Final Report

COMPUTATIONAL GEOMETRY

CS6319.001

Authors:

Nicholas Zolton (ngz200000)

April 24, 2024

Contents

Introduction

1 Reason for Study

Throughout this semester I've been working on an indepedent study project that has used AI embeddings to create a tailoring system. This caused me to quickly realize the main problem with the current state of AI vector databases: they, despite focusing on nearest neighbor queries, primarily run in linear time. This quickly becomes an issue at scale, as the number of vectors necessary for many projects can grow quite quickly.

Luckily, however, during class while discussing the Voronoi diagram I started to consider the potential of using it to solve the nearest neighbor problem for embeddings. This led me to the idea of using the Voronoi diagram to create a database that could be used to solve the nearest neighbor problem in logarithmic time. This project is the result of that idea.

2 Initial Ideas

The initial idea for a solution to this problem that I had would be to solve the following steps:

1. Embed text into 2D space using a pre-trained model.
2. Visualize the text embeddings to make sure they are in a usable format in low dimensions.
3. Create a Voronoi diagram of the text embeddings.
4. Create a function that would allow for the querying of the nearest neighbor to a given point.
5. Generalize the solution to work in higher dimensions.

So, with this in mind, I set out to follow these steps and create the Voronoi diagram database.

3 Embedding Text into 2D Space

For starters, I needed to embed the text into 2D space. Normally, I would love to create a custom trained model from scratch, but due to the lack of resources at my disposal (on a fairly low-end laptop) I decided to instead use a pre-trained model to handle the embedding process. I do not believe this is a major issue, as the goal of this project is the computational geometry aspect, not the AI aspect. With this in mind, I decided to use OpenAI's "text-embedding-3-small" model. This model is known for being fairly accurate and is also quite small so it can be run quite cheaply (in total I only spent around 5 cents on this project).

There is one small issue with using this model, however. The model is trained to embed text into 1536 dimensions, which is far too high for the purposes of this project, since the space complexity of the Voronoi diagram is $O(n^{d/2})$. This would, in theory, cause my laptop to run out of memory when trying to create even a small Voronoi diagram. So, I set out to reduce the dimensionality of the embeddings to 2D.

3.1 First Attempt at Dimensionality Reduction

Before I began to attempt to reduce the dimensionality of the embeddings after they were created, I decided to try and reduce the dimensionality of the embeddings at their time of creation. While this would not be possible just one year ago with OpenAI's text embedding models, they have since added a feature that allows for the embeddings to be created in a given dimensionality. So, I decided to try and utilize the OpenAI library to create the embeddings in 2D space from the start. This did indeed work in that it returned embeddings in 2D space, but the embeddings were a bit strange. Below is a figure of the embeddings of all the named colors (according to Wikipedia) in 2D space:

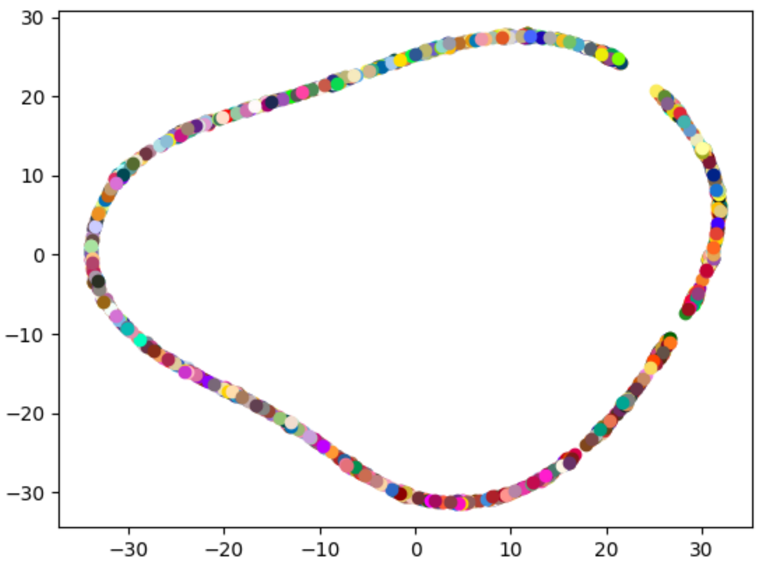


Figure 1: OpenAI's Embeddings of named colors in 2D space. The color of each point corresponds to the color it represents.

