GDA HW 3

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1 Metric Tree Curvature

Want to show that a metric tree space has negative curvate, where a metric tree space (M, d) is a metric space such that:

$$\forall x, y \in M, \exists \text{a unique path } x \rightsquigarrow y \text{ that is homeomorphic to } [0, 1]$$

Proof. We will show that a metric tree space (M, d) has negative curvature by showing that for all $x, y, z \in M$:

$$d(x, y) + d(y, z) - d(x, z) \geq 0$$

We will prove this by cases. First, consider the case where x, y, z are all on the same path. Then, $d(x, y) + d(y, z) = d(x, z)$, so $d(x, y) + d(y, z) - d(x, z) = 0$. Thus, the inequality holds.

Now, consider the case where x, y, z are not all on the same path. Then, there are two cases: either x and y are on the same path, or y and z are on the same path. Without loss of generality, assume that x and y are on the same path. Then, $d(x, y) = d(x, z) - d(y, z)$. Thus, $d(x, y) + d(y, z) - d(x, z) = d(x, z) - d(y, z) + d(y, z) - d(x, z) = 0$. Thus, the inequality holds. $\qquad\square$

2 Hausdorff and Gromov-Hausdorff Metrics

Want to show that Hausdorff and Gromov-Hausdorff metrics are indeed metrics. Recall that a metric space is defined as (M, d) for set M and metric (distance) function d such that for all $x, y, z \in M$:

$$
\begin{aligned}
&d_M(x, y) = 0 \iff x = y && \text{(equality)} \\
&d_M(x, y) > 0 \text{ for } x \neq y && \text{(positivity)} \\
&d_M(x, y) = d_M(y, x) && \text{(symmetry)} \\
&d_M(x, z) \leq d_M(x, y) + d_M(y, z) && \text{(triangle inequality)}
\end{aligned}
$$

2.1   Hausdorff Metric

The Hausdorff distance is defined on two non-empty subsets X, Y of a metric space (M, d_M) as:

$$d_H(X, Y) = \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x, y), \sup_{y \in Y} \inf_{x \in X} d_M(x, y) \right\}$$

Want to show that the Hausdorff distance d_H is a metric that satisifes the four properties above.

Proof. We will prove all four properties of a metric in a metric space for the Hausdorff distance.

1. **Equality:** To show the property of equality we prove both directions. If $X = Y$ then:

$$
\begin{aligned}
d_H(X, Y) &= d_H(X, X) \\
&= \max \left\{ \sup_{x \in X} \inf_{x' \in X} d_M(x, x'), \sup_{x \in X} \inf_{x' \in X} d_M(x, x') \right\} \\
&= \max \{0, 0\} \qquad \text{by } d_M(x, x') = 0 \text{ for } x = x' \\
&= 0
\end{aligned}
$$

If $d_H(X, Y) = 0$ then:

$$
\begin{aligned}
d_H(X, Y) &= 0 \\
&= \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x, y), \sup_{y \in Y} \inf_{x \in X} d_M(x, y) \right\}
\end{aligned}
$$

By the max operation, one or both arguments must be equal to zero. However, since metric-distances are non-negative, both arguments must be zero:

$$\sup_{x \in X} \inf_{y \in Y} d_M(x, y) = \sup_{y \in Y} \inf_{x \in X} d_M(x, y) = 0$$

By the definition of the sup and inf operators, this implies that for all $x \in X$ and $y \in Y$, $d_M(x, y) = 0$. Since d_M is a metric, this implies that $x = y$ for all $x \in X$ and $y \in Y$. Thus, $X = Y$.

Therefore d_H satisfies the property of equality.

