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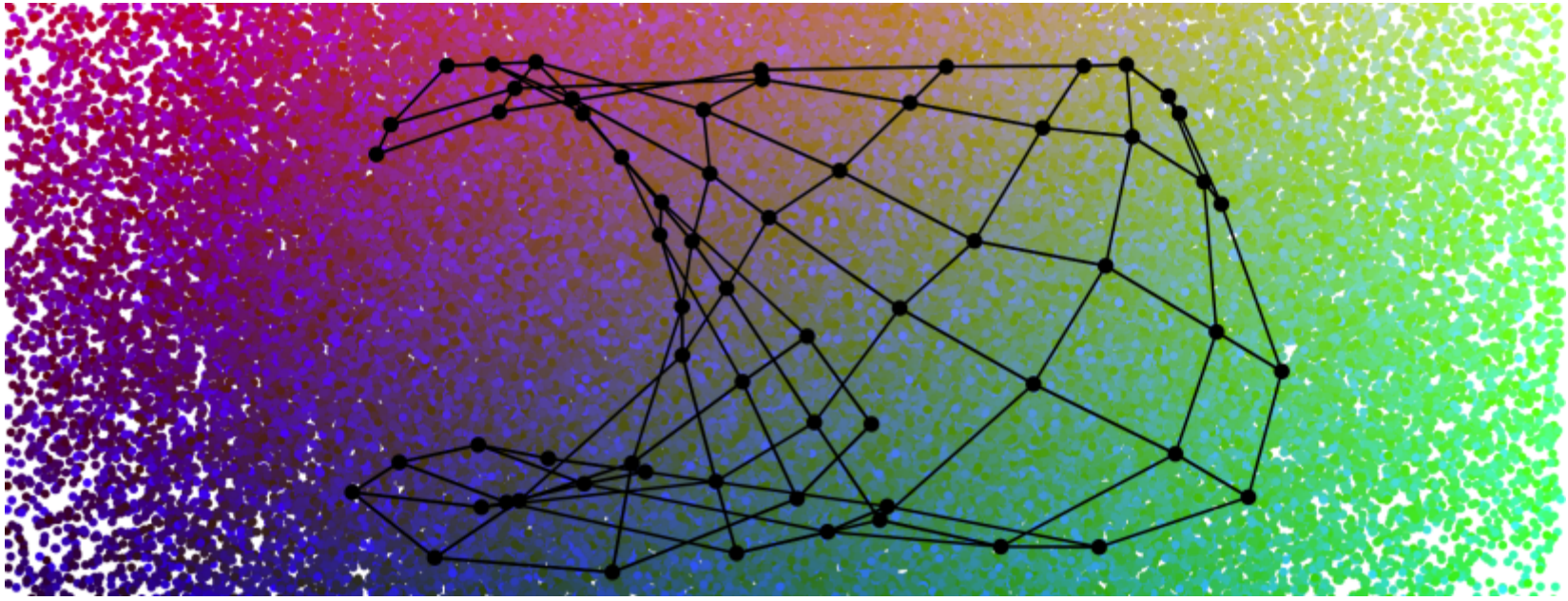

Self-Organizing Maps Tutorial

November 2, 2017November 3, 2017

The term ‘self-organizing map’ might conjure up a militaristic image of data points marching towards their contingents on a map, which is a rather apt analogy of how the algorithm actually works.

A *self-organizing map* (SOM) is a clustering technique that helps you uncover categories in large datasets, such as to find customer profiles based on a list of past purchases. It is a special breed of unsupervised neural networks, where neurons (also called *nodes* or *reference vectors*) are arranged in a single, 2-dimensional grid, which can take the shape of either rectangles or hexagons.

