Introduction to Topological Data Analysis

Persistent Homology

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Mathematical Theory Not Presented

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- We'll skip the abstract, math grad student-level theory. :-)
- Much of it of limited relevance to the simple method I'll use here as my running example.

Broad Overview

- Determine "what is connected to what" in dataset.
- Definition of *connected* depends on the application and possibly the ingenuity of the analyst.
- Do this in each of a sequence of steps.
- Each step produces some kind of data summarizing connectivity in that step. The data is collectively called a *filtration*.
- Use that output data as features, e.g. to do classification.

Image Classification Example

Image Classification Example

- TDA can be applied to many kinds of data, but we'll focus mainly on image classification here.
- The famous MNIST data, hand-drawn digits. Predict what digit it is, by analyzing the pixels (28×28).
- Not just greyscale, but mainly black-and-white. Here I'll look only at pixels > 192 level.

Filtration Method in This Example

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- For simplicity, I'll first use a somewhat nonstandard TDA method, which I'll call the *Sweep method*.
- May or may not be better than other methods.
- But is simple, easy to explain and draw.
- **Just an example**.

Crucial Need for Dimension Reduction

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- In MNIST case, we are predicting digit from $28^2 = 784$ features.
- 784 way too large: (a) Overfitting. (b) Horrendous computation needs.
- So, we need to convert the existing 784 features to a smaller number (*dimension reduction*). But how?

Dimension Reduction Methods for Images

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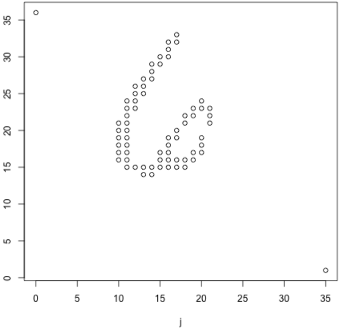
- Principal Components Analysis (PCA)
    - A traditional approach. Project the data from R^{784} to, say, R^{50}, using eigenanalysis.
    - Tacitly linear, but can form polynomial terms before compute PCA.
- Convolutional Neural Networks (CNNs)
    - Currently most fashionable.
    - Not new! The "C" part of CNN is just **traditional image smoothing**: break image into tiles, and then finding the median or max pixel intensity in each tile. In MNIST, take 4×4 tiles, stride 4, so now have $7^2 = 49$ predictors.
- Geometric methods:
    - Runs statistics (RLRN): counts of how many consecutive vertical, horizontal or diagonal pixels are black, etc.
    - TDA.

A '6'

A '6'



Filtration plan:

- Draw a series of horizontal lines.
- See how many components are formed in the figure by a line.

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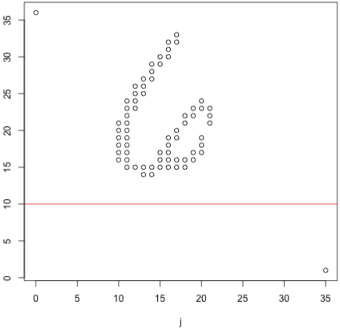
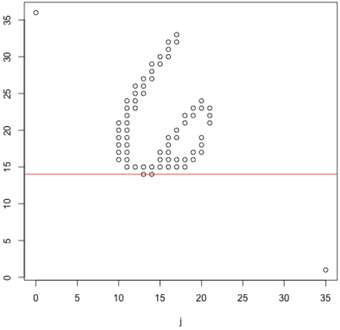


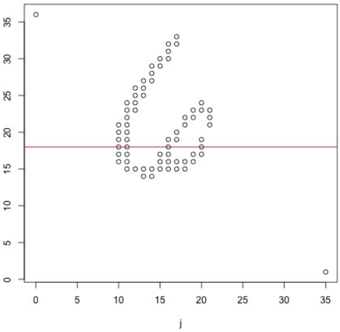
E.g. line at row 10. 0 components

A '6'



Line at row 14: 1 component.

A '6'



Line at row 18: 3 components

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Birth, Death Times

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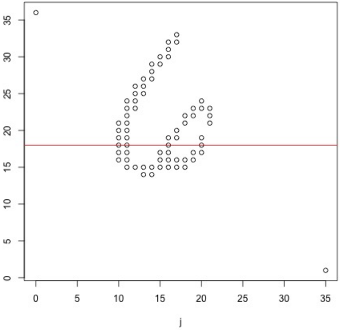
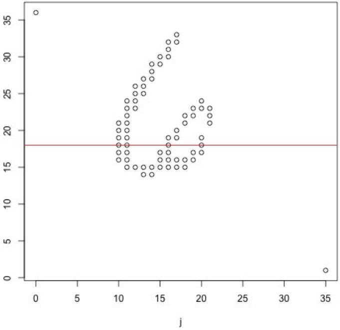


We talk about *birth* and *death* times. E.g. the first 3-component line is "born" at row 17 and "dies" at row 25.

