Similarity Measures for Graph Adjacency with Sets

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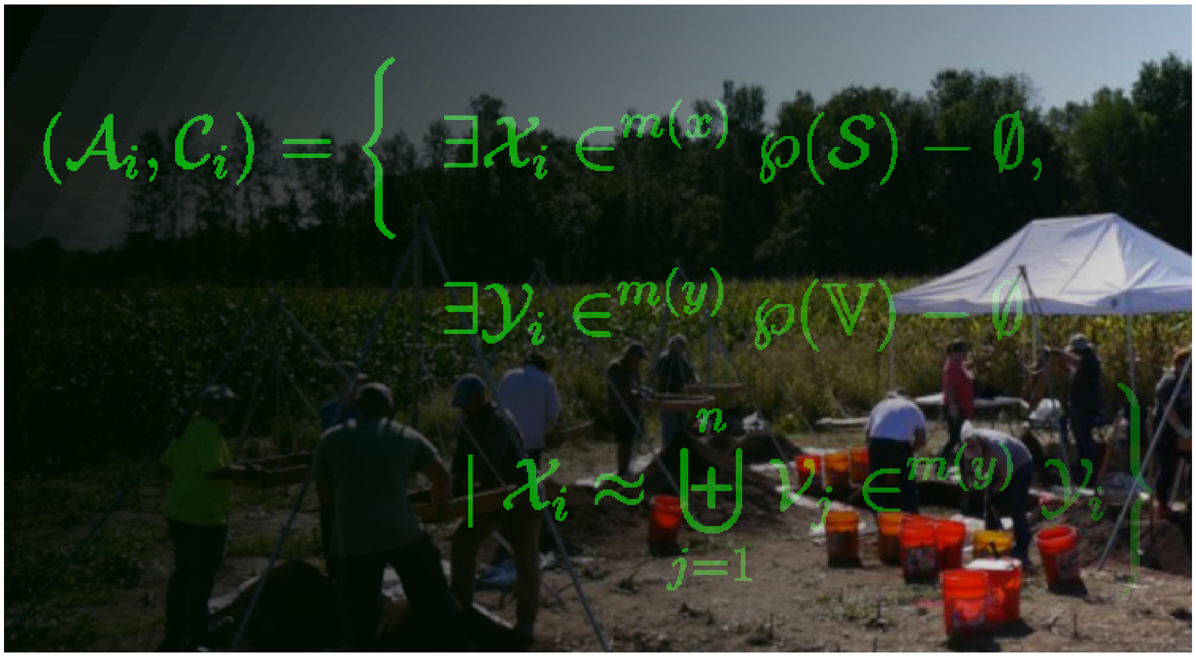
10/14/2021


$(\mathcal{A}_i, \mathcal{C}_i) = \{ \exists \mathcal{X}_i \in^{m(x)} \wp(\mathcal{S}) - \emptyset,$
$\exists \mathcal{Y}_i \in^{m(y)} \wp(\mathbb{V}) - \emptyset$
$| \mathcal{X}_i \approx \biguplus_{j=1}^{n} \mathcal{V}_j \in^{m(y)} \mathcal{Y}_i \}$

In my last installment (Part I), I introduced you to a bit about the process of analyzing an archaeological site with data science. I talked about the frustratingly complex nature of "Old Things in Space" and how the network of artifacts and locations constitute a bipartite graph.

As we worked through the process of creating a two-mode graph and projecting it into its constituent one-mode graphs, however, we ended on something of a cliff-hanger... *everything* ended up connected to *everything else*!

Well, sort of. I have to confess that I intentionally lead you down a primrose path straight into a cul-de-sac. All part of my cunning plan, of course, to get to the much more interesting topic of thinking about just what it means for two things to be "similar" and similarity metrics for *sets.*

In my defense, I did briefly mention that `igraph` doesn't really have the best of tools to actually *do* much of anything interesting with bipartite graphs. The problem is that the method it uses in its `bipartite_projection` simply sums the pairwise occurrences in the incidence matrix. That, as it turns out, is less than useful in a lot of cases.

Instead, we need to explore some more robust methods for evaluating *similarity* between sets. Unlike numerical methods of calculating correlation or distance, there are some conceptual peculiarities when comparing correspondence and similarity between sets that need to be considered. In this article, we'll look at some of the most commonly used set-based similarity metrics and reason through *how* to choose the appropriate metric for our goals.