2. **Positivity:** To show the property of positivity we prove the following: if $X \neq Y$ then $d_H(X,Y) > 0$. We will prove this by contradiction. Suppose $d_H(X,Y) = 0$ for $X \neq Y$. Then:

$$d_H(X,Y) = 0$$
$$= \max\left\{\sup_{x \in X} \inf_{y \in Y} d_M(x,y), \sup_{y \in Y} \inf_{x \in X} d_M(x,y)\right\}$$

By the max operation, one or both arguments must be equal to zero. However, since metric-distances are non-negative, both arguments must be zero:

$$\sup_{x \in X} \inf_{y \in Y} d_M(x,y) = \sup_{y \in Y} \inf_{x \in X} d_M(x,y) = 0$$

By the definition of the sup and inf operators, this implies that for all $x \in X$ and $y \in Y$, $d_M(x,y) = 0$. Since d_M is a metric, this implies that $x = y$ for all $x \in X$ and $y \in Y$. Thus, $X = Y$.

This contradicts the assumption that $X \neq Y$. Therefore d_H satisfies the property of positivity since d_M is always non-negative.

3. **Symmetry:** To show the property of symmetry, prove that $d_H(X,Y) = d_H(Y,X)$. If $X = Y$, this proof is trivial because $d_H(X,Y) = 0$ and $d_H(Y,X) = 0$. If $X \neq Y$, then:

$$d_H(X,Y) = \max\left\{\sup_{x \in X} \inf_{y \in Y} d_M(x,y), \sup_{y \in Y} \inf_{x \in X} d_M(x,y)\right\}$$
$$= \max\left\{\sup_{y \in Y} \inf_{x \in X} d_M(x,y), \sup_{x \in X} \inf_{y \in Y} d_M(x,y)\right\}$$
$$= d_H(Y,X)$$

4. **Triangle Inequality:** To show the property of triangle inequality, prove that $d_H(X,Z) \leq d_H(X,Y) + d_H(Y,Z)$. If $X = Y$ or $Y = Z$, this proof is trivial because $d_H(X,Y) = 0$ or $d_H(Y,Z) = 0$ and $d_H(X,Z) = 0$. If $X \neq Y$ and $Y \neq Z$, then:

$$d_H(X,Z) = \max\left\{\sup_{x \in X} \inf_{z \in Z} d_M(x,z), \sup_{z \in Z} \inf_{x \in X} d_M(x,z)\right\}$$

Because d_M is a metric, it satisfies the triangle inequality for x, y, z for all choices of x, y, z. In particular, any choice of y holds, letting us pick $y' := \inf_{y \in Y} d_M(x, y)$ and $y'' := \inf_{y \in Y} d_M(y, z)$:

$$
\begin{aligned}
d_H(X, Z) &= \max \left\{ \sup_{x \in X} \inf_{z \in Z} d_M(x, z), \sup_{z \in Z} \inf_{x \in X} d_M(x, z) \right\} \\
&\leq \max \left\{ \sup_{x \in X} \inf_{z \in Z} \left(d_M(x, y') + d_M(y', z) \right), \sup_{z \in Z} \inf_{x \in X} \left(d_M(x, y'') + d_M(y'', z) \right) \right\} \\
&= \max \left\{ \sup_{x \in X} d_M(x, y') + \inf_{z \in Z} d_M(y', z), \sup_{z \in Z} d_M(y'', z) + \inf_{x \in X} d_M(x, y'') \right\} \\
&\leq \max \left\{ \sup_{x \in X} d_M(x, y'), \inf_{x \in X} d_M(x, y'') \right\} + \max \left\{ \inf_{z \in Z} d_M(y', z), \sup_{z \in Z} d_M(y'', z) \right\} \\
&\leq \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x, y), \inf_{x \in X} d_M(x, y'') \right\} + \max \left\{ \inf_{z \in Z} d_M(y', z), \sup_{z \in Z} \inf_{y \in Y} d_M(y, z) \right\} \\
&\leq \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x, y), \inf_{x \in X} \sup_{y \in Y} d_M(x, y) \right\} + \max \left\{ \inf_{z \in Z} \sup_{y \in Y} d_M(y, z), \sup_{z \in Z} \inf_{y \in Y} d_M(y, z) \right\} \\
&= d_H(X, Y) + d_H(Y, Z)
\end{aligned}
$$