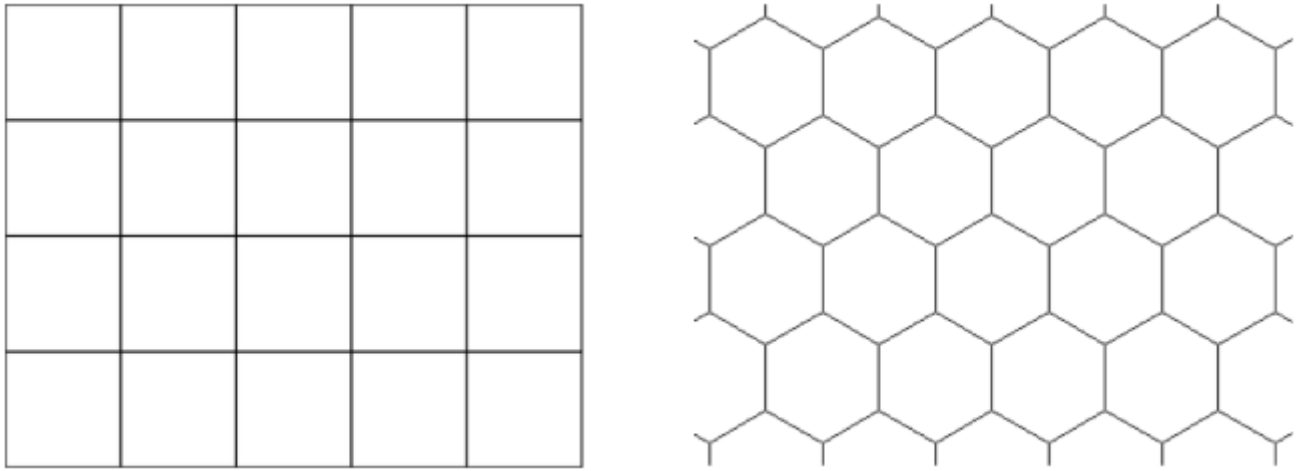

Figure 1. SOM grids can either be rectangular or hexagonal. Each square or hexagon is a neuron.

Through multiple iterations, neurons on the grid will gradually coalesce around areas with high density of data points. Hence, areas with many neurons might reflect underlying clusters in the data. As the neurons move, they inadvertently bend and twist the grid to more closely reflect the overall topological shape of our data.

Let's see a visual example of how SOM works. The accompanying SOM code in R is on our GitHub page. (https://github.com/algobeans/Self-Organizing-Map/blob/master/analysis.R)

A Visual Walkthrough

One example of a data type with more than two dimensions is color. Colors have three dimensions, typically represented by RGB (red, green, blue) values. In this example, we will see how SOM can distinguish two color clusters.

Data Generation

We picked two colors—yellow and green—around which to generate random samples to form two clusters. We can visualize our color clusters using blue and green values, which are the dimensions along which the clusters are most differentiated.