For those just joining in, this is the Part II of a series in archaeological data science covering:

- Part I – Creating and exploring bipartite and one-mode graphs,
- Part II – Similarity measures for sets and graph adjacency,
- Part III – Graph structure and community detection methods,
- Part IV – Geo-spatial networks

I'll continue using R for the coding, but again all of this could be done with Python just as easily.

Introduction

Before we get into the weeds of metrics, methods, and combinatorics (i.e., the mathematics of *sets*) let's stop to think for a moment about just what we mean when we say that two things are *similar.*

In general, we refer to things as *similar* when they are neither the quite the same nor are they entirely different. Similar things are alike-*ish.* It means that some measure of shared features or attributes is suggesting *association* but not necessarily *commonality* or *identity.* It denotes a resemblance or correspondence, but there's a certain fuzziness about it – i.e., similarity implies a subjective or qualitative assessment.

Our goal, then, is twofold. Firstly, we need to determine what set similarity metric most closely reflects the *relationship* between set elements. Secondly, we have to determine an appropriate method for determining the *threshold* of similarity between those entities. In other words, we need to choose our criteria for *resemblance* and set the *limits* of what is (or isn't) considered similar between our sets.

Sets and Similarity

Unlike real-valued vector spaces in which distance or similarity can be readily calculated, sets consist of an un-ordered collection of unique members or elements. Those member elements can be anything – e.g., numbers, letters, words, objects, categories – so there isn't always an obvious numerical solution such as vector norms or coordinates that can be used for comparison of elements.

Instead, we have to compare the membership of elements between sets. More specifically, we compare the size or *cardinality* of certain attributes of or operation on the sets such as their intersections and unions. Luckily, there are numerous metrics available for comparing similarity between sets. For our purposes, I will discuss only a few that are most common:

- Overlap or Szymkiewicz-Simpson coefficient
- Jaccard similarity coefficient (a.k.a. Tanimoto coefficient)
- Sørensen–Dice coefficient

Each of these similarity measures was derived specifically to address the peculiarities of dealing with sets. The difference between them is just the way in which they weight common elements (i.e., intersections) against differences.

It is important to consider, however, exactly what relationships between sets you are trying to capture before choosing a method. If your samples all contain approximately the same number of elements, you might choose differently than if each sample has widely different numbers of members. How likely are complete subsets, and are those important to capture? Are differences more important than commonalities, or the other way around?

As with any data analysis, it's necessary to explicitly consider your *methodology* as well as your methods. The rationale and justification for the selection of methods is a critical part of the process. That is, after all, why we call it data *science*.

Revisiting Bipartite Graphs and Projections

First, lets go back and recreate our bipartite graph of sampling locations (called "proveniences") and artifact types found at those locations like we did in Part I.

```r
require(tidyverse)
require(igraph)
require(ggraph)

# Read in edgelist into data frame
dat <- read_csv("Catalog_SiteA.csv",
                col_select = c(LEVEL_ID, CODE))
```

```
# Create graph
g_assemblages_bpg <-
  graph_from_data_frame(unique.data.frame(dat),
                        directed = FALSE)

# Assign bipartite node types
V(g_assemblages_bpg)$type <-
  bipartite_mapping(g_assemblages_bpg)$type
```

Again, we have our graph of connections between artifact types and locations, and can already see some rough grouping in each of the vertex types (one type at the top and one at the bottom of the plot). The graph is densely connected, with many nodes and edges.

```
# Plot bipartite graph
g_assemblages_bpg %>%
  ggraph(layout = "bipartite") +
  geom_edge_link(color = "gray", alpha = 0.25) +
  geom_node_point(aes(color = type), size = 2) +
  scale_color_manual(
    values = c("green", "blue"),
    name = "Node Type",
    breaks = c(FALSE, TRUE),
    labels = c("Provenience", "Artifact")) +
  ggtitle("Bipartite network of Provenience and Artifact Type")
```

