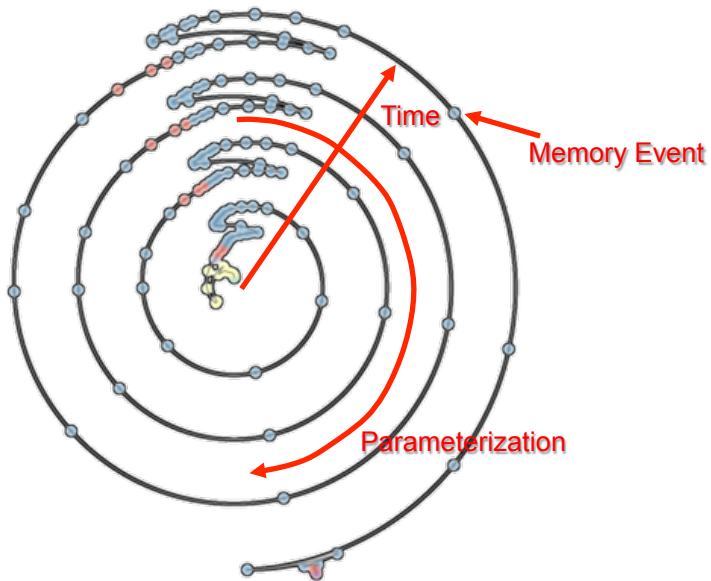
# Capture a memory reference trace

```
File: sort.cpp
1: void bubblesort(std::vector<double>& v){
2:   for(unsigned end=v.size()-1; end >= 0; end--){
3:     bool swapped = false;
4:     for(unsigned i=0; i<end; i++){
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9:     }
10:    if(!swapped) break;
11:  }
12:}
```



Write	0x7fffac539ed8
Write	0x7fffac539ed0
Write	0x7fffac539ecc
Write	0x7fffac539ec8
Read	0x7fffac539ecc
Read	0x7fffac539ec8
Write	0x7fffac539eb8
Write	0x7fffac539eb0

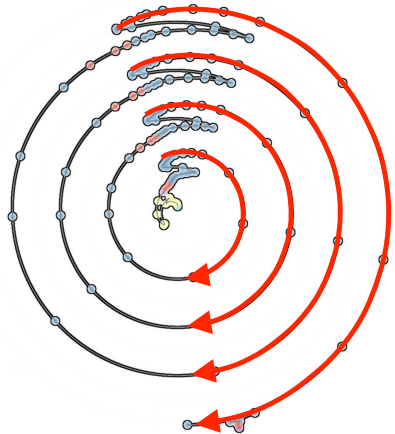
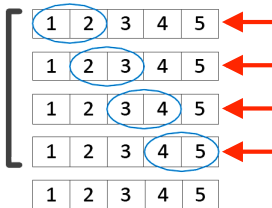
# Visualization



# Data dependent structure

# loops = # comparisons

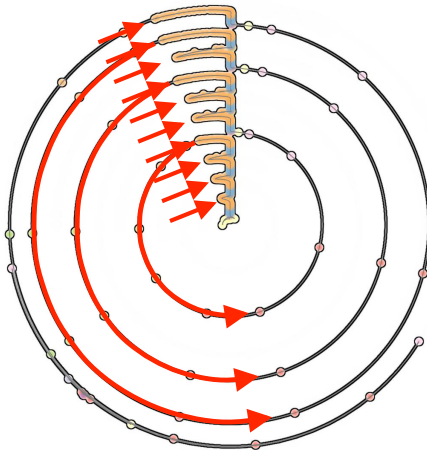
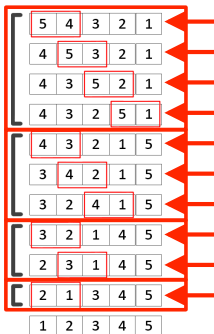
```
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7:         swapped = true;
8:       }
9:     }
10:    if(!swapped) break;
11:  }
12: }
```



# Data dependent structure

# teeth = # swaps

```
File: sort.cpp
1: void bubblesort(std::vector<double>& v){
2:   for(unsigned end=v.size()-1; end >= 0; end--){
3:     bool swapped = false;
4:     for(unsigned i=0; i<end; i++){
5:       if(v[i] > v[i+1]){
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7:         swapped = true;
8:       }
9:     }
10:    if(!swapped) break;
11:  }
12: }
```