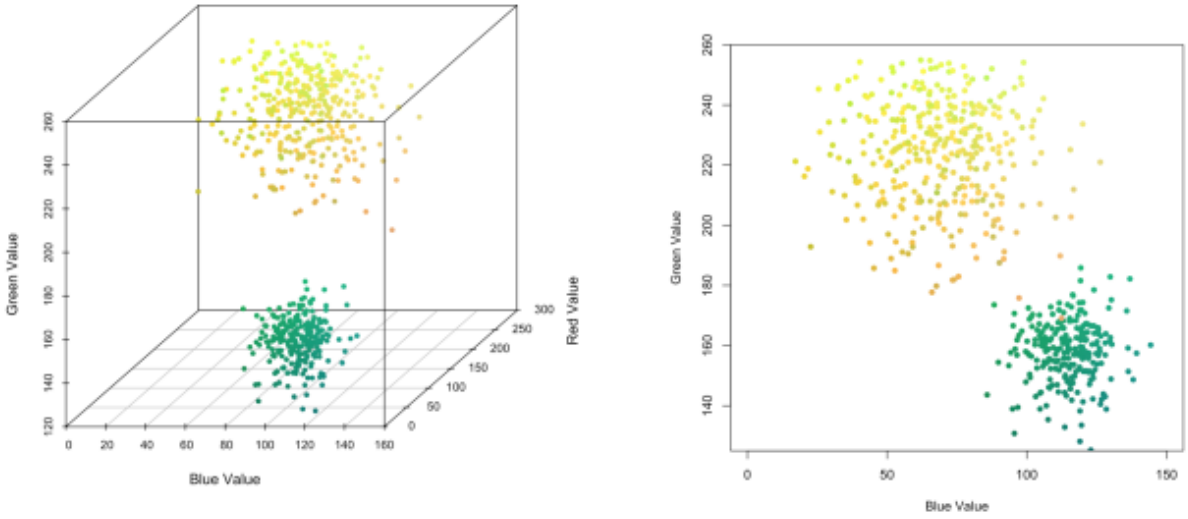

Figure 2. Two color clusters of yellow and green, in 3D and 2D spaces.

Data Analysis

It’s time to build our SOM. We used an 8 x 8 rectangular grid, so there were 64 neurons in total. Initially, neurons in the SOM grid start out in random positions, but they are gradually massaged into a mould outlining the shape of our data. This is an iterative process, which we can watch from the animated GIF below:

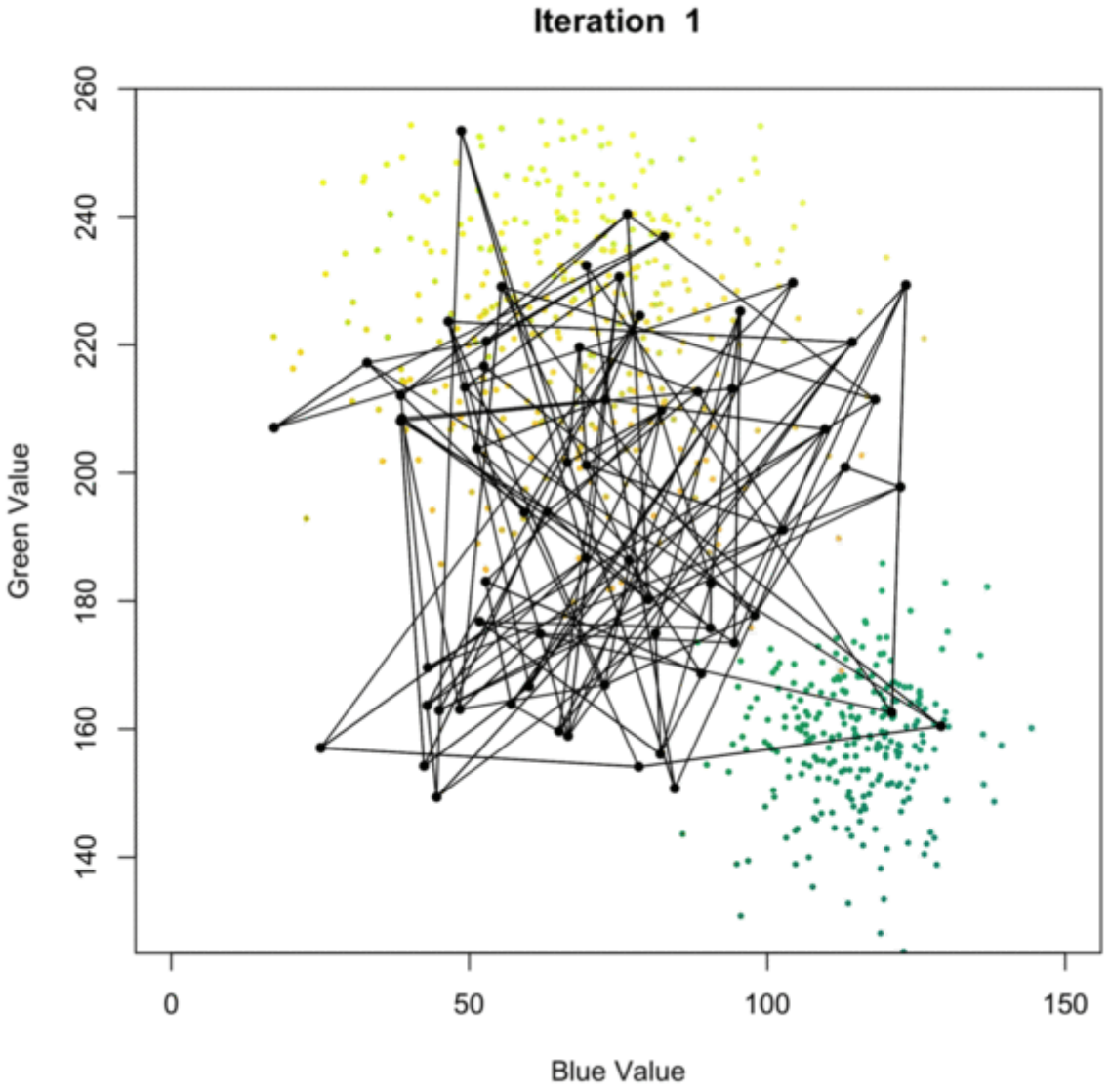

Figure 3. Animated GIF showing how an SOM grid evolves to take the shape of our data. Note that the visualization is a top-down view of the data, and the neurons are actually moving in three dimensions

We can see that the grid's shape stabilizes after a couple of hundred iterations. To check that the algorithm has converged, we can plot the evolution of the SOM's energy—initially, the SOM evolves rapidly, but as it reaches the approximate shape of the data, the rate of change slows down.

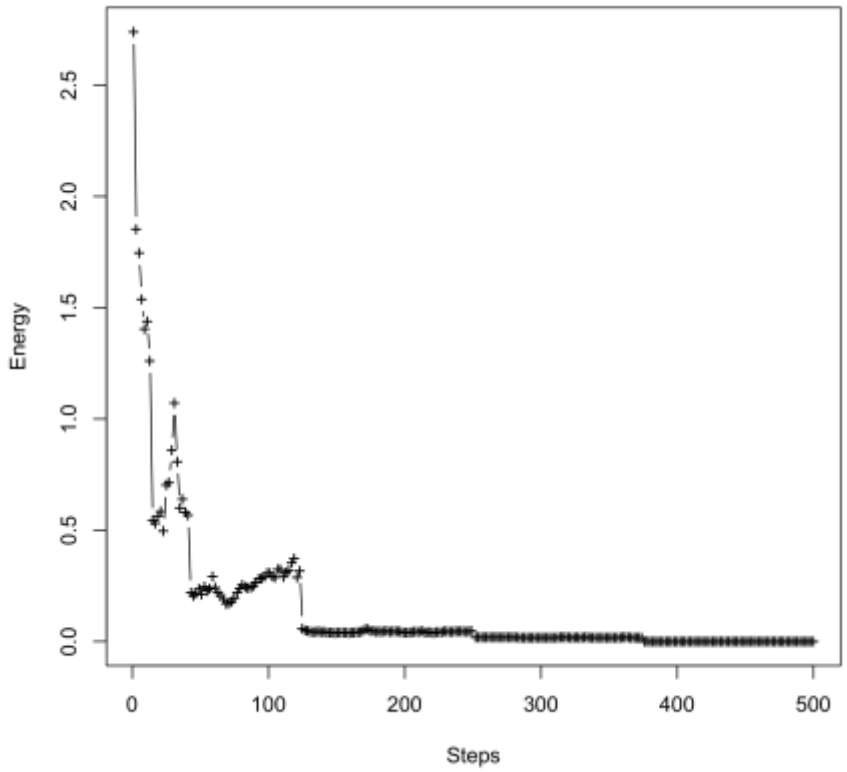

Figure 4. Evolution of the SOM's energy. It took about 150 iterations for neurons in the SOM grid to stabilize.

To get an overview of how many data points each neuron corresponded to, we can plot a frequency map of the grid, shown below. Each neuron is represented by a square, and the pink region within the square represents the relative number of data points that neuron is positioned closest to—the larger the pink area, the more data points represented by that neuron.

