Greedy Principal Flows

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Acknowledgements

My 7 soft toys. And my desk lamp for being the light of my life.

Abstract

Principal Flows are a great tool to use when we want to extend the notion of Principal Component analysis to multivariate datasets that we know lie on non-linear manifolds. We restrict this problem to constructing principal flows on hyperspheres. We use a different, easier method to obtain the principal flow that is even closer to its canonical PCA interpretation.

Contents

Chapter 1

Introduction

1.1 Motivation

With the advent of Big Data, using machine learning on multivariate datasets to solve problems from disparate fields has grown in popularity. Although most problems take the form of classification or regression problems, Unsupervised learning has also grown in popularity, Principal Component Analysis being the most popular algorithm. However, if it is given data that lie on some manifold, or a non-linear space, PCA fails to achieve good results. This is why we want to use Principal flows: in essence they are a generalisation of PCA to manifolds. Furthermore, in keeping with the trends of the data science field, we want to use a popular language, python to construct these principal flows.

1.2 Notation

We first define notation and some important concepts we will use later.

Notation	**Explanation**
$\mathbb{R}^D$	Ddimensional space of real numbers.
$\mathbf{X}$	Data Matrix, D dimensions
D	The original dimension of the data matrix
d	Dimension of lower dimensional data which $\mathbf{X}$ is reduced to
$\mathcal{M}^d$	Denotes a connected and complete d-dimensional manifold embedded in $\mathbb{R}^D$
p	Denotes a point on the manifold, $\mathcal{M}^d$.
$\mathbf{v}$	Denotes a vector.
T_pM	Denotes the Tangent space of a point p on $\mathcal{M}^d$.
$\mathbf{C}$	Denotes a Covariance matrix.
$\{x_1, ...x_n\}$	Denotes a collection of n data points.
$\mathbf{1}$	Denotes a vector of 1s.
$\mathbf{I}$	Denotes the identity matrix.
M^T	Denotes the transpose of a some matrix M.

1.3 Definitions

1.3.1 Vector Fields

A vector at point p, $p \in \mathbb{R}^D$ is a pair $\mathbf{a} = (\mathbf{p}, \mathbf{v})$, $\mathbf{v} \in \mathbb{R}^D$, such that $\mathbf{v}$ is the vector v translated so that its tail is at p instead of the origin. All vector operations are defined such that the first item of the pair remains the same, and the second item is the result of the operation. The length and angle between 2 vectors are the same as normal vectors rooted in the origin.

Definition: A *vector field* $\mathbf{F}$ on $U \subset \mathbb{R}^D$ is a function which assigns to each point of U a vector at that point. Then

$$\mathbf{F}(p) = (p, F(p))$$

for some function $F : U \longrightarrow \mathbb{R}^D$. Vector fields on $\mathbb{R}^D$ are often most easily described by specifying this associated function F. A pictoral example of a vector field is below.

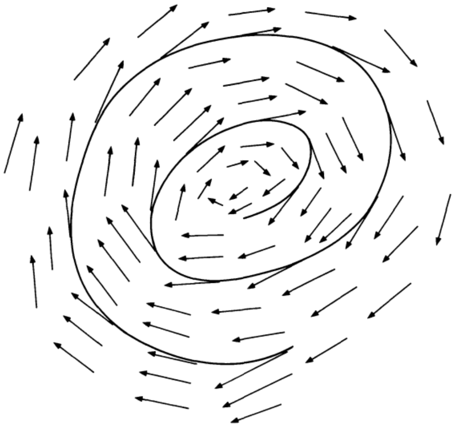


Figure 1.1: An example of a vector field, $\mathbb{R}^3$

1.3.2 Logarithm Maps

Logarithm Map: For each $p \in M$, let

$$log_p(\mathbf{v}) : \mathcal{M}^d \longrightarrow T_pM$$

x is a vector be the logarithm map. The log map is a function that projects a point x_i on the manifold $\mathcal{M}^d$ onto the plane tangent to $\mathcal{M}^d$ at p, by producing a vector which indicates the direction in which p should move to obtain the projection of $x \in \mathcal{M}^d$ onto T_pM.