Therefore, because the Hausdorff distance has all four properties of a metric, it is inded a metric. $\square$

2.2 Gromov-Hausdorff Metric

The Gromov-Hausdorff distance is defined for two metric spaces (X, d_X) and (Y, d_Y) with two isometric functions $\phi : X \to A$ and $\psi : Y \to A$ as:

$$
d_{GH}(X, Y) := \inf_{\phi, \psi} d_H(\phi(X), \psi(Y))
$$

Want to show that the Gromov-Hausdorff distance d_{GH} is a metric that satisifies the four metric properties above.

Proof. We will prove all four proerties of a metric in a metric space for the Gromov-Hausdorff distance.

Equality: We will prove both directions of $d_{GH}(X, Y) = 0 \iff X = Y$

First, let $d_{GH}(X, Y) = 0$. Because $d_H \geq 0$, we know by the def of infimum that $d_H(\phi(X), \psi(Y)) = 0$. Because d_H is a metric, we know that $\phi(X) = \psi(Y)$ only when $X = Y$. Therefore, $d_{GH}(X, Y) = 0 \implies X = Y$.

Now let $X = Y$. By the metric property of the Hausdorff distance, we know $d_H(X, Y) = 0$ for $X = Y$. Therefore, no matter the isometric embeddings ϕ and ψ, there is always an isometric embedding $\phi = \psi$ such that $d_H(\phi(X), \psi(Y)) = 0$. Therefore, $d_{GH}(X, Y) = 0$.

2. **Positivity:** We will prove that $d_{GH}(X,Y) > 0$ for all $X \neq Y$.

   Because d_H is a metric, we know that $d_H(\phi(X), \psi(Y)) > 0$ is always true when $X \neq Y$. Therefore, no matter the isometric embedding, the infimum of $d_H(\phi(X), \psi(Y))$ is always positive. Thus $d_{GH}(X,Y) > 0$.

3. **Symmetry:** We will prove that $d_{GH}(X,Y) = d_{GH}(Y,X)$. This is trivially true by relabeling X and Y since the isometric embedding functions ϕ, ψ can be anything.

4. **Triangle Inequality:** We will prove that $d_{GH}(X,Z) \leq d_{GH}(X,Y) + d_{GH}(Y,Z)$ for all X, Y, Z.

   By the metric property of the Hausdorff distance we know for spaces $\phi(X), \theta(Y), \psi(Z)$ that:

$$d_H(\phi(X), \psi(Z)) \leq d_H(\phi(X), \theta(Y)) + d_H(\theta(Y), \psi(Z))$$

   Taking the infimum of both sides, we get:

$$d_{GH}(X,Z) \leq d_{GH}(X,Y) + d_{GH}(Y,Z)$$

   Thus we have shown that the Gromov-Hausdorff distance is a metric. $\quad\square$

3   Bounding Gromov-Hausdorff Distance With Diameter

Want to bound the Gromov-Hausdorff distance $d_G H$ in terms of the diameter of metric spaces X and Y:

$$\operatorname{diam}(X) := \max_{x,x' \in X} d_X(x,x') \qquad \operatorname{diam}(Y) := \max_{y,y' \in Y} d_X(y,y')$$

Proof. Let $\tilde{R}$ be an arbitrary relation.

$$\begin{aligned}
d_{GH}(X,Y) &= \inf_{\phi,\psi} d_H(\phi(X),\psi(Y)) \\
&= \frac{1}{2} \inf_{R} \sup_{\substack{(x,y)\in R \\ (x',y')\in R}} |d_X(x,x') - d_Y(y,y')| \\
&\leq \frac{1}{2} \sup_{\substack{(x,y)\in \tilde{R} \\ (x',y')\in \tilde{R}}} |d_X(x,x') - d_Y(y,y')| \\
&\leq \frac{1}{2} \sup_{\substack{(x,y)\in \tilde{R} \\ (x',y')\in \tilde{R}}} \{d_X(x,x'), d_Y(y,y')\} \\
&= \frac{1}{2} \max\{\mathrm{diam}(X), \mathrm{diam}(Y)\}
\end{aligned}$$