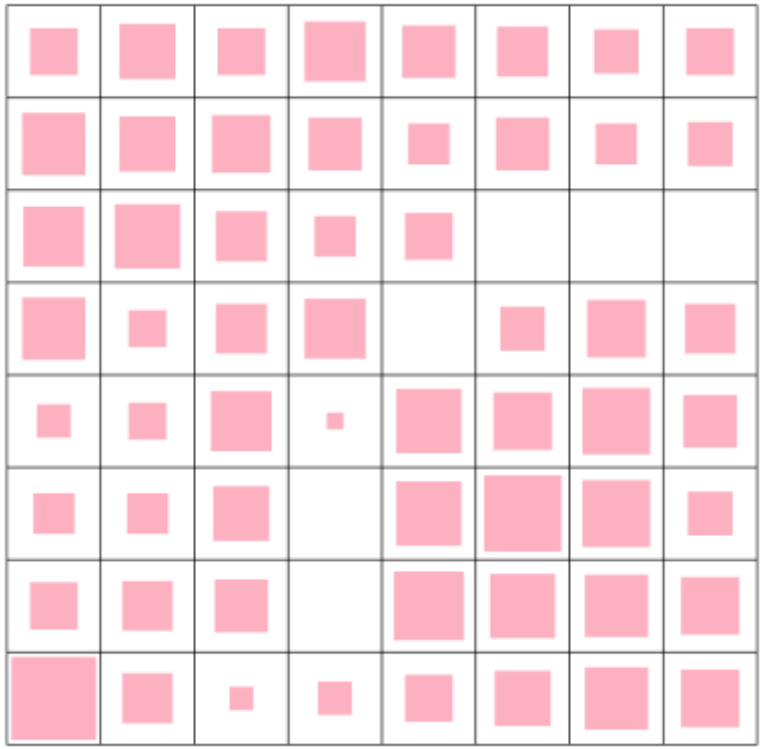

Figure 5. Frequency map of neurons in an 8 x 8 SOM grid.

From the frequency map, we can see a clear divide separating a top left neuron cluster from a smaller bottom right cluster. This divide is represented by the neurons in-between with small or no pink squares.

To verify that there is indeed a divide, we can plot what's called a *U-matrix*, which visualizes how much neurons differ from each other in 2-dimensional space. When two neurons correspond to vastly different sets of data points, they would be separated by a larger distance, denoted by a pink color. On the other hand, neurons representing similar data points are separated by shorter distances, denoted by a blue color.