Exponential Map: For each $p \in M$, let

$$exp_p(\mathbf{v}) : T_pM \longrightarrow \mathcal{M}^d$$

be the exponential map. Exponential maps are the inverse of the logarithm maps. Given a point p, the exponential map w.r.t $\mathcal{M}^d$, a manifold, is a function that projects a point from the plane tangent to $\mathcal{M}^d$ at p onto x on the manifold $\mathcal{M}^d$.

1.3.3 Tangent Space

Define graphically. For a smooth function $f : U \longrightarrow \mathbb{R}$ where U is an open set $\in \mathbb{R}^D$, a vector u is said to be *tangent to the level set* if there is a well defined tangent space consisting of all velocity vectors at p of all parametrized curves in $f^{-1}(c)$ passing through p, and this tangent space is precisely the subspace consisting of all vectors orthogonal to $\nabla f(p)$. In the context of this report, the tangent space T_pM is the hyperplane in which all vectors which are tangent to the point p on the $\mathcal{M}^d$ lie.

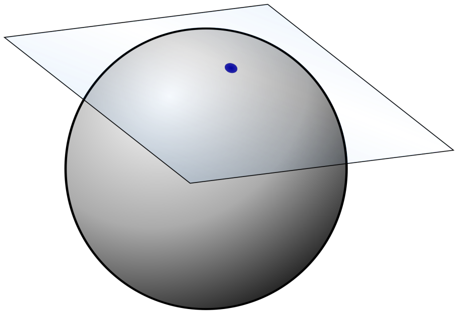


Figure 1.2: Tangent Space of a sphere, $\mathbb{R}^3$

1.3.4 Geodesics

Geodesics are curves on $\mathcal{M}^d$ which play the same role as straight lines in $\mathbb{R}^d$. They can be thought of as the "shortest path between 2 points on the manifold, $\mathcal{M}^d$.

The Euclidean distance between 2 points p, q is defined as $\|p - q\|$, or the 2-norm of the vector $p - q$. Geodesic distance extends this concept of Euclidean, straight line distance in the Euclidean space to Manifolds.

1.3.5 Eigenvalues and Eigenvectors

Now we define eigenvalues and eigenvectors.

Definition: Let $\mathbf{A} \in \mathbb{R}^{n \times n}$. Then a non-zero vector $\mathbf{v}$ is an eigenvector of $\mathbf{A}$ if there exists some scalar λ such that $\mathbf{Av} = \lambda\mathbf{v}$. Then λ is known as the eigenvalue corresponding to vector $\mathbf{v}$.

In this report, we talk only about the eigenvectors and eigenvalues of some Covariance matrix, $\mathbf{C}$. Here we also note that for any 2 eigenvectors v_i and v_j, $i \neq j$, $v_i \cdot v_j = 0$, or any 2 eigenvectors are orthogonal to each other, and that $v_i \cdot v_i = 1$.

1.3.6 Diagonalisation

We say that a matrix is diagonalisable if $\exists \mathbf{V}$, an orthonormal matrix such that the rows of $\mathbf{V}$ are the eigenvectors of $\mathbf{C}$, and a diagonal matrix $\mathbf{E}$ whose diagonal values are the eigenvalues of $\mathbf{C}$. In the context of this report, we only consider symmetric matrices given by $\mathbf{C} \in \mathbb{R}^{D \times D}$, which are always diagonalisable.

$$\mathbf{C} = \mathbf{V}\mathbf{E}\mathbf{V}^T$$

Chapter 2

Literature Review

2.1 Linear Dimension Reduction

2.1.1 Principal Component Analysis

Principal Component analysis is a linear dimension reduction method which tries to obtain a lower-dimensional representation of the data that retains as much variation as possible present in the data set. PCA does this by constructing principal components (PCs) which are linear combinations of the centered original variables. Note that centering each column is the same as finding the "mean" observation and subtracting that from every observation: $x_i - \bar{x}$, since $\bar{x}$ contains the means of every column. These PCs are uncorrelated (orthogonal) and ordered in descending order by the amount of variation retained. Then, reducing some high-dimensional data of dimension D to a lower dimensional d is simply a matter of computing the first d principal components.