$\square$

4 Bounding Gromov-Hausdorff Distance With ϵ-Nets

Want to bound the Gromov Hausdorff distance $d_{GH}(X,Y)$ for metric spaces X and Y. Here, $Y \subset X$ is an ϵ-net such that:

$$\forall x \in X, \exists y \in Y \text{ such that } d(x,y) < \epsilon$$

Proof.

$$\begin{aligned}
d_{GH}(X,Y) &= \inf_{\phi,\psi} d_H(\phi(X),\psi(Y)) \\
&= \inf_{\phi,\psi} \max \left\{ \sup_{x\in\phi(X)} \inf_{y\in\psi(Y)} d(x,y), \sup_{y\in\psi(Y)} \inf_{x\in\phi(X)} d(x,y) \right\} \\
&\leq \inf_{\phi,\psi} \max \left\{ \sup_{x\in\phi(X)} \inf_{y\in\psi(Y)} \epsilon, \sup_{y\in\psi(Y)} \inf_{x\in\phi(X)} \epsilon \right\} \\
&= \inf_{\phi,\psi} \max\{\epsilon, \epsilon\} \\
&= \epsilon
\end{aligned}$$

$\square$

5 Intrinsic Dimensionality Estimation

I estimate the intrinsic dimensionality of a multidimensional Gaussian and hypercube from estimating the tangent plane. I do this by examining the nearest

neighbors of a point and computing its rank – this is an appoximation of the intrinsic dimension. I then take the average of the intrinsic dimension of all points in the dataset.

I use $n = 5000$ data points and an ambient dimension of $D = 50$. I use $k = 2 * ambient\text{-}dim$ nearest neighbors. I then use intrinsic dimensions of $d = \{2, 4, 8, 16, 32\}$ and estimate it with my method. The results are plotted below, with the figures demonstrating the accuracy of my method.
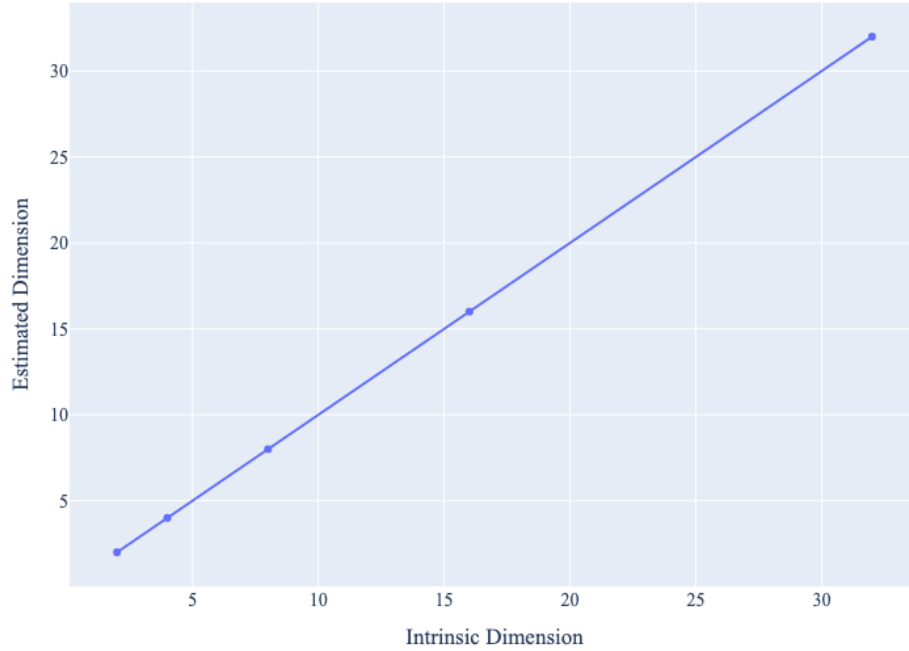