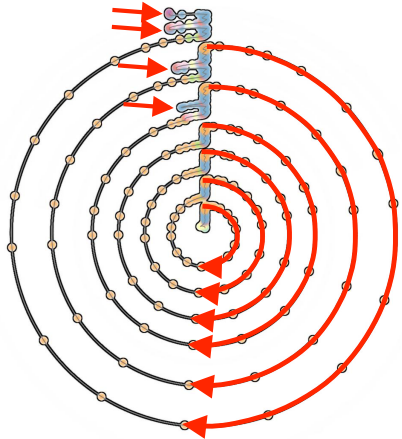
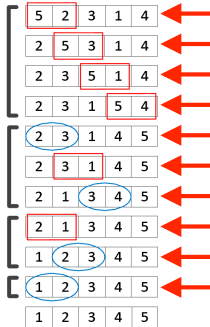


# Data dependent structure

# teeth = # comparisons

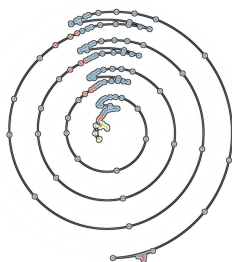
# loops = # comparisons and swaps

```
File: sort.cpp
1: void bubblesort(std::vector<double>& v){
2:   for(unsigned end=v.size()-1; end >= 0; end--){
3:     bool swapped = false;
4:     for(unsigned i=0; i<end; i++){
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6:         std::swap(v[i], v[i+1]);
7:         swapped = true;
8:       }
9:     }
10:    if(!swapped) break;
11:  }
12: }
```

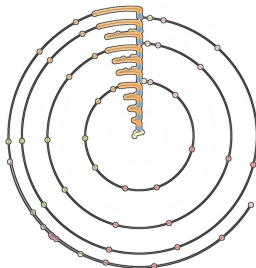


# Data dependent structure

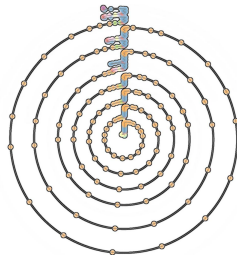
1	2	3	4	5
1	2	3	4	5
1	2	3	4	5
1	2	3	4	5
1	2	3	4	5



5	4	3	2	1
4	5	3	2	1
4	3	5	2	1
4	3	2	5	1
4	3	2	1	5
3	4	2	1	5
3	2	4	1	5
3	2	1	4	5
2	3	1	4	5
2	1	3	4	5
1	2	3	4	5

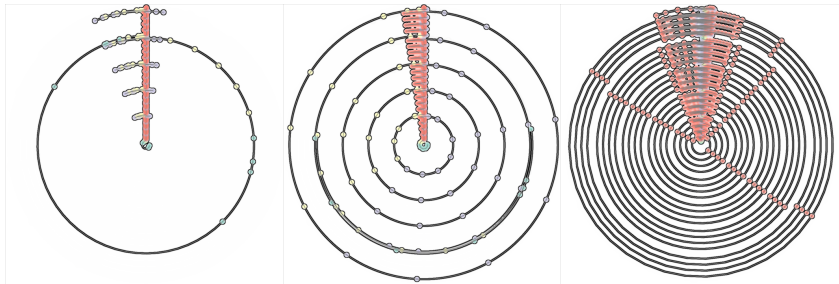


5	2	3	1	4
2	5	3	1	4
2	3	5	1	4
2	3	1	5	4
2	3	1	4	5
2	3	1	4	5
2	1	3	4	5
2	1	3	4	5
1	2	3	4	5
1	2	3	4	5



# Algorithm dependent structure

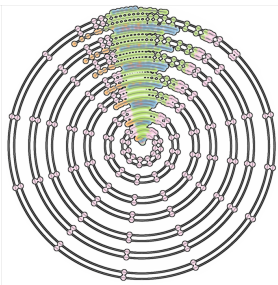
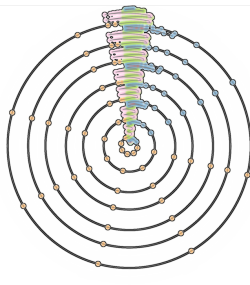
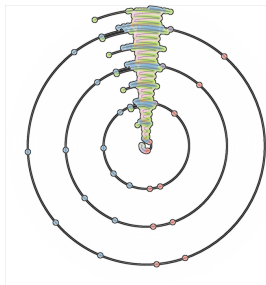
```
File: matmult.cpp
1: unsigned int i, j, k;
2: for (i = 0; i < N; i++)
3:   for (j = 0; j < N; j++)
4:     for (k = 0; k < N; k++)
5:       linC[i*N + j] += linA[i*N + k] * linB[k*N + j];
```