Algorithm

- 1. First we center the data matrix, $\mathbf{X}$, by centering each column of $\mathbf{X}$.

- 2. Next we compute the covariance matrix of the centered data matrix.

- 3. Now we diagonalise the covariance matrix and take the first$D$eigenvectors. Let these$D$eigenvectors be the columns of a matrix $\mathbf{V}_d$.

- 4. Multiply $\mathbf{X}$ by $\mathbf{V}_d$ to obtain the$D$principal components.

2.1.2 Classical MDS, Euclidean Distance

Multidimensional Scaling is a linear dimensionality reduction method. Its main aim is to take some high dimensional data, $\mathbf{X}$ and find some low dimensional points so as to minimize the discrepancy between the pairwise distances in the original space and the pairwise distances in the lower-dimensional space.
Let a squared dissimilarity matrix between n points be $\mathbf{M} \in \mathbb{R}^{n \times n}$, let the matrix of coordinates be denoted by $\mathbf{X} \in \mathbb{R}^{n \times D}$, and let $\mathbf{B} = \mathbf{X}^T\mathbf{X}$. Since dissimilarities do not change under translations, we assume that $\mathbf{X}$ has column means equal to 0. MDS seeks to find a lower dimensional representation $\mathbf{X}_{(d)} \in \mathbb{R}^{n \times d}$.
Algorithm: from 2005 Book Modern Multidimensional Scaling, pg 262

- 1. Compute or obtain the dissimilarity matrix, $\mathbf{M}$.
- 2. Let $\mathbf{J}$ be the centering matrix: $\mathbf{J} = \mathbf{I} - n^{-1}\mathbf{1}\mathbf{1}^T$. Compute $\mathbf{B} = -\frac{1}{2}\mathbf{JDJ}$.
- 3. Then, compute the eigendecomposition of $\mathbf{B}$: $\mathbf{B} = \mathbf{V\Lambda V}^T$.
- 4. Then $\mathbf{X} = \mathbf{\Lambda}^{1/2}\mathbf{V}^T$ and for a d-dimensional representation of $\mathbf{X}$: $\mathbf{X}_{(d)}$, $\mathbf{X}_{(d)} = \mathbf{\Lambda}_d^{1/2}\mathbf{V}_d^T$, where $\mathbf{\Lambda}_d^{1/2}$ is the first $d \times d$ submatrix of Λ, and $\mathbf{V}_p^T$ is the first$D$columns of $\mathbf{V}^T$, i.e the first d eigenvectors and their corresponding eigenvalues.

Note that using Euclidean distances, the result of MDS is the same as PCA.

2.2 Non-Linear Dimension Reduction

Non-linear dimensionality reduction methods are particularly useful when the multivariate data we obtain is sampled from a smooth non-linear manifold $\mathcal{M}^d$, e.g a manifold in an

S-shape, obtains better estimates than linear methods like PCA and MDS, which implicitly assume that the data is sampled from a linear space. Certain data sets contain essential nonlinear structures that are invisible to PCA and MDS.

2.2.1 Principal Geodesic Analysis

Principal Geodesic Analysis(PGA) is a generalization of principal component analysis to connected, complete manifolds. The main aim of PGA is to be able to describe the variability of some data lying on some manifold $\mathcal{M}$. More formally, the goal is to find a sequence of lower-dimensional subspaces, which on manifolds are nested geodesic submanifolds that maximize the projected variance of the data. These submanifolds are called the principal geodesic submanifolds, which are analogous to linear subspaces for PCA.