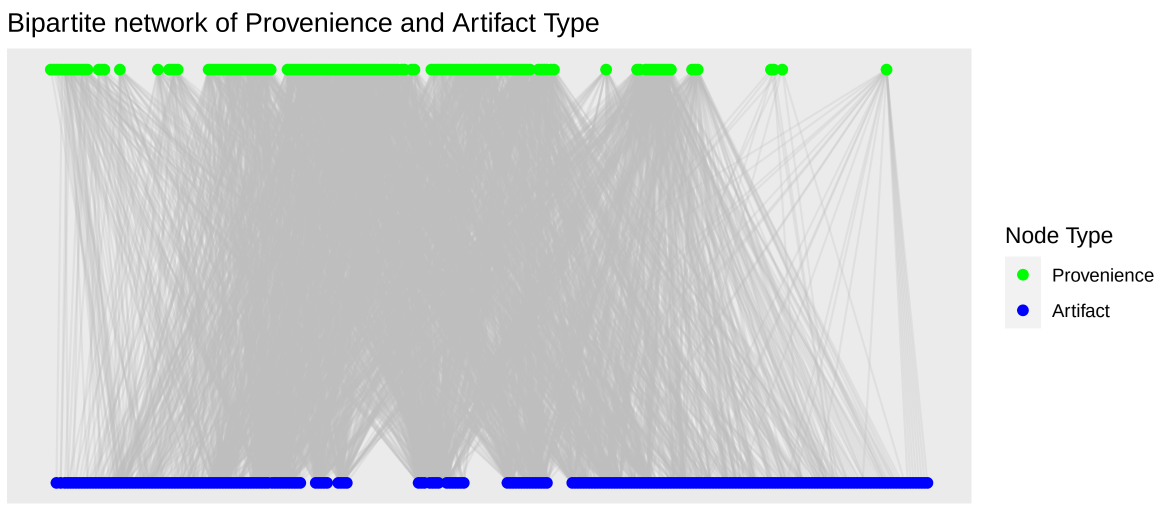


Figure 1: Bipartite graph of artifact-provenience connections.

Now we retrieve the binary incidence matrix of proveniences and artifact types from the graph, which we will use as the data for our similarity measures. Remember, we are only considering presence (`1`) or absence (`0`) of an artifact type at each provenience.

```r
g_assemblages_bpg_inc <- as_incidence_matrix(g_assemblages_bpg)

# View the first few rows and columns
g_assemblages_bpg_inc[1:5, 1:15]
```

```
     UDB TOOT CS OCH BNUT UIS TWN UWN MCN UCN CWN BLT CAP SCR TACK
1726   1    1  1   0    1   1   0   1   1   1   1   1   0   1    1
1725   1    1  0   1    0   1   1   0   1   1   0   0   1   0    1
1306   0    0  0   1    0   1   0   1   1   1   1   0   0   0    1
1307   0    0  0   1    0   1   0   0   0   0   1   0   0   0    0
1737   1    0  0   0    1   1   0   0   1   1   1   1   0   1    0
```

Depending on which way we orient our incidence matrix, we now have a collection of the sets of artifact types found at each provenience (by row) or sets of proveniences at which each artifact type was found (by column).

The goal is to find a partitioning of this system of sets such that each subset of provenience contains a coherent collection of artifact types (i.e., what archaeologists call an *assemblage*) and each subset of artifact types are found together in a coherent spatial collection of proveniences (we call those a *context*).

What we're trying to do now is to look at the ways we compute that "coherence" within the projected modes of our bipartite graph. In order to project our bipartite node types into two separate one-mode graphs, we want to evaluate similarity measures between pairwise comparisons of these sets.

Archaeological Objectives

I've introduced you to a couple archaeological concepts, as well as a few concepts about sets and graphs. Now I'd like to pause to explain why we're so interested in finding these subsets and partitions. You see, archaeologists don't really interpret artifacts *per se*.

We're interested in interpreting human activities across time and space, which gives us a window into far more abstract concepts like *behavior* or *culture*. The way we do that, since we don't have a time machine to go back and observe what people were actually doing, is by looking for patterns of associations between the physical remnants (i.e., the debris or *trash*) left behind by those activities. Weird, I know, but it works surprisingly well.

Just think for a moment about what your trash might show about *your* daily behavior!

Anyway, the reason we're so interested in finding groupings in artifacts (the things) and provenience (the location in 3-dimensional space) is that those are just the samples we collect. We want to know about the *populations* from which those samples are drawn. In this case, those populations are the *assemblages* and *contexts*. We want to see if we can differentiate one assemblage or context from another, then see what patterns that reveals.

For example, does an identified assemblage of artifacts have a specific range of dates so that it uniquely identifies *when* or *how long* a site was occupied? Does one assemblage relate to domestic activities while another reflects economic activities, and are those spaces (i.e., their contexts) separate or commingled? If the site was occupied multiple times or by multiple households, were they continuous or intermittent? Different assemblages might be mixed into the same context if they were continuous.