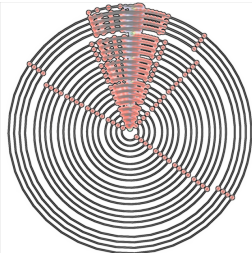
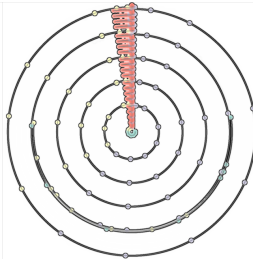
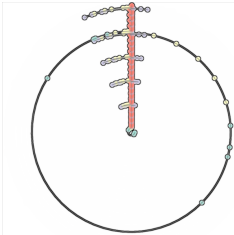
# Algorithm dependent structure

```
File: blocked-matmult.cpp
1: unsigned int i, j, k, j0, k0;
2: for (k0 = 0; k0 < N; k0 += b)
3:   for (j0 = 0; j0 < N; j0 += b)
4:     for (i = 0; i < N; i++)
5:       for (k = k0; k < min(k0 + b, N); k++) {
6:         r = linA[i*N + k];
7:         for (j = j0; j < min(j0 + b, N); j++)
8:           linC[i*N + j] += r*linB[k*N + j];
9:       }
```

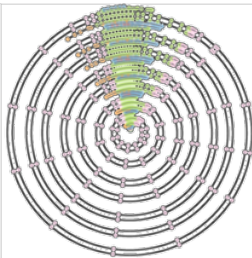
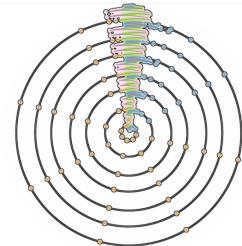
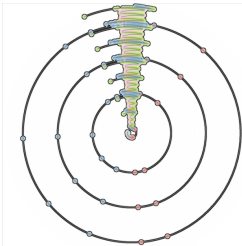


# Algorithm dependent structure

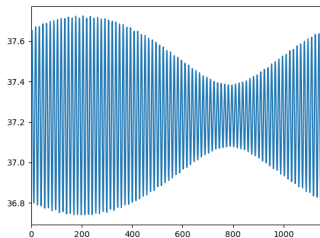
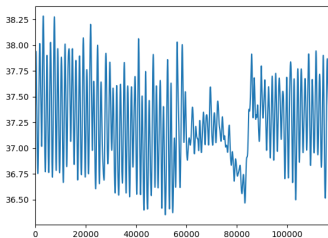
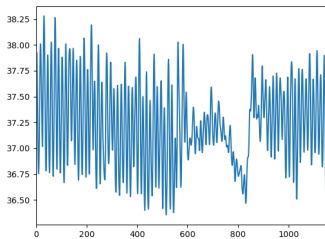
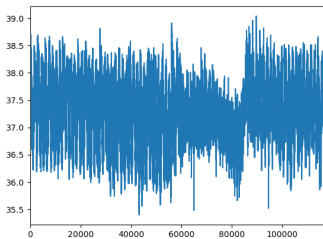
Naïve Matrix  
Multiply