Let T_pM be the tangent space of $\mathcal{M}$ at the intrinsic mean p of the x_i. The intrinsic mean of some data $\mathbf{X}$ lying on some manifold is obtained by first setting the initial mean to a random data point, then iteratively obtaining a better estimation of the intrinsic mean by computing the average of the vectors obtained using the log map at the current mean on all data points, then taking the next estimate of the intrinsic mean as the projection of that average using the exponential map at the current estimate.

Let $U \subset T_pM$ be a neighbourhood of 0 in which our data, $\{x_1, ...x_n\}$ lies, such that projection is well defined for all geodesic submanifolds of $exp_p(U)$.These principal geodesic submanifolds are obtained by by first constructing an orthonormal basis of tangent vectors $v_1, ..., v_d \in T_pM$ that span the tangent space. These vectors are then used to form the principal geodesic subspaces H_k where $H_k = exp_p(V_k)$, and V_k is intersection of the subspace spanned by vectors $1..k$ and U. subspace $V_k = span(\{v_1, ..., v_k\}) \bigcap U$.

Algorithm:

- 1. Obtain the intrinsic mean, $p \in \mathcal{M}^d$ of $\{x_1, ..x_n\}$.
- 2. Calculate the vectors $u_i = log_p(x_i)$.
- 3. Calculate the covariance matrix $\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n} u_i u_i^T$.
- 4. Diagonalise the covariance matrix to obtain $\{v_k, \lambda_k\}$ the eigenvectors and eigenvalues respectively, which represent the principal directions in the tangent space T_pM and the variances.

2.2.2 Locally Linear Embedding

Locally Linear Embedding

The main idea of LLE is to construct a neighbourhood preserving mapping of the original points of dimension D to the reconstructed points of dimension d. We assume that for some data $\mathbf{X} \in \mathbb{R}^D$, the data lie on or near a smooth manifold of dimensionality $d << D$. Locally, LLE assumes the embedding is linear, and thus for each data point $p \in \mathbb{R}^D$, we aim to use a linear combination of its K nearest neighbours to reconstruct a lower-dimensional $p \in \mathbb{R}^d$. LLE does this by first learning some reconstruction weights from the D-dimensional data: $\mathbf{W}$ where $\mathbf{W}_{ij}$ represents the contribution of the j-th data point in reconstructing the i-th one. These weights obey an important symmetry: for any particular data point, they are invariant to rotations, rescalings, and translations of that data point and its neighbors. They thus reflect intrinsic geometric properties of the data that are invariant to exactly such transformations, and therefore, we expect their characterization of local geometry in the original data space to be equally valid for local patches on the manifold. This is what motivates $\mathbf{W}_{ij}$ to be used to reconstruct the embedded manifold coordinates in d dimensions. At the end of LLE, each D-dimensional observation $\mathbf{X}_i$ is mapped to a low dimensional vector $\mathbf{Y}_i$ representing global internal coordinates on the manifold.

LLE Algorithm:

- 1. Compute the K nearest Neighbors of each original data point $\mathbf{X}_i$, where K is a hyperparameter.

- 2. Compute the weights $\mathbf{W}_{ij}$ that best reconstruct each data point from it's neighbours minimizing the **Reconstruction Error** below by constrained linear fits.

$$\varepsilon(\mathbf{W}) = \sum_i |\mathbf{X}_i - \sum_j \mathbf{W}_{ij}\mathbf{X}_j|^2$$

- 3. Compute the vectors $\mathbf{Y}_i$ best reconstructed by the weights $\mathbf{W}_{ij}$ by minimising the embedding cost function:

$$\Phi(\mathbf{Y}) = \sum_i |\mathbf{Y}_i - \sum_j \mathbf{W}_{ij}\mathbf{Y}_j|^2$$

This is minimised by solving a sparse $N \times N$ eigenvector problem whose bottom d non-zero eigenvectors provide an ordered set of orthogonal coordinates centered on the origin.

2.2.3 Isomap

Isomap is an extension of MDS to manifolds in which embeddings are optimized to preserve geodesic distances between pairs of data points. It combines the major algorithmic features of PCA and MDS — computational efficiency, global optimality, and asymptotic convergence guarantees — with the flexibility to learn a broad class of nonlinear manifolds. Isomap achieves this by estimating the geodesic distance between data points, given only input-space distances, e.g euclidean distance between points.