So many questions, but parsing the artifact and provenience data into assemblages and contexts is the first step. We want to be sure that our analytic methods are appropriate.

Similarity Measures for Projections

We found out in the last installment (Part I) that the `bipartite_projection` method in `igraph` only sums the number of pairwise coincidences. That means, though, that even one shared element between sets is enough to link them. It doesn't, at all, factor in how many elements of the sets are *different* or the *total* number of elements being considered.

In the end, every node in each projection was linked to almost every other node with no good way to evaluate the *strength* of those connections. Not particularly useful.

Now we can start looking more closely at set-based similarity measures, and how use them to project our bipartite graph. We could use existing packages for these, but I'd like instead to build our own functions in order to get a better sense of what is going on "under the hood" so to speak.

Do note that these functions are intended for binary incidence matrices. Different approaches would be needed for sets with multiplicities or counts (i.e., multisets or m-sets).

Overlap or Szymkiewicz-Simpson Coefficient

This similarity measure is simply the number of common elements of the intersection between two sets divided by the total number of members in the *smaller* of the two sets. Remember, the number of unique members or elements that make up a set are its size or (more formally) its cardinality.

$$Overlap(A,B) = \frac{|A \cap B|}{\min(|A|,|B|)}$$

For example, say we have two sets: $X = \{a, b, c\}$ and $Y = \{b, c, d, e, f\}$. Their intersection is $X \cap Y = \{b, c\}$ and the sets have cardinality $|X| = 3$ and $|Y| = 5$. Their overlap coefficient would be:

$$\begin{aligned} Overlap(X, Y) &= \frac{|\{b, c\}|}{\min(|\{a, b, c\}|, |\{b, c, d, e, f\}|)} \\ &= \frac{2}{\min(3, 5)} \\ &= \frac{2}{3} \approx 0.67 \end{aligned}$$

Easy, right? It's just the proportion of the smaller set's members that are also members of the larger set (thus, *overlap*).

Notice, though, that if *all* of the elements of the smaller set were in the larger set – i.e., if we were to drop element a from set X so that it was a complete *subset* of Y – then the coefficient would equal 1 regardless of how many additional members were in Y.

So, this similarity measure is defining *similarity* in a very specific way. It includes an assumption that *any* subset is effectively *equivalent* to its superset. That little quirk of definition can be quite useful, depending on your application.

The overlap coefficient is a common set similarity metric used in everything from gene sequencing to topic modeling. It's also quite easy to calculate across our binary incidence matrix.

```
# Szymkiewicz-Simpson overlap coefficient for binary incidence matrices

overlap_coef_bin <- function(x) {
  # Calculate the pairwise sums of non-zero matrix elements to find the number
  # of intersecting elements between each input column
  bin_intersect_mat <- t(x) %*% x

  # Calculate the input column sums to find the individual size of each set
  col_sum <- apply(x, 2, function(xx)
    sum(xx != 0))

  # Find the smaller of each pair of sets by taking the matrix outer minimum
  min_set_size_mat <- outer(col_sum, col_sum, FUN = pmin)

  # Szymkiewicz-Simpson overlap coefficient is the pairwise intersection of two
  # sets divided by the size of the smaller set
  ssoc <- bin_intersect_mat / min_set_size_mat
  # Set diagonal to identity
  diag(ssoc) <- 1

  # Assign input column names to rows and columns of return matrix
  dimnames(ssoc) <- list(colnames(x), colnames(x))

  return(ssoc)
}
```

Jaccard (or Tanimoto) Similarity Index

The Jaccard index is probably the most well-known and used of the set similarity measures. You may also see this one referenced as the Tanimoto (or even Jaccard-Tanimoto) index, owing to its independent formulation through time in different fields of study. All versions, however, refer to a measure of similarity based on the ratio of cardinality between the *intersection* of two sets and their *union*.

$$J(A,B) = \frac{|A \cap B|}{|A \cup B|} = \frac{|A \cap B|}{|A| + |B| - |A \cap B|}$$

Unlike the overlap coefficient, you can see that the Jaccard index considers the *total* membership of both sets being compared in the denominator. That means that this index will *always* penalize differences between sets, even if one is a proper subset of the other.

To demonstrate, let's go back to our toy example sets $X = \{a, b, c\}$ and $Y = \{b, c, d, e, f\}$ to calculate the Jaccard index value.

$$\begin{aligned} J(X,Y) &= \frac{|\{b,c\}|}{|\{a,b,c\}| + |\{b,c,d,e,f\}| - |\{b,c\}|} \\ &= \frac{2}{3+5-2} \\ &= \frac{2}{6} \approx 0.33 \end{aligned}$$

By considering the total cardinality of the sets, the Jaccard index comes back a fair bit *lower* than the Overlap Coefficient (≈ 0.67). Next, let's go ahead and drop element a to make X a proper subset of Y and see what happens. Whereas the Overlap Coefficient was 1, we find that

$$\begin{aligned} J(X,Y) &= \frac{|\{b,c\}|}{|\{b,c\}| + |\{b,c,d,e,f\}| - |\{b,c\}|} \\ &= \frac{2}{2+5-2} \\ &= \frac{2}{5} = 0.4 \end{aligned}$$

That's a significant difference! Even though X is a proper subset of Y, the Jaccard index emphasizes the *differences* between the sets over their commonalities. The greater the disparity between sets, the lower the index value. Again, depending on your use case, that extra penalization of difference may be to your advantage.

The Jaccard similarity index is perhaps, as already mentioned, the most common and versatile of the set similarity measures. It's often used for comparing categorical data, and frequently found in ecological or social science applications.

Our function to calculate the index is very similar to that for the overlap coefficient, but substituting summation for minimum value in our outer product and changing the denominator.

```r
# Jaccard/Tanimoto similarity index for binary incidence matrices

jaccard_sim_bin <- function(x) {
  # Calculate the pairwise sums of non-zero matrix elements to find the number
  # of intersecting elements between each input column
  bin_intersect_mat <- t(x) %*% x

  # Calculate the input column sums to find the individual size of each set
  x_col_sum <- apply(x, 2, function(xx)
    sum(xx != 0))

  # Calculate the matrix outer sums for pairwise sum of set sizes
  set_size_sum_mat <- outer(x_col_sum, x_col_sum, FUN = "+")

  # Jaccard index is intersection of set sizes over the size of the union of
  # sets
  jacc <- bin_intersect_mat / (set_size_sum_mat - bin_intersect_mat)

  # Set diagonal to identity
  diag(jacc) <- 1

  # Assign input column names to rows and columns of return matrix
  dimnames(jacc) <- list(colnames(x), colnames(x))
  return(jacc)
}
```

Sørensen–Dice Similarity Coefficient

Similar to the Jaccard index, the Sørensen–Dice similarity coefficient compares the ratio of the intersection to the total membership of both sets. The difference is that the denominator for Sørensen–Dice is the sum of the cardinalities rather than that of the union of the sets as it is for Jaccard. Another difference is that Sørensen–Dice doubles the intersection in the numerator, which has the effect of "weighting" the commonalities between sets a little bit more than the differences.

$$DSC(A,B) = \frac{2 \times |A \cap B|}{|A| + |B|}$$

Let's see how Sørensen–Dice similarity compares with our toy example $X = \{a, b, c\}$ and $Y = \{b, c, d, e, f\}$ again.

$$\begin{aligned} DSC(X,Y) &= \frac{2 \times |\{b,c\}|}{|\{a,b,c\}| + |\{b,c,d,e,f\}|} \\ &= \frac{2 \times 2}{3+5} \\ &= \frac{4}{8} = 0.5 \end{aligned}$$

As expected, our calculated similarity $DSC = 0.5$ is somewhat higher than Jaccard but lower than the Overlap Coefficient. What happens now if we make X a proper subset of Y again (*i.e.*, drop element a)?

$$\begin{aligned} DSC(X,Y) &= \frac{2 \times |\{b,c\}|}{|\{b,c\}| + |\{b,c,d,e,f\}|} \\ &= \frac{2 \times 2}{2+5} \\ &= \frac{4}{7} \approx 0.57 \end{aligned}$$

Like Jaccard, the Sørensen–Dice similarity coefficient does *not* equate a proper subset to identity but does calculate it as a stronger similarity than the Jaccard similarity index. The difference is that while Jaccard is the ratio of intersection to union, Sørensen–Dice is the ratio of the intersection to the *disjoint* union (*i.e.*, union minus intersection) of the two sets.

Effectively, it's the ratio of matches to mismatches rather than Jaccard's ratio of matches to the overall membership. As before, this may be better suited depending on your particular application.

The setup for the function for our binary incidence matrix should be familiar by now.

```r
# Sørensen-Dice Coefficient for binary incidence matrices

soren_dice_sim_bin <- function(x) {
  # Calculate the pairwise sums of non-zero matrix elements to find the number
  # of intersecting elements between each input column
  bin_intersect_mat <- t(x) %*% x

  # Calculate the input column sums, to find the individual size of each set
  col_sum <- apply(x, 2, function(xx)
    sum(xx != 0))

  # Calculate the matrix outer sums for pairwise sum of set sizes
  set_size_sum_mat <- outer(col_sum, col_sum, FUN = "+")

  # Sorenson-Dice index is twice the size of the intersection divided by the
  # sum of the size for each set
  sd <- (2 * bin_intersect_mat) / set_size_sum_mat

  # Set diagonal to identity
  diag(sd) <- 1

  # Assign input column names to rows and columns of return matrix
  dimnames(sd) <- list(colnames(x), colnames(x))
  return(sd)

}
```

Choosing Similarity

We now have three very specific ways to measure similarity, so how do we choose which measure to use? Well, there's no "one size fits all" answer so we have to decide what we mean by "similarity" for our particular scenario.

We have to think through our data-generating processes, and decide what we *sort* of similarities we are trying to capture depending on what we believe to be the inherent structuring. More importantly, we need to *justify* that decision from the data.

Revisiting the Data Distributions

Recall from Part I that when we looked at the degree and edge-weight distributions, for both provenience and artifact type, that we have high-density connections formed by relatively low-strength edges. We're looking at similarity measures to rectify that, but just how "sparse" is our goal (i.e., our threshold value for similarity)?

When looking at the various similarity metrics and their intuitions, we found that the relative weighting of commonalities to differences made a significant difference. The cardinality involved for each calculation, though, is fully dependent on how many members are likely to be in each sample. That also implies that *diversity* in sample sizes will effect our similarity measures. Let's see what those look like.

```r
require(gridExtra)
```

```
Loading required package: gridExtra


Attaching package: 'gridExtra'


The following object is masked from 'package:dplyr':

    combine
```

```r
grid.arrange(
  ggplot(
    data = data.frame(x = rowSums(g_assemblages_bpg_inc)),
    aes(x = x)) +
    geom_histogram(color = "gray", fill = "green", bins = 20) +
    ggtitle("Artifact Types per Provenience"),

  ggplot(
    data = data.frame(x = colSums(g_assemblages_bpg_inc)),
    aes(x = x)) +
    geom_histogram(color = "gray", fill = "blue", bins = 20) +
    ggtitle("Occurence per Artifact Type"),

  ncol = 2
)
```

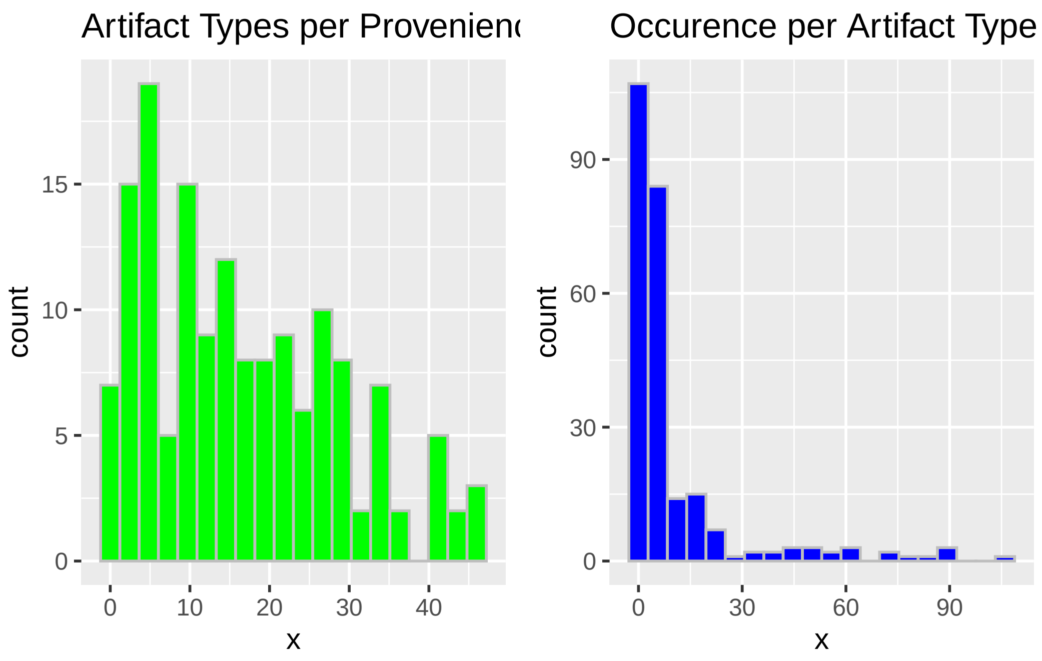


Figure 2: Sample size distribution.

On the left, we have the density distribution of how many artifact types tend to be found within a single provenience. On the right, we have the number of proveniences in which any single artifact type is found.

One thing immediately jumps out – a substantial proportion of our proveniences contain a rather diverse collection of artifact types, but most of those individual types are found in very few proveniences. It's also worth noting that it seems that some artifact types are showing up in a very high proportion of proveniences. Remember, our sample contains only 152 proveniences and 251 unique artifact types at our site.

Both distributions are right-skewed, though, which is promising for our attempt to find hidden network structure. Why? Well, it means that all of those values on the right-hand tails aren't especially likely to be particularly informative.

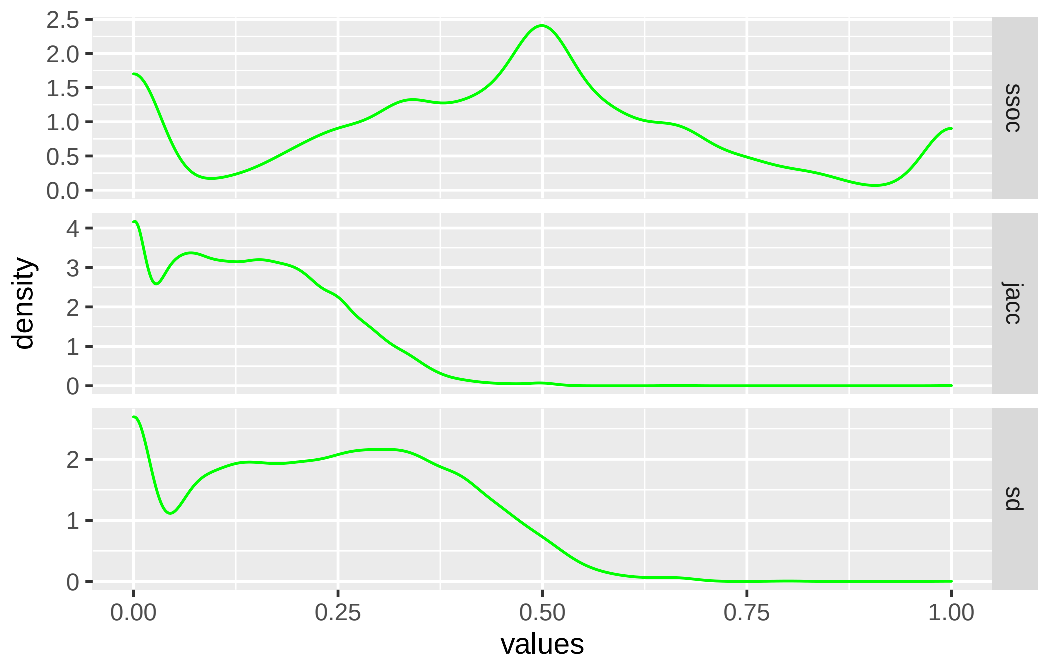
An artifact type that shows up *everywhere* tells us very little about the associations between *other* artifact types, and next to nothing about the differences or similarities between proveniences. Similarly, proveniences that contain a little bit of everything don't help us in finding spatial distinctions and are quite likely locations in which different assemblages may be mixed together.

The inherent *structure* that we're looking for isn't likely to be found in those samples. Luckily, we now know that the *bulk* of the samples should (when projected as one-mode graphs) have a much smaller graph node *degree* than what we found in our "everything-to-everything" projections from before.

Comparing Similarity Measures

Comparing similarities for proveniences

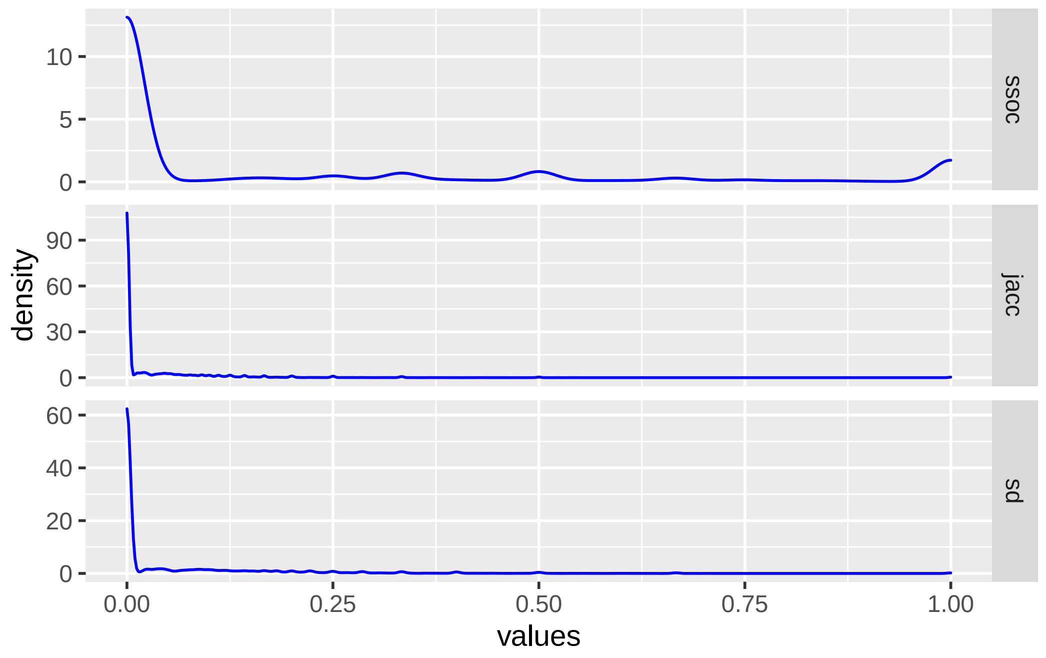
```r
# Overlap coefficient, provenience
prov_adj_ssoc <- overlap_coef_bin(t(g_assemblages_bpg_inc))

prov_ssoc_vals <-
  prov_adj_ssoc[lower.tri(prov_adj_ssoc, diag = FALSE)]

# Jaccard, provenience
prov_adj_jacc <- jaccard_sim_bin(t(g_assemblages_bpg_inc))

prov_jacc_vals <-
  prov_adj_jacc[lower.tri(prov_adj_jacc, diag = FALSE)]

# Sorenson-Dice
prov_adj_sd <- soren_dice_sim_bin(t(g_assemblages_bpg_inc))

prov_sd_vals <-
  prov_adj_sd[lower.tri(prov_adj_sd, diag = FALSE)]

# Make data frame to compare
prov_sims <-
  data.frame(ssoc = prov_ssoc_vals,
             jacc = prov_jacc_vals,
             sd = prov_sd_vals)

# Plot densities by similarity measure
prov_sims %>% stack() %>%
  ggplot(aes(x = values)) +
  geom_density(color = "green",
               alpha = 0.4) +
  facet_grid(ind ~ ., scales = "free")
```



Comparing similarities for artifact types

```r
# Overlap coefficient, artifact types
artifact_adj_ssoc <- overlap_coef_bin(g_assemblages_bpg_inc)

artifact_ssoc_vals <-
  artifact_adj_ssoc[lower.tri(artifact_adj_ssoc, diag = FALSE)]

# Jaccard, artifact types
artifact_adj_jacc <- jaccard_sim_bin(g_assemblages_bpg_inc)

artifact_jacc_vals <-
  artifact_adj_jacc[lower.tri(artifact_adj_jacc, diag = FALSE)]

#Sorenson-Dice, artifact types
artifact_adj_sd <- soren_dice_sim_bin(g_assemblages_bpg_inc)

artifact_sd_vals <-
  artifact_adj_sd[lower.tri(artifact_adj_sd, diag = FALSE)]

# Make data frame to compare
```

```
artifact_sims <-
  data.frame(ssoc = artifact_ssoc_vals,
             jacc = artifact_jacc_vals,
             sd = artifact_sd_vals)

# Plot densities by similarity measure
artifact_sims %>% stack() %>%
  ggplot(aes(x = values)) +
  geom_density(color = "blue",
               alpha = 0.4) +
  facet_grid(ind ~ ., scales = "free")
```


density
values
ssoc
jacc
sd