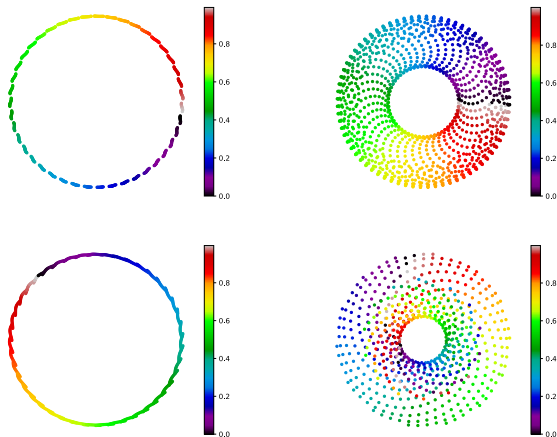
Blocked Matrix  
Multiply



# A story from mice pregnancy detection

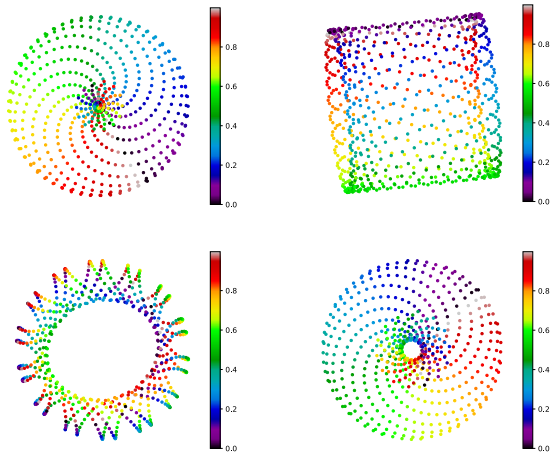


# A story from mice pregnancy detection



Which mice are pregnant? Joint work with Benjamin Smarr.  
Data from Smarr et al. (2016).

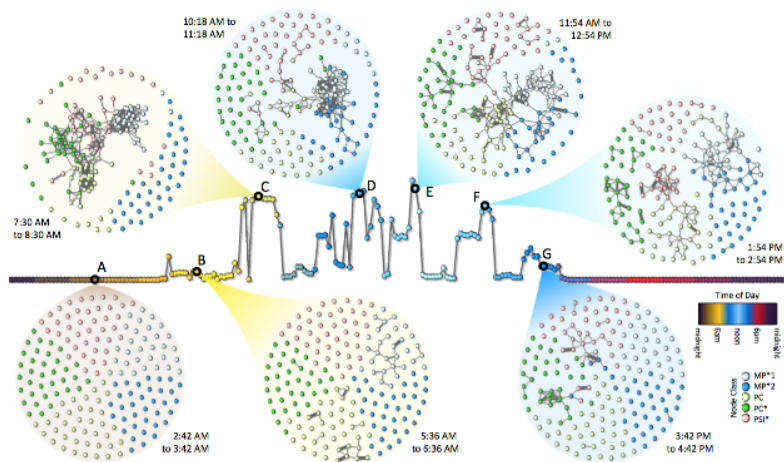
# Jet lagged mice



Which jet lagged mice are pregnant?

# Persistent homology of time-varying networks

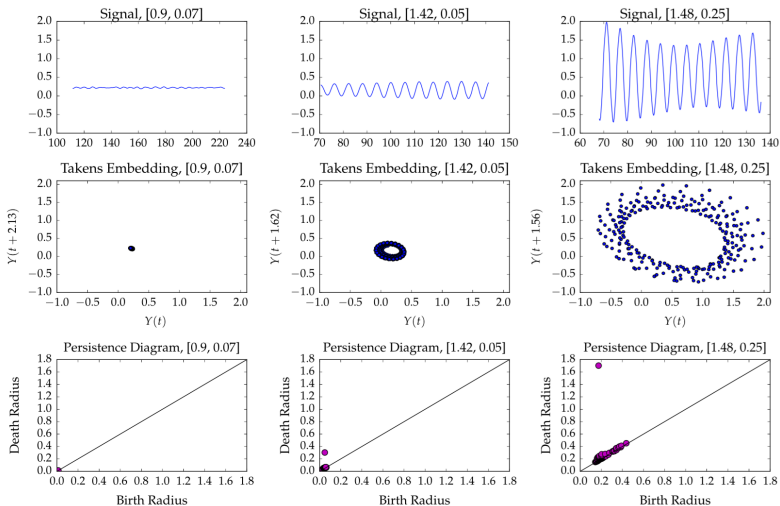
Visual detection of structural changes in time-varying graphs using persistent homology.