This relies on the fact that for neighboring points, input-space distance provides a good approximation to geodesic distance. For faraway points, Isomap approximates geodesic distance by adding up a sequence of “short hops” between neighboring points, computed efficiently by finding shortest paths in a graph with edges connecting neighboring data points. This approximation relies on the proof that for a sufficiently high density of data points, we can always choose a neighborhood size (e or K) large enough that the graph will (with high probability) have a path not much longer than the true geodesic, but small enough to prevent edges that “short circuit” the true geometry of the manifold.

Isomap Algorithm:

- 1. Construct neighbourhood graph G: First, we need to compute the distances between points: for any node i and j, connect the 2 nodes if $d(i, j) < \epsilon$ or if j is one of the k-nearest neighbours of i.
- 2. Compute all-pairs shortest paths on G. There are many algorithms to do this, but we use the Floyd-Warshall algorithm.
- 3. Construct d-dimensional embedding, using MDS.

Chapter 3

Greedy Principal Flows

3.1 Problem Statement

The main objective for greedy principal flows was to quantify or describe multivariate data on the manifold: we cannot simply fit a line, as this is not Euclidean space. Instead, we want some curve or path such that, locally, and globally, it follows the path of maximal variation of the data. The first principal flow can be thought of as the manifold extension of the 1st principal component in euclidean space. This has already been done in [4], where the principal flows were constructed by solving a problem in variational calculus. Here, we focus on constructing the principal flow using a novel, simpler to implement approach: a greedy algorithm.

3.2 An explanation of the algorithm

Throughout we will assume that $\mathbf{X}$ lies on the hypersphere. To find our principal flow, we first need a starting point. Since our principal flow follows the path of maximal variation of our data, we know it should pass through the centroid of the data. Thus, we first aim to find or estimate this centroid. Although there are many ways of doing this, we opt to make use of the fact that the first principal component passes through the centroid of the data. Thus, if we iteratively project all the data onto the tangent space of the hypersphere, find the 1st principal direction, move in that direction, and find the projected point on the hypersphere, we will eventually converge on the centroid.

Centroid Algorithm:

- 1. Let $p = x_i$, a random data point.
- 2. Compute $log_p(x_i)$ for all x_i, and let these vectors be the rows of the matrix $\bar{\mathbf{X}}$.
- 3. Calculate the covariance matrix of $\bar{\mathbf{X}}$.
- 4. Diagonalise the matrix, then save the eigenvector corresponding to the largest eigenvector, $\mathbf{v}_1$.
- 5. Move in the direction of $\mathbf{v}_1$ a step size of ϵ, $p' = p + \epsilon\mathbf{v}_1$.
- 6. Let $p = exp_p(p')$.

Then we start from that centroid, and build our principal flow from there. Our aim is to find the path of maximal variation of the data.

Problem:

What if our data stretches all around the hypersphere? How do we deal with projecting data through the sphere?

Instead of taking all data into consideration, we choose a small neighborhood around our centroid, whose size is controlled by h. This neighbourhood is determined by some kernel function: either binary or gaussian. The binary kernel includes points in some neighbourhood and excludes points outside, while the gaussian kernel weights nearer points in some neighbourhood much more than those outside the neighbourhood. Thus, we project the data within some neighbourhood $\mathbf{X}_h$ onto the tangent space at the centroid, p: T_pM. We use the logarithm map, log_p to do this. Then the path of maximal variation in this neighbourhood of points is the first principal direction of this data from PCA. This direction is obtained by diagonalising the covariance matrix of the data on this tangent space.

Problem:

This direction clearly is not accurate if we only move in this direction, since it will eventually lead us out of the surface of the hypersphere, and even on the hypersphere, the neighbourhood of points may differ, and change the direction of the path of maximal variation.