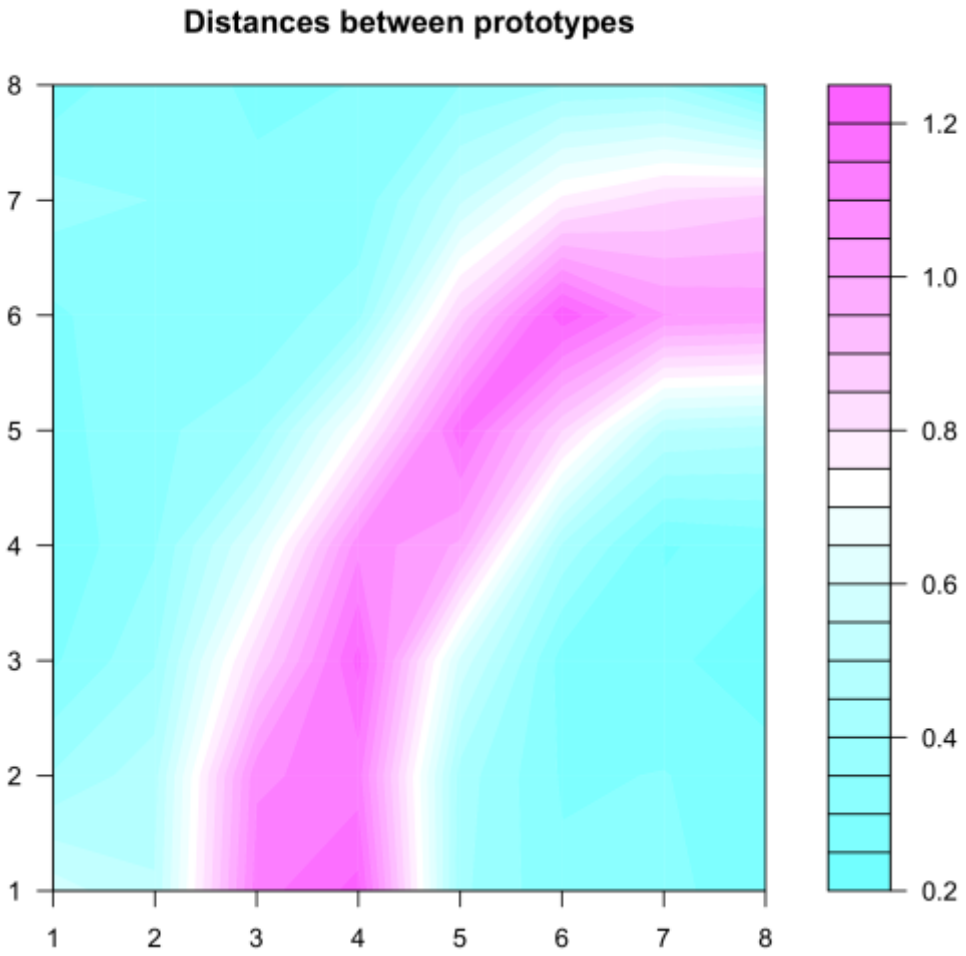

Figure 6. U-matrix showing similarity and dissimilarity between neurons. Useful for identifying clusters.

Comparing the sizes of neuron clusters, we can infer that the bigger cluster in the top left probably corresponds to the larger group of yellow data points, leaving the smaller bottom right cluster to correspond to green data points.

To check if we labelled the clusters correctly, we can infer a color profile for each neuron, by averaging the RGB values of data points associated with that neuron:

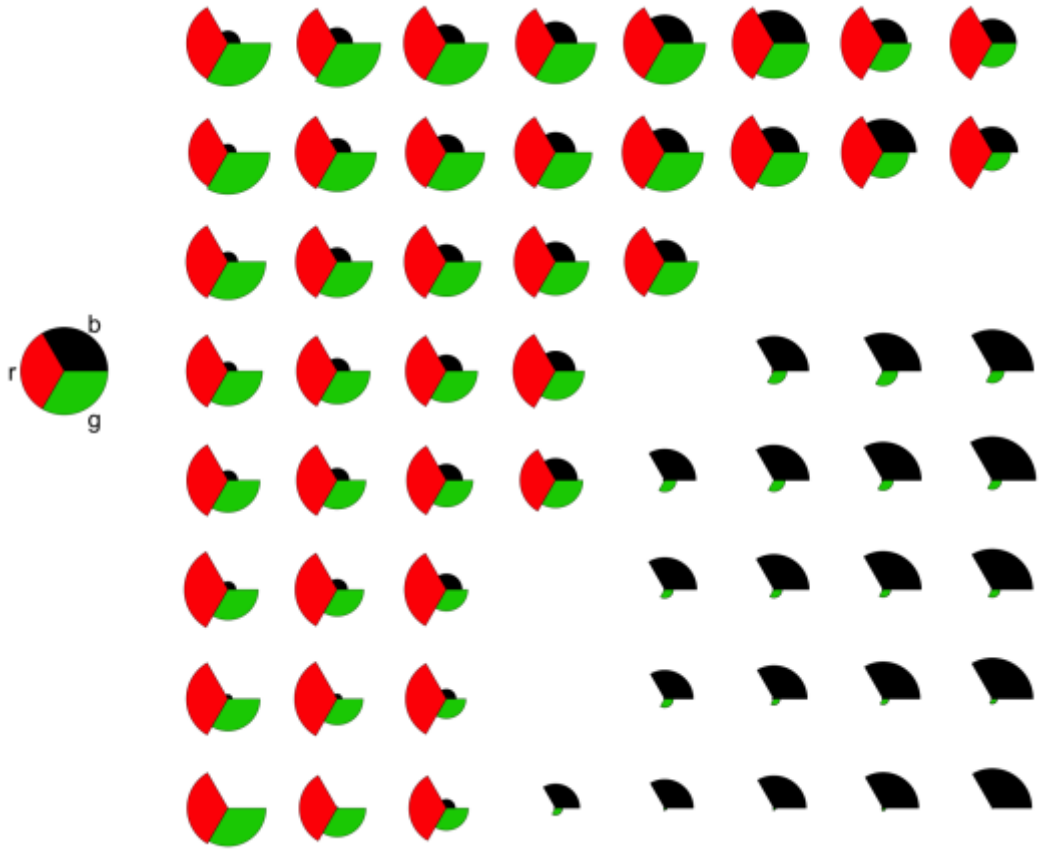

Figure 7. Radar plots showing the aggregated profile of each neuron, as determined by their constituent data points.

From the radar plots, we can observe that the neurons in the top left have data points of high red and green values, and combining these two colors in light gives us, as you'd have guessed, yellow. Conversely, the remaining neurons on the bottom right are characterized by data points with high values of blue and a slight tinge of green, which would give us a bluish green hue.

By representing data with multiple variables in just two dimensions, the SOM grid is well-suited for data visualization (it works similarly to another famous technique called *t-SNE*). While the 2-dimesional space is popular due to its use for visualization, the SOM is a general dimension reduction technique that can simplify a dataset to any number of variables, and is closely related to what we learned previously on principal components analysis (https://algobeans.com/2016/06/15/principal-component-analysis-tutorial/).

Now that you've seen how SOM effectively identifies clusters, we will explain how it works under the hood.

How does SOM Work?

In a nutshell, an SOM comprises neurons in the grid, which gradually adapt to the intrinsic shape of our data. The final result allows us to visualize data points and identify clusters in a lower dimension.

So how does the SOM grid learn the shape of our data? Well, this is done in an iterative process, which is summarized in the following steps, and visualized in the animated GIF below:

Step 0: Randomly position the grid's neurons in the data space.

Step 1: Select one data point, either randomly or systematically cycling through the dataset in order

Step 2: Find the neuron that is closest to the chosen data point. This neuron is called the Best Matching Unit (BMU).

Step 3: Move the BMU closer to that data point. The distance moved by the BMU is determined by a *learning rate*, which decreases after each iteration.

Step 4: Move the BMU's neighbors closer to that data point as well, with farther away neighbors moving less. Neighbors are identified using a radius around the BMU, and the value for this radius decreases after each iteration.

Step 5: Update the learning rate and BMU radius, before repeating Steps 1 to 4. Iterate these steps until positions of neurons have been stabilized.

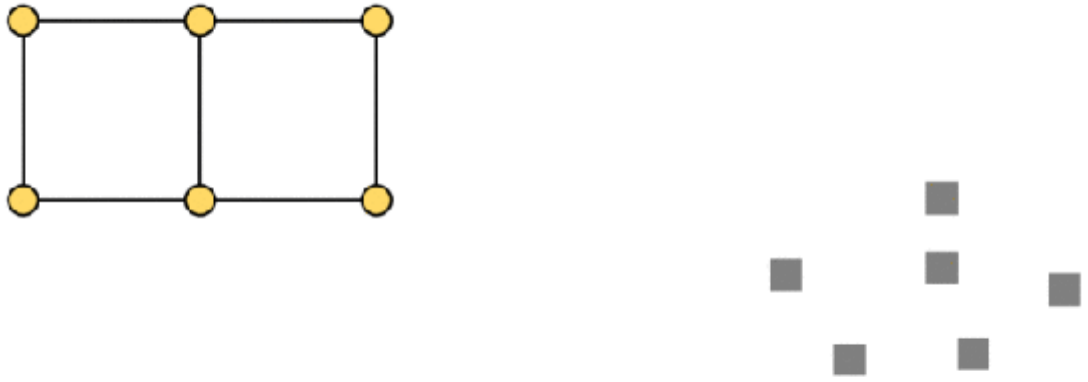

Figure 8. Iterative process of an SOM.