Figure 1: Intrinsic Dimension Estimation for Gaussian
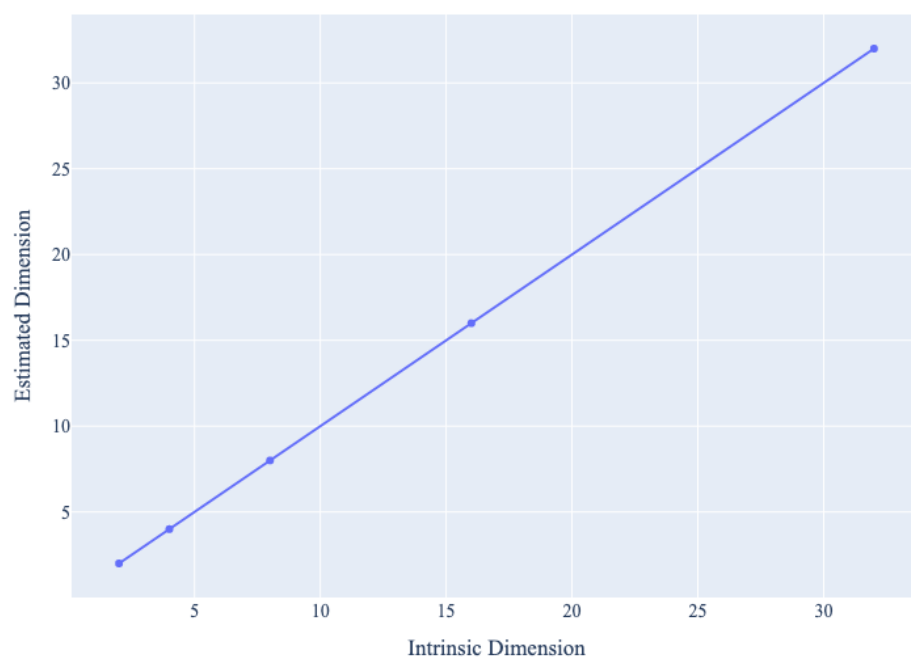
Figure 2: Intrinsic Dimension Estimation for Hypercube

6 Numerical Exploration of Johnson-Lindenstrauss Lemma

Recall the Johnson-Lindenstrauss Lemma:

Lemma: For $0 < \epsilon < 1$, set $X = \{x_1 \ldots x_m\}$ with $x_i \in \mathbb{R}^N$, and $n > 8\ln(m)/\epsilon^2$ there exists a linear map $f : \mathbb{R}^N \to \mathbb{R}^n$ such that:

$$(1 - \epsilon)||u - v||^2 \leq ||f(u) - f(v)||^2 \leq (1 + \epsilon)||u - v||^2$$

for all $u, v \in X$.

Furthermore, the linear map that satisifies this condition is given by $A \in \mathbb{R}^{n \times N}$ where $A_{ij} \sim \mathcal{N}(0, 1/n)$.

To test this out numerically, I simulated the original data X, a projection matrix A, and then actually projected the data to AX.

By the JL Lemma, we expect the distortion of distances to be bounded. Thus, for every pair of points $u, v \in X$, I computed the lower bound $(1 - \epsilon)||u - v||^2$, the upper bound $(1 + \epsilon)||u - v||^2$, and the true distortion $||Au - Av||^2$. I numerically confirmed that the true distortion is between the upper and lower bounds for all pairs of points $u, v \in X$ for multiple dimensions.