Thus, instead of only using this direction, we move infinitesimally in this first direction, then carry out the same procedure again. Thus we iteratively find the "local" direction of maximal variation, move in that direction, and re-compute the next direction of maximal variation. We continue doing this until we have obtained a flow through the entire data set. This does indeed follow the framework that isomap and LLE abide by as well: that obtaining the best option locally becomes the best option globally as well. This is exactly the idea of this Greedy Principal flow algorithm.

3.3 Algorithm Steps

Defn: The Principal Flow of the dataset is basically an integral curve that is always tangent to the direction of 'maximal variation' at any given point it contains.

- We assume the underlying structure of the data is a hypersphere. Starting from the centroid of the data set (user defined or calculated below), we apply the following procedure:

- 1. Project the data residing on the hypersphere onto the hyperplane tangent to the centroid of the data (p). We use the log map of p, obtaining a matrix of vectors on the tangent plane that point from p to the projected points. These are the plane vectors.

- 2. Compute the largest principal component of the points using the plane vectors, applying weights as necessary via the kernel function provided.

- 3. The largest principal component is the new directions that the principal flow moves in. We determine it's sign by making sure it is moving in the same direction as the previous principal direction.

- 4. We take a small step in each direction on the plane, then project it back to the hypersphere.
- 5. We do 1-4 for the point on the opposite end of the growing principal flow.
- 6. Store both points.
- 7. Repeat 1-6 until max_iter is reached.

Chapter 4

Greedy Principal Boundary

In the section above, we have already seen the principal flow. Now we extend the idea of Principal flows to attempt to find some boundary of the data. Let us imagine that the data is contained on some ellipse of the manifold $\mathcal{M}$. Then our aim is to find some boundary around this ellipse. We proceed similarly to the principal flow, except that we also take the 1st and 2nd largest eigenvector and eigenvalues. Here in this context

- We assume the underlying structure of the data is a hypersphere. Starting from the centroid of the data set (user defined or calculated below) we iteratively do the steps below:
- 1. Project the data residing on the hypersphere onto the hyperplane tangent to the centroid of the data (p). We use the log map of p, obtaining a matrix of vectors on the tangent plane that point from p to the projected points. These are the plane vectors.
- 2. Compute the 1st and 2nd largest eigenvector and their associated eigenvalues of the covariance matrix of the points using the plane vectors, applying weights as necessary via the kernel function provided.
- 3. Use the eigenvalues obtained to calculate the radius of the
- ellipse of the data. Then we move a distance of this radius, in the direction

- indicated by the 2nd largest eigenvector.

- 4. We take a small step in each direction on the plane, then project it back to the hypersphere.

- 5. We do 1-4 for the point on the opposite end of the growing principal flow.

- 6. Store both points.

- 7. Repeat 1-6 until max_iter is reached.

4.1 Algorithm

Chapter 5

Applications

Writing the algorithm is meaningless without testing that it also functions as we want it to. First we start with simple applications on toy data to confirm that our algorithm works as intended, then we apply it on some real world data to show how the principal flow can be used there as well.

5.1 Toy Data

5.1.1 Without Noise

As a sanity check or proof of concept of our principal flow, we first want to test our algorithm on some toy data that we know lies on the 3-dimensional unit sphere. This will help us visualise the flow created and determine if it follows the pattern of the data, and thus act as a proof of concept of our algorithm. We generate some data artificially.