The learning rate and BMU radius should be tuned via validation. If values for both are too high, neurons will be shoved around constantly without settling down. But if values are too low, the analysis will take too long as neurons inch towards their optimal positions. Hence, it is ideal to start with larger learning rate and BMU radius first, before reducing them over time.

Another feature that we need to validate is the optimal number of neurons in the grid. Recall that because each neuron has multiple data points associated with it, it can be treated as a mini-cluster. We can thus validate each neuron to see if its associated data points correspond to known sub-clusters of, say, consumer profiles. In order for such clusters to be distilled however, there should be fewer neurons than data points, so that similar data points can be mapped to each neuron.

One thing to note before we apply SOM: Variables measured in different units could interfere with the speed and accuracy of our analysis. For example, a variable measured in centimeters would have a value 100 times larger than the same one measured in meters. To prevent any variable from overpowering the others, we need to *standardize* all variables. Standardization is analogous to expressing each variable in terms of percentiles, meaning to shift them onto a uniform standard scale, so that they are of the same measurement unit.

Limitations of SOM

SOM simplifies datasets with many variables, which is useful for visualization and identifying clusters. However, it has several drawbacks:

Does not handle categorical variables well. To obtain a scatterplot with good data spread to identify clusters, SOM will have to assume that all variables in the dataset are continuous. Plotting categorical values will result in data points lining up at discrete values instead of spreading across the plot.

Computationally expensive. A dataset with more variables would require longer times to calculate distances and identify BMUs. To expedite computations, we could improve our initial positions of neurons from a random state to a more informed approximation with the help of a simpler dimension reduction technique, such as principal components analysis (https://algobeans.com/2016/06/15/principal-component-analysis-tutorial/). By starting the neurons off closer to the data points, less time would be needed to move them to their optimal locations.

Potentially inconsistent solutions. As initial positions of neurons differ each time the SOM analysis is run, the eventual SOM map generated will also differ. Sometimes, overly large clusters may be split up and represented by two separate clusters of neurons. Therefore, before concluding on the number of clusters, the SOM analysis can be repeated to check for consistency, and resulting clusters should be validated against actual cases.

Summary

- A *self-organizing map* (SOM) is a grid of neurons which adapt to the topological shape of a dataset, allowing us to visualize large datasets and identify potential clusters.
- An SOM learns the shape of a dataset by repeatedly moving its neurons closer to the data points. Distinct groups of neurons may thus reflect underlying clusters in the data.
- SOMs are best for datasets with continuous variables, and it should be repeated to check for consistency. Resulting clusters should also be validated.

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1. **GIORGI** says: October 25, 2018 at 1:14 am REPLY
   great post

3. Pingback: Machine Learning to Explore Geographical Data – Geo Blog – Geoscienstists sharing their ideas and projects
   SPENCER says: July 5, 2018 at 6:55 am REPLY
   Hi, great post! Can I ask for an explanation on the R code where you remove the crisscross pts? How do we know that these points will crisscross? The logic written makes it so that for every pt %% 8 == 0 or 1 a value +/- 1 from the pt will be removed from the pt_neighbor variable.
4. **SERGEI** says: April 25, 2018 at 12:22 am REPLY
   that is awesome!

5. Pingback: Do you know about Self-Organizing Maps? – Data Mining / Machine Learning / Data Analysis
   DANIEL says: November 16, 2017 at 2:09 am REPLY
   Great tutorial. How do you define the energy for the SOM?

7. Pingback: Layman’s Tutorial to Self-Organizing Maps | A bunch of data