Notice how the embeddings are in a very specific, clean polygonal shape. This is not what we would expect from embeddings of colors, even though they are all colors. Instead, we would expect groupings of similar colors. While there is a little bit of grouping, it is not nearly as strong as we would expect. For this reason, it would seem that we cannot rely on OpenAI's text embedding model to create embeddings in 2D space.

3.2 Second Attempt at Dimensionality Reduction

So, although the OpenAI dimensionality method was promising, it did not fill the requirements of the project. Instead, I decided to investigate other methods of dimensionality reduction. From this, I found the T-SNE algorithm. T-SNE is a fairly popular algorithm for dimensionality reduction and is known for being able to reduce the dimensionality of embeddings while still keeping the groupings of similar items. So, I decided to try and use T-SNE to reduce the dimensionality of the embeddings from 1536 to 2. This worked quite well, and the embeddings of the named colors in 2D space looked much more like what we would except:

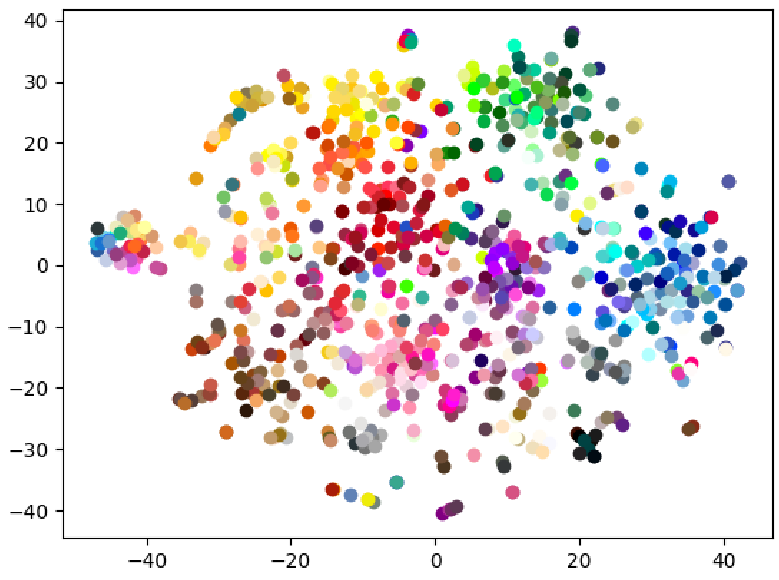


Figure 2: T-SNE's Embeddings of named colors in 2D space.

Here we can absolutely see more clear groupings of similar colors, and with a lot more variation in the x and y dimensions. This is perfect for our use case. So, with this in mind, I decided to use T-SNE to reduce the dimensionality of the embeddings to 2D space. There are, however, a few issues with this approach that we will need to address later on. The first is that T-SNE is a fairly slow algorithm, so it reduces the speed increase that we would hope for by using the Voronoi diagram, but only in the creation process of the diagram. Regardless, this would allow us to begin targeting the other steps of the project since we can focus on the overarching plan to generalize nearest neighbor queries in our data structure. Second, T-SNE is a stochastic algorithm, so it will not always produce the same results. This is not a major issue, but it is something to keep in mind when we are testing the system. Finally, T-SNE is not perfect, so we may lose some information in the dimensionality reduction process (this is not only expected, but necessary for low dimensional reduction so we do not need to worry about it). Luckily, all of these issues should not affect our generalized nearest neighbor query function, so we can move on to the next step of the project and simply consider the database to be "static" for now.

4 Creating the Voronoi Diagram

As seen both in class and throughout computational geometry literature, the Voronoi diagram is a powerful tool for solving nearest neighbor queries. Because of this, it's an extremely well-studied data structure and there are many algorithms for creating it. This poses an interesting question: which algorithm should we use to create the Voronoi diagram? Should we even program it ourselves? Part of the problem as well is that the future data structure we will be creating will hopefully be both generalized and incremental, so we need to make sure that the Voronoi diagram creation algorithm we choose will allow for this (although, in practice, we could theoretically create the Voronoi diagram using one algorithm and then modify it with another algorithm). For now, however, I decided to use Quick Hull to create the Voronoi diagram, since it is fairly simple, generalizable to higher dimensions, and is incremental. Running a very simple version of Quick Hull on the named colors embeddings, we get the following Voronoi diagram:

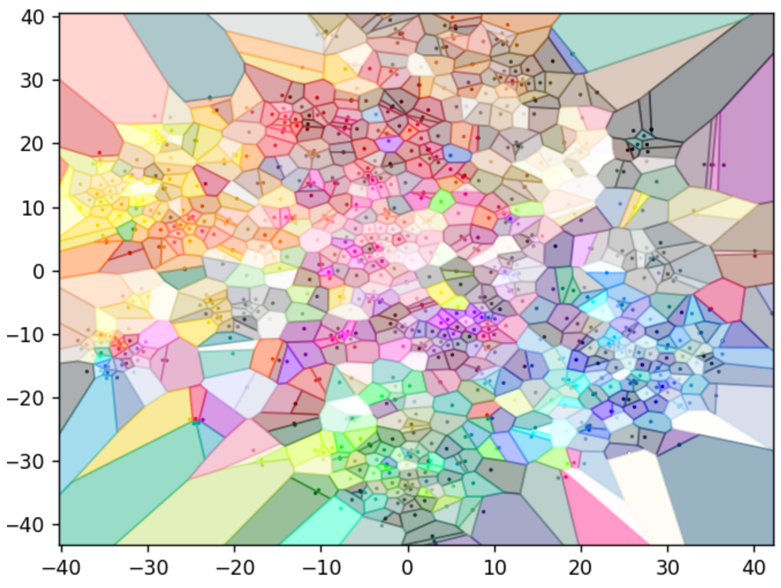


Figure 3: Voronoi Diagram of named colors embeddings.

This, while being fairly simple and mostly just a visualization, shows that we can create the Voronoi diagram quite cleanly. Now, we will need to create a function that will allow us to query the nearest neighbor to a given point. This will be quite easy, as we can simply find the cell that the new point is in and then accept that cell's point as the nearest neighbor. However, it's also common to find the nearest n neighbors to a given point, so we will also need to explore nearby cells to find more neighbors. Regardless, this is a promising start to the project and we will now move on to the next steps: creating the querying function and generalizing the function.

5 Querying the Voronoi Diagram

Now that we have the Voronoi Diagram, we need to create a function that will allow us to query the nearest neighbor to a given new point. The problem, however, is that up until now we have been using T-SNE to reduce the dimensionality of the embeddings to 2D space, but T-SNE is not able to add new points to the embeddings moving forward because it does not actually use parametric mapping from the original space to the new space. This makes it impossible to query the nearest neighbor to a truly new point. So, we will need to make a small change to how we are reducing dimensionality. Instead of simply using T-SNE to reduce the dimensionality of the embeddings, we will instead need to either create a multivariate regressor to predict the 2D space embeddings from the 1536D embeddings or use a regressor to minimize the loss between the 2D space embeddings and the 1536D embeddings directly, as was done in a paper by Laurens Matten[5].

Luckily for us, however, this was already implemented in openTSNE, a Python library that allows for the training of a regressor to predict the 2D space embeddings from the 1536D embeddings. This is perfect for our use case, as it enables us to create a query point inside of the 2D space without having to worry about the dimensionality reduction process. So, with this in mind, we can now move on to creating the querying function. This function will simply follow a few steps:

1. Take in a new input (string).
2. Embed the input into 1536D space.
3. Use the regressor to predict the 2D space embeddings.
4. Find the cell that the new point is in.
5. Return the point in that cell as the nearest neighbor.

6. If we want more than one nearest neighbor, explore nearby cells and return those as well.

This is a fairly simple process at a high level, but it will require a bit of work to implement. First, we will need to sanity-check the regressor to make sure it is working correctly.

5.1 Sanity-Checking the Regressor

To sanity-check the regressor, we will need to embed a new point into 1536D space, predict the 2D space embeddings, and then plot the new point into our Voronoi diagram to make sure it is in the correct cell. While I know this is not the most solid method of checking the validity of the method, it is a good first step for making sure that the queries make at least a little bit of sense. So, with this in mind, I decided to embed the word "lime". Below is the result of the sanity check test:

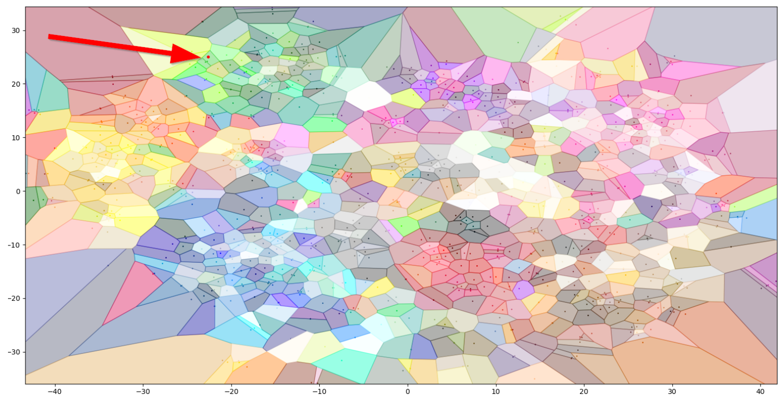


Figure 4: Sanity Check of the regressor. The word "lime" is embedded into 2D space and plotted into the Voronoi diagram.