I then plotted these distortion values for a given dimension to visually demonstrate this result: on the vertical axis, the embedding distortion (in black) falls between the upper and lower distortion bounds (in blue).
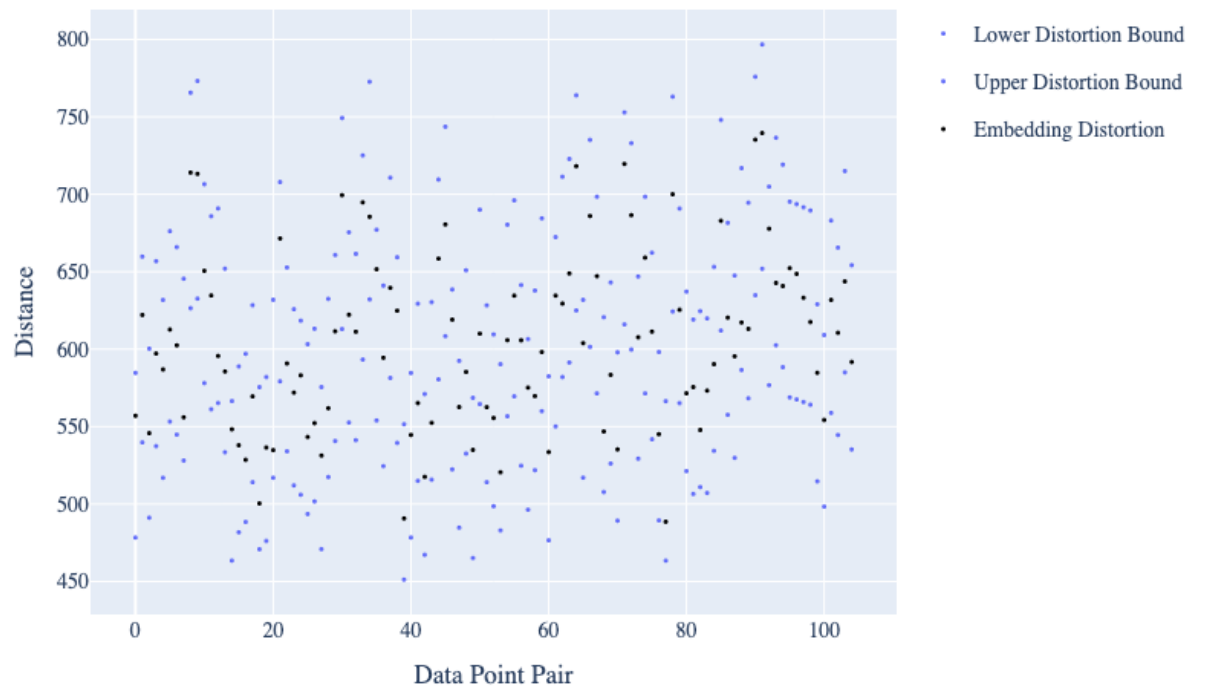
Figure 3: Distortion of Distances for JL Lemma

7 Centroid in Wasserstein Space

I found the centroid in Wasserstein space and plotted it for the MNIST dataset and a few univariate Gaussians. (I used the Python Optimal Transport library to do so.)

7.1 MNIST

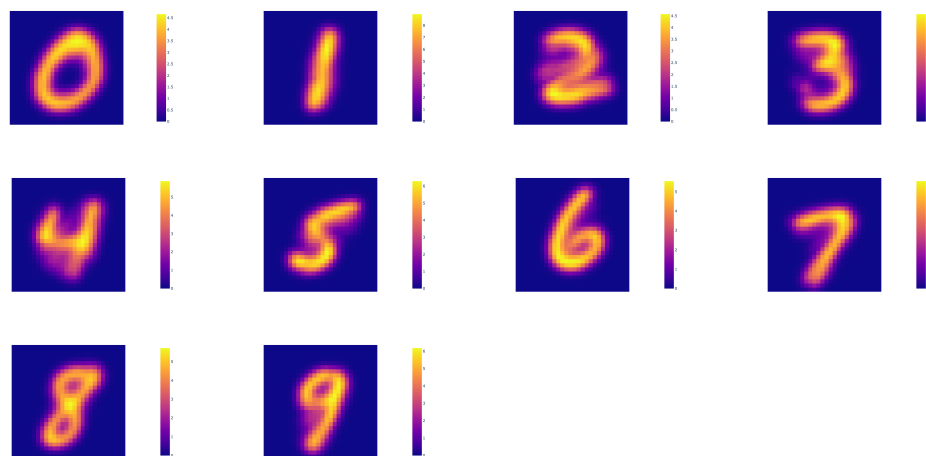Finding the centroid in Wasserstein space for each digit in the MNIST dataset.