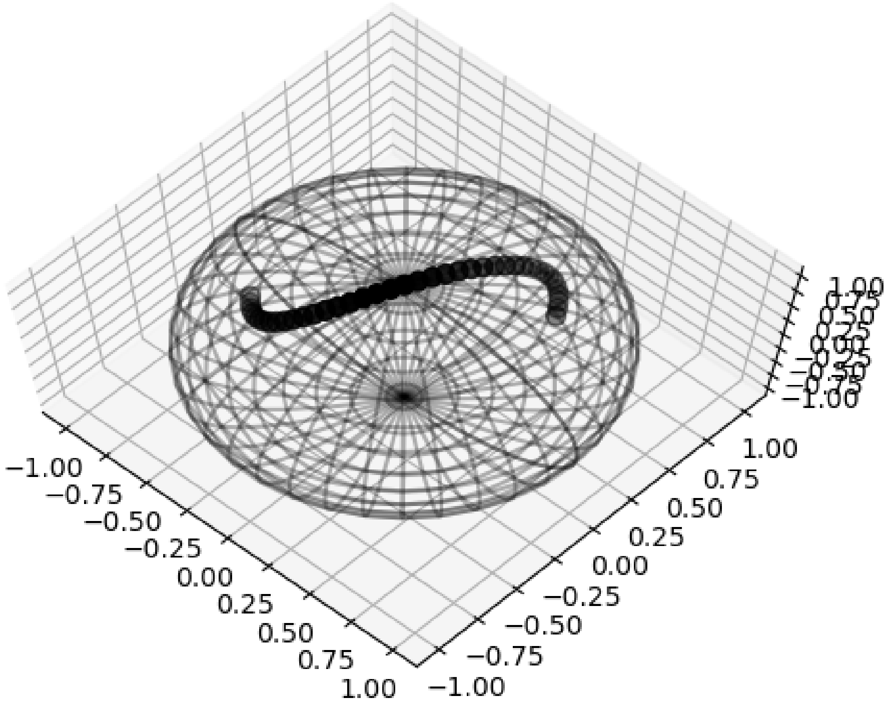


Figure 5.1: Toy data 13, $\mathbb{R}^3$

For example, this dataset is created by setting the first coordinate of the i-th point to $\frac{i-n/2}{n}$, the second to $sin(4*1st)/2$, and the third to $\sqrt{1-(1st)^2-(2nd)^2}$, where n is the number of points we want to generate.
Now that we have seen the Toy Data, let us apply the Principal Flow algorithm to the data above.

This 3D plot shows the original data in black, and the principal flow in red. With some tuning of h, the size of the neighbourhood, we can see that we have constructed a principal flow that follows the original data almost exactly, reconstructing an S with some slight differences at the curves of the s-shape of the original data. We have now seen that proof that our principal flow algorithm works: it is able to accurately reconstruct the toy data,

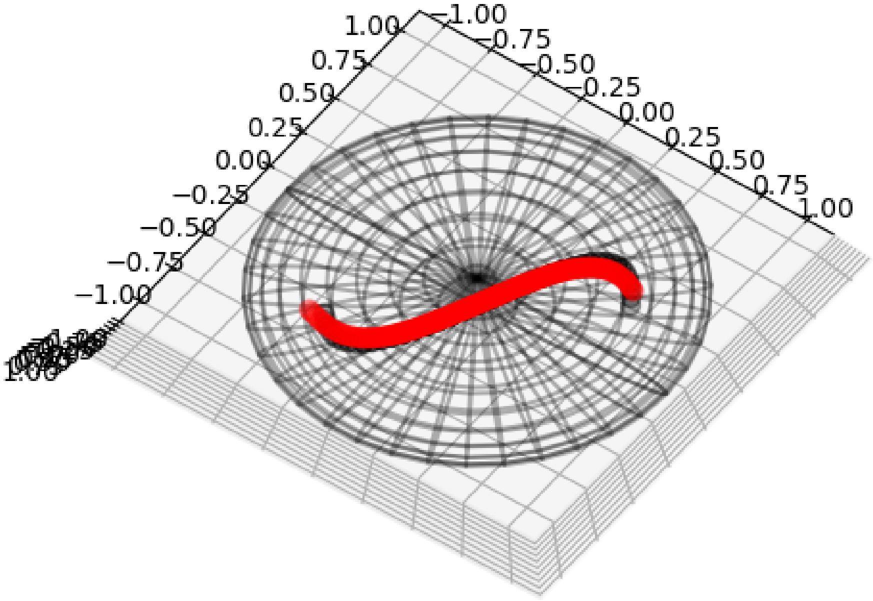