While it is a bit difficult to quantify how well the overall process is working, it is clear that the regressor is at least somewhat working since we can see that the new point for "lime" is in the correct area, as it is grouped with the majority of the other "green" colors and is paired specifically with a bright green! Personally, I also tried this with a few other colors and received similarly accurate results, but due to brevity I will leave those out for now. So, now that we have proven that placing new points into the Voronoi diagram is viable, we can move on to the next step of doing planar point location to actually find what the nearest neighbor is for our new queried point.

5.2 Planar Point Location

Planar point location is a well-studied and clearly thought out problem in computational geometry, so my first thought was that programming an algorithm for planar point location, in this case the Kirkpatrick-Seidel algorithm, would be quite easy. However, after looking into the algorithm a second time, I realized that it is a bit more complex than I had originally thought. Not only that, but the high constants in the algorithm would make it quite slow for smaller datasets. Because of this, I decided that it would be best to avoid heavily investing in the Kirkpatrick-Seidel algorithm and instead look for a library that implements it. Finally, I would compare the results of the library to the results of the final implmentation that I would create. It's also worth noting that the Kirkpatrick-Seidel algorithm is incredible at reducing the space required for creating the planar point location data structure with a space complexity of $O(n)$, so it still may be worth implementing on a case-by-case basis.

5.2.1 The Planar Point Location Library

To start, I began to search for libraries that implement the Kirkpatrick-Seidel algorithm. Immediately I stumbled upon an 11-year-old library called simply called point-location[4], which is a Python library that implements the Kirkpatrick-Seidel algorithm directly, but also creates its own geometry classes to handle the data. While this isn't ideal, as it would be nice to directly use the polygons I created for the Voronoi diagram directly, it was a good start. So, I decided to begin testing the library with the named colors. Unfortunately, I immediately hit an issue: it required a dependency named "Poly2Tri", or P2T for short. When I first tried installing it from PyPI (as it was present in the PyPI registry), I had an error and was unable to install it. So, I figured I would try to install it directly from the source instead. Upon going to the repostory, I realized that it was a Cython library, something that I had never worked with personally before. Not only this, but it also did not have a ‘setup.py‘ file so I knew that I would have to do some manual work to get it installed and, to validate my suspicions, the GitHub issues showed that I was not the only one having issues installing it. After a few hours of trying to get it to work with no luck, I figured that perhaps there was another maintained version of the library that I could use since it appeared to be a well-used library before it was abandoned. After a little bit more investigating, I found a couple different options. The first was a library called "pypoly2tri". This library had no documentation, but did have a ‘setup.py‘ file and similar code to the original library, so I figured it would be worth a shot. Luckily, after a bit of tinkering with the code (since the library was originally written for Python 2), I was able to get it to install. Further, I was even able to get it to do the basic tests that the original library was able to do. So, with this in mind, I decided to try and use the point-location library with the new pypoly2tri library.

This was, in hindsight, a costly mistake. After a bit of tinkering with the triangulation functions, I realized that the library had different names for many of the functions that the point-location library was using. Despite this, I decided to push through and try resolving all of these issues by hand. After a couple more hours of work, I was able to test a few simple functions of the library that did similar things to the point-location library, but I had also learned that the original poly2tri library had a couple functions with no exact equivalent in the pypoly2tri library. This was, of course, a major issue since the point-location library relied on these functions. So, with this in mind, I decided to try and find another library that would work. Next, I found a library named "poly2tri.python" that was a more direct port of the original poly2tri library, but modified to work with Python 3.

With a few more hours of work, I was even able to get the poly2tri library to work with the point-location library. Unfortunately, I realized a little too late that the point-location library itself also had a few difficult-to-resolve issues. Notably, the library made a few strange assumptions about the data that was being passed to it. For example, it assumed that the data was integers and not floats, which caused a few rounding errors. This also spiraled into a few other issues, such as the library not being able to handle overlapping points, and vertices in the polygons with degrees greater than, or equal to, 8. While this wouldn’t normally be an issue with most Voronoi diagrams, I decided that it would be best to try and find another library that would work better with the general use case of the Voronoi Database.