Figure 4: Centroids in Wasserstein Space for MNIST Digits

7.2 Gaussians

Finding the centroid in Wasserstein space for a few Gaussians.

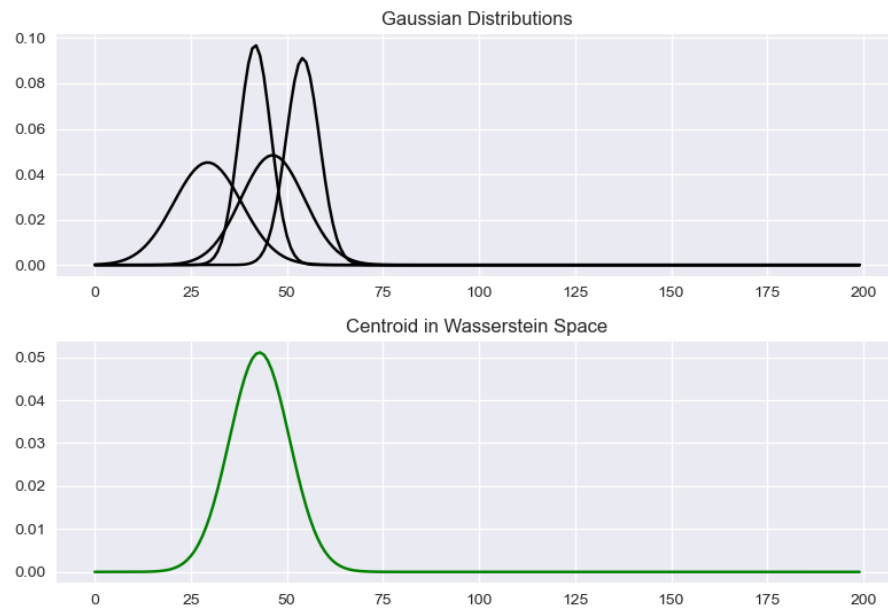Figure 5: Centroid in Wasserstein Space for Gaussians

8 Cluster Tooth and Bone Datasets With Gromov-Hausdorff Metric

I clustered the tooth dataset. First, I read in the data, and subsampled the points for computational efficiency. Then, for each point, I constructed an adjacency matrix comprised of its k nearest neighbors. Next, to compute a distance matrix, I used the approximate Gromov-Hausdorff metric between each pair of adjaency matricies. (Implementation of approximate Gromov-Hausdorff metric can be found here) Finally, I clustered the points using the distance matrix with spectral clustering. The results are shown below.
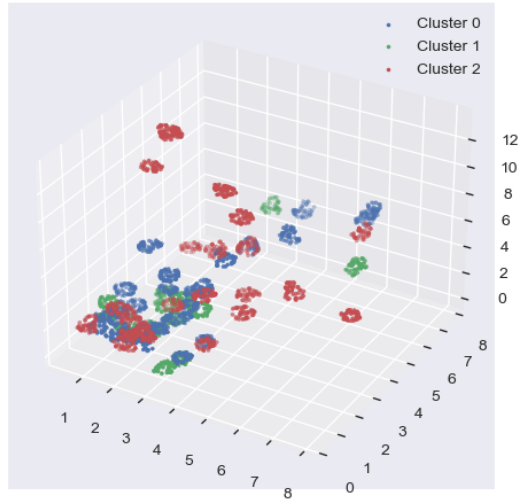

Figure 6: Clusters for Tooth Dataset with Gromov-Hausdorff Metric