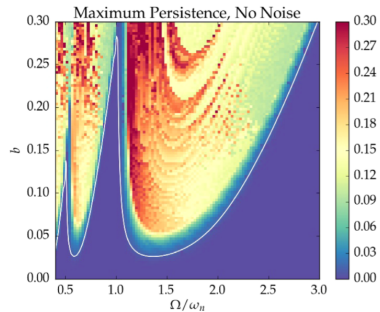
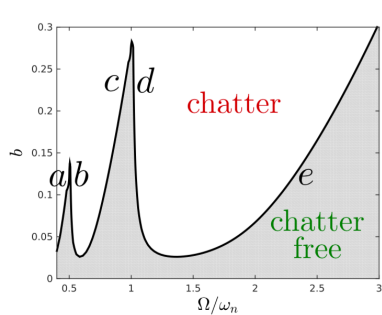
Hajj et al. (2018)

# Takens embedding

Maximal persistence: Khasawneh and Munch (2016)



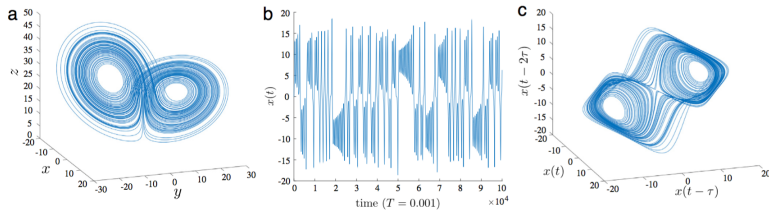
# Chatter detection



Khasawneh and Munch (2016)



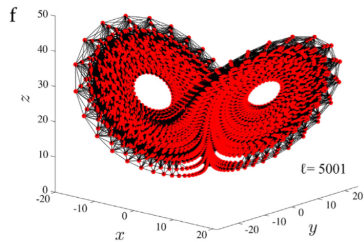
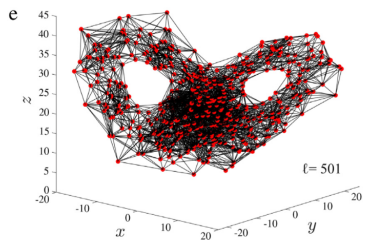
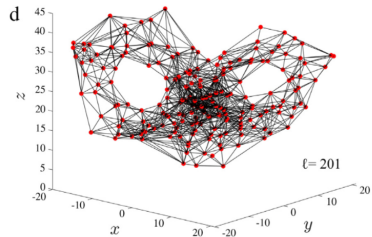
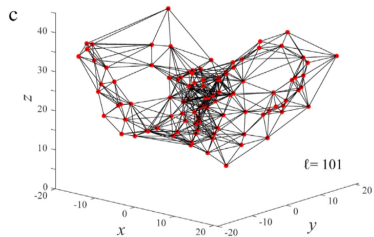
# Reconstruct dynamics using witness complexes



**Fig. 1.** Classic Lorenz attractor ( $r = 28$ ,  $b = 8/3$ ,  $\sigma = 10$ ): (a) A  $10^5$ -point trajectory in  $\mathbb{R}^3$  generated using fourth-order Runge-Kutta with a time step of  $T = 0.001$ . (b) A time-series trace of the  $x$  coordinate of that trajectory. (c) A 3D projection of a delay-coordinate embedding with dimension  $m = 5$  and delay  $\tau = 174T$ , following (1).

Garland et al. (2016)

# Reconstruct dynamics using witness complexes



Garland et al. (2016)

- Choudhury, A. I., Wang, B., Rosen, P., and Pascucci, V. (2012). Topological analysis and visualization of cyclical behavior in memory reference traces. *IEEE Pacific Visualization Symposium (PacificVis)*, pages 9–16.
- Garland, J., Bradley, E., and Meiss, J. D. (2016). Exploring the topology of dynamical reconstructions. *Physica D: Nonlinear Phenomena*, 334(1):49–59.
- Hajij, M., Wang, B., Scheidegger, C., and Rosen, P. (2018). Visual detection of structural changes in time-varying graphs using persistent homology. *IEEE Pacific Visualization Symposium (PacificVis)*.
- Khasawneh, F. A. and Munch, E. (2016). Chatter detection in turning using persistent homology. *Mechanical Systems and Signal Processing*, 70-71:527–541.
- Smarr, B. L., Zucker, I., and Kriegsfeld, L. J. (2016). Detection of successful and unsuccessful pregnancies in mice within hours of pairing through frequency analysis of high temporal resolution core body temperature data. *PLoS One*.