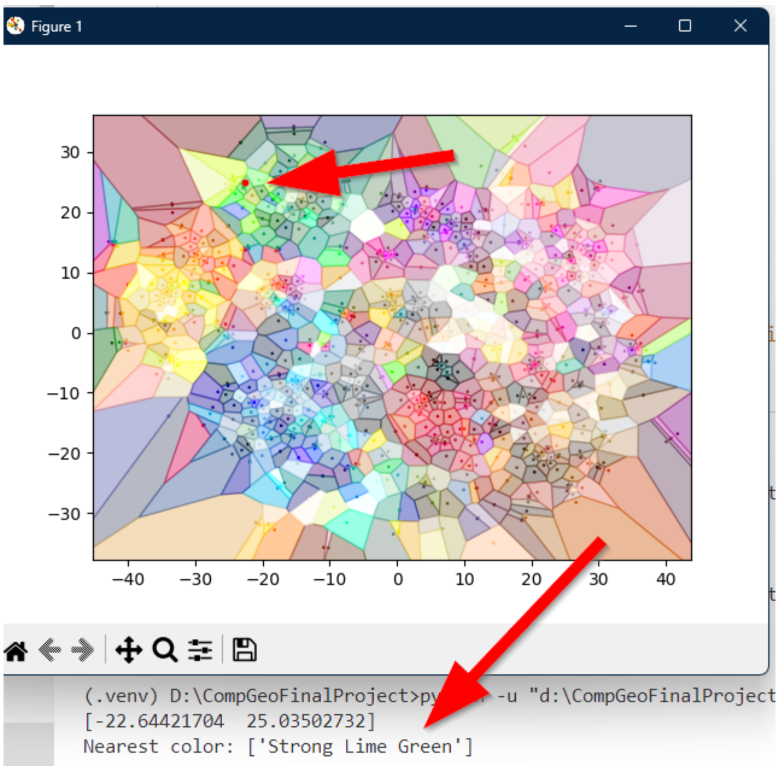
5.2.2 Theodore Ando's Kirkpatrick Library

The next library I stumbled upon was a library created by Theodore Ando that implemented the Kirkpatrick-Seidel algorithm too[1]. Luckily for me, this library was a bit more modern too and had a few nice features. First, it had a "requirements.txt" file that made it easy to install the dependencies. Second, it had detailed documentation and some examples that made it easy to understand how to use the library. This allowed me to get up to speed much faster than with the point-location library and I only had to make one or two small changes to the library to account for the difference it Python versions. With the examples working as well, I decided to try and use the library with the Voronoi diagram. Unfortunately, I quickly realized that the library was not as general as I had hoped. The library was designed to work with some general assumptions about the data just like the point-location library, but it also had a few other issues. For whatever reason, the library implemented it's own version of Quick Hull that had a big issue with some of the polygons that were created by the Voronoi diagram and it would infinitely loop. Luckily, I was able to fix this by reimplementing the Quick Hull algorithm with the use of Scipy. Next, I realized that the polygons would also fail during the triangulation process. This was a bit more difficult to fix, and after a few hours of debugging with no luck, I decided to once again pivot away from the library. With very few choices left for libraries that implement the Kirkpatrick-Seidel algorithm, I decided to try a fully different technique and, after some searching, I landed on R trees.

5.2.3 R Trees

R trees are functionally able to do point location in logarithmic time on average. Of course, this means that their worst possible case is linear time, but for the purposes of this project, that is not a major issue. So, I decided to try and use a variant of the R tree algorithm to do the point location for the Voronoi diagram. This led me to learning that Shapely, a library that I've commonly used for other computational geoemtry problems, has an R tree variant called "STRTree", or (as described by the Shapely documentation) "a query-only R-tree spatial index created using the Sort-Tile-Recursive (STR) algorithm"[2][3].

With all this in mind, it was time to finally implement the R tree algorithm and finish the querying function for the Voronoi Database. This was, luckily, a fairly simple process due to how well the Shapely library is documented and the similarity between how Shapely handles polygons and how the Voronoi Database up to this point has handled polygons. So, with a couple conversions from the polygons we already had to the Shapely polygons, I was able to create the querying function. Below is the result of the query "lime" in the Voronoi Database:



```
(.venv) D:\CompGeoFinalProject>py     -u "d:\CompGeoFinalProject
[-22.64421704  25.03502732]
Nearest color: ['Strong Lime Green']
```

Figure 5: Result of the query "lime" in the Voronoi Database. The nearest neighbor is the bright green point.