Birth, Death Times



We talk about *birth* and *death* times. E.g. the first 3-component line is "born" at row 17 and "dies" at row 25. Those pairs, e.g. (17,25), form our dimension-reduced data.

A '7'

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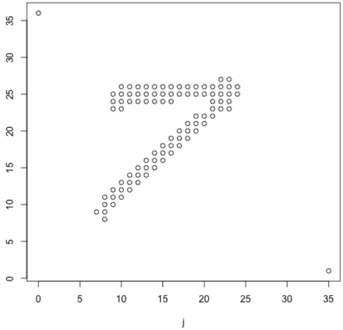
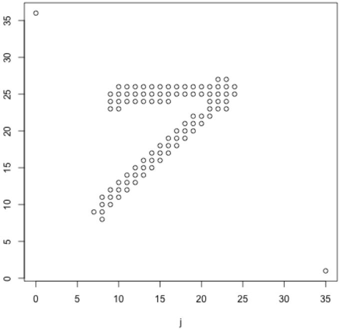


A 1-component line will be born at row 8, then die at row 23.

A '7'



A 1-component line will be born at row 8, then die at row 23. Then we get a 2-component birth, not long-lived, rows 23-24 only.

'6' vs. '7'

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'6'	3-comps., then 1-comps.
'7'	1-comps., then 2-comps.

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- But what if the top bar of a '7' is angled slightly up, not down? Then only have 1-comps.

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So, our new features could be the two sets of BD data, horizontal and vertical sweeps.

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- In the CNN case, the tiles have weights, which vary over the iterations. But these weights have direct analogs in the other ML methods, e.g. coefficients in logit.

Notes

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- For color images, calculate BD data for R, G, B.
- Various *persistence diagrams* to plot BD data.
- Have lots of non-image applications too. E.g. Kurlin *et al*, (2018) use moisture data at various altitudes to predict atmospheric rivers.

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- **Vectorization:** Different images for the same digit have different numbers of BD pairs. But ML methods require the feature vector to have a constant number of features from one data point to another (in this case one image to another), the 49 in our 65000×49 example above.

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- **Anomalous BDs:** Sometimes have fainter pixels than our 192 threshold. E.g. row 20 in the '6' had a gap. Causes an incorrect birth/death.
- **Vectorization:** Different images for the same digit have different numbers of BD pairs. But ML methods require the feature vector to have a constant number of features from one data point to another (in this case one image to another), the 49 in our 65000×49 example above.
- **Orientation:**The above filtration scheme largely assumed:
  - Mainly black-and-white image, not really greyscale.
  - Image has a notion of left-right, up-down.

  Not true for, e.g., histology slides.

Possible Solutions: Anomalous BDs

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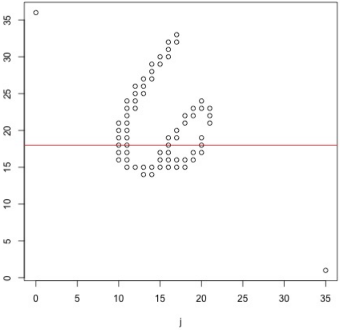

- Ignore row 20 in the BD calculation (e.g. D - B = 1).
- But what if the row is real? Are there 1-row comps. in most images of this digit?
- Maybe do BD at each of several pixel intensity thresholds, e.g. 64, 128, 192.

Possible Solutions: Vectorization

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- **Grid counts:**
  - Say have 35-row, 35-column images, so that (B,D) pairs are in the range 1 to 35.
  - Construct a "2-D histogram" (counts only, not graphed), with bin size, say, 5×5.
  - So we have a grid, $1 \leq i \leq j \leq 7$), a total of 28 points.
  - For each image, calculate the count of (B,D) pairs at each grid point. Do the same for the red vertical lines.
  - Our new data matrix is 65000×56. Feed that into SVM, NN, RF, logit, whatever.

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- **Ad hoc:**
  - For a large, detailed images, the above method may need voluminous computation and/or lead to overfitting.
  - Some analysts devise their own *ad hoc* method.
  - E.g. Garside (2019) compute a vector consisting of the number of pixels, average lifetime, area under the persistence function, and four measures based on polygons drawn in the persistence graph.

Possible Solutions: Orientation

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Most filtration methods for images don't assume the image has a left and right, up and down. (More on this shortly.)

(Vietoris-)Rips Filtrations

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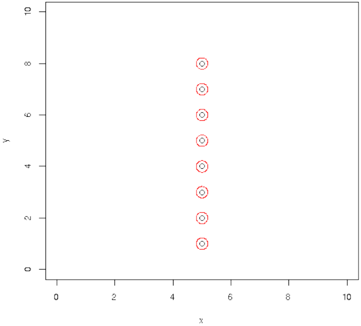
- We've seen one filtration method so far (my Sweep method). Here's another, very widely used.
- Draw a red circle around each data point, same radius for all.
- The filtration consists of drawing an increasing sequence of radii.
- Points in overlapping circles are considered to be in the same component.
- Use with any metric, not just Euclidean distance and not just on image data.

An 'I'

An 'I'



- radius 0.2
- 8 1-components

An 'I'

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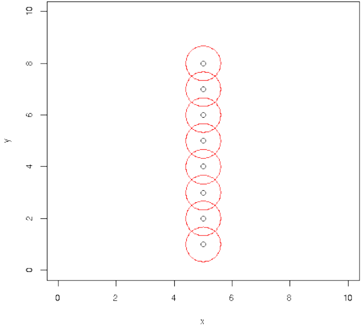
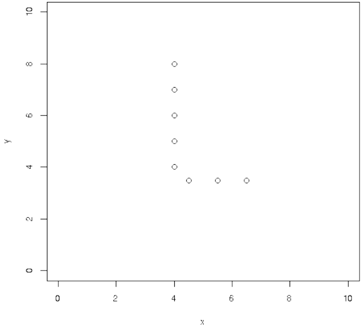


- radius 0.6
- 1 8-component
- the 8 1-components died at 0.5, the 1-component was born at 0.5

An 'L'

An 'L'

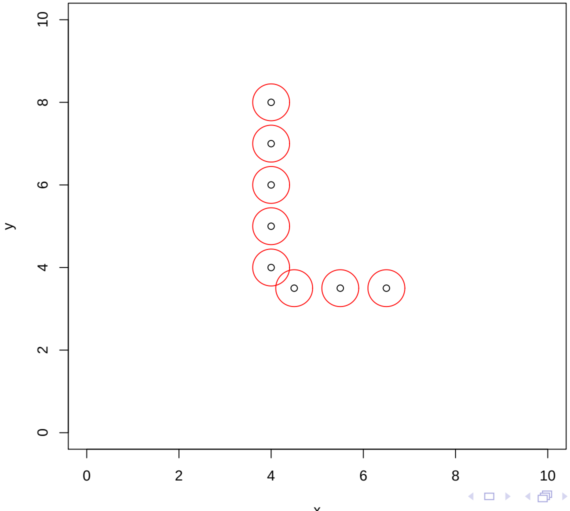


- I took the 'I' and just bent it; linear distance between points still 1.0
- but now there will be a birth at $0.5(0.5\sqrt{2}) = 0.35$, not 0.5
- originally 8 1-components, then 7 components (1 2-comp., 6 1-comps.), then 1 8-comp. — different pattern than for 'I'

An 'L'

An 'L'

Radius 0.4:



Rips Senses Angles!

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The point:

> *Rips filtration does more than topology; it does geometry. (Math: curvature)*

An Approach to General Images Using Rips

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E.g. do this:

- Do a separate analysis at each of several (or many) threshold values.
- In each one, do a Rips filtration.
- Combine (i.e. concatenate) the BD data for the various thresholds to get the feature vector for an image.

A "Topographic" Method

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- Consdider, e.g., the image classification context.
- Analogous to a topographic map. At each altitude, have contours at that height.
- Treat the (row,col) data as being the X-Y plane, and the pixel intensities as the Z-axis.
- Instead of a moving red line, now have a red plane, moving in the Z direction but always parallel to the X-Y plane.
- Pixels that survive the red-plane cutoff op and that are adjacent then considered in the same component.
- Computer BD data as before.

Nongeometric Applications

Nongeometric Applications

- Association of diet with cancer.
- Data on age, gender, race, various dietary measures.
- Still can do, say, Rips, using distance in the same way as k-Nearest Neighbors.

Betti Numbers

Betti Numbers

- Most of the math theory behind persistent homology centers around this concept.
- β_i is data on "holes" at dimension $i = 0, 1, 2, ...$
- Dimension 0 is number of components (with the holes being gaps between components in a line).
- Dimension 1 is holes in a plane, e.g. the 2 holes in an '8'.
- Dimension 2 is holes in 3-dimensional objects. In the image classification context, this would be the volume of spheres in voxel data.
- Higher dimensions not visualizable, but e.g. can use Rips on data (not images, just regular data) of d columns, with the holes being considered dimension $d - 1$.
- Software typically gives the user a choice of maximum dimension to use. Too high a value may result in overfitting.

Betti Numbers (cont'd.)

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- TDA software will typically report BD data separately for each dimension.
- E.g. for a 2-dim. image, the dimension 0 BD will be reported, followed by dimension 1. But one will probably use all of it.
- Where does the Sweep method fit into this? Since have both horizontal and vertical sweeps, it is inherently 2-D (Betti dimension 1), so Betti-type separation wouldn't make sense.

R Software

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- **TDA**
- **TDAstats**
- **TDAsweep** (mine, in preparation)