And with that, the querying function was complete. Not only that, but because of the method of using a parametric T-SNE to predict the 2D space embeddings, the querying function works for any dimension. Therefore, the Voronoi Database is now fully generalized and can be used for any dimension.

6 Conclusion (final limitations/next steps)

Now that we have the Voronoi Database implemented, I want to talk about the current operating state of the project, the limitations of the project, and the next steps that could be taken to improve the process.

6.1 Current Operating State

First, the project is currently in a working state with a couple neat features. The first is that the project is fully generalized and can be used for any dataset with any dimension. This is a major win, as it allows for the project to be used in a wide variety of applications. Second, the project allows for the querying of the nearest neighbor to a given point in logarithmic time. This is a major improvement over the linear time that is normally required for nearest neighbor queries in AI vector databases. Third, the project is fairly simple to use and can be easily implemented in a wide variety of applications. Fourth, the project is extremely visual and can be used to learn more about the data, as seen in the named colors example. Finally, the project has a ton of useful insights and data that can be used to extend the project in the future.

6.2 Limitations

The project is not without its limitations, however. The first is that we are currently using T-SNE to reduce the dimensionality of the embeddings to 2D space. While a lot of the issues with T-SNE are mitigated by the use of the parametric variant, the time taken to reduce the dimensionality is still quite high and could be a major issue for making large initial databases that we are querying against. It is certainly possible, however, to use a different technique to reduce the dimensionality of the embeddings, such as PCA or UMAP and try to reduce the time taken to create the database. Second, the database does not allow for adding or removing points. This isn't a major issue in terms of usability, but it does limit the current use cases. We could even get around this with some clever work on both the Quick Hull and R tree algorithms, but it would be a major undertaking. Third, we haven't even begun trying to fine-tune the T-SNE algorithm itself to make the embeddings more accurate, so there may be larger issues with trying to query multiple nearest neighbors. This is because we may not be accurately preserving the global structure of the data. Finally, we have not extensively tested the database with a wide variety of datasets. While I firmly believe that the method will work for any dataset, I am not confident in the accuracy of the queries yet. This is something that will need to be tested in the future.

6.3 Next Steps

The next steps for the project are fairly clear. The first is to try and reduce the time taken to create the database. This could be done by using a different dimensionality reduction technique, as mentioned before, or by trying to parallelize a lot of the work that is being done. Second, we need to try and add the ability to add and remove points from the database. The Quick Hull algorithm does allow for incremental construction, but not incremental removal. The Voronoi diagram itself has the same limitation. Once these two issues are resolved, we could certainly allow for the database to be used in a much wider variety of applications (though I am not sure of the time complexity for these operations, so it may still be slow). Third, we need to try and fine-tune the T-SNE algorithm to make the embeddings more accurate. This could be done by trying to find the best hyperparameters (perplexity, learning rate, etc.) for the T-SNE model. Finally, we need to test the database with a wide variety of datasets to make sure that it is working as intended and focus on the general accuracy of the queries. Once this is done, it should also be possible to do n nearest neighbor queries, which would be a major improvement over the current state of the database.

7 Final Thoughts

Overall, I am quite happy with the progress that I have made on this project. While it is not perfect, I believe it could be a major improvement in some very specific use cases. I am also quite happy with the amount of learning that I have done throughout the project. There are so many different algorithms and techniques that I didn't know existed prior to this project, and I am quite excited to continue learning about them and implementing them in the future. Lastly, if you want to check out the code for the project, it is available on my GitHub at the following link: .

References

[1] Ando, T. (2018). Kickpatrick's algorithm python library. https://github.com/theodore-ando/kirkpatrick.

[2] Gillies, S. and Contributors (2021). Strtree. https://shapely.readthedocs.io/en/stable/strtree.html.

[3] Leutenegger, Scott T. Edgington, J. M. and A., L. M. (1997). Str: A simple and efficient algorithm for r-tree packing. https://ia600900.us.archive.org/27/items/nasa_techdoc_19970016975/19970016975.pdf.

[4] Marsh, C. (2013). Point location. https://github.com/charliermarsh/point-location.

[5] van der Maaten, L. (2009). Learning a parametric embedding by preserving local structure. https://lvdmaaten.github.io/publications/papers/AISTATS_2009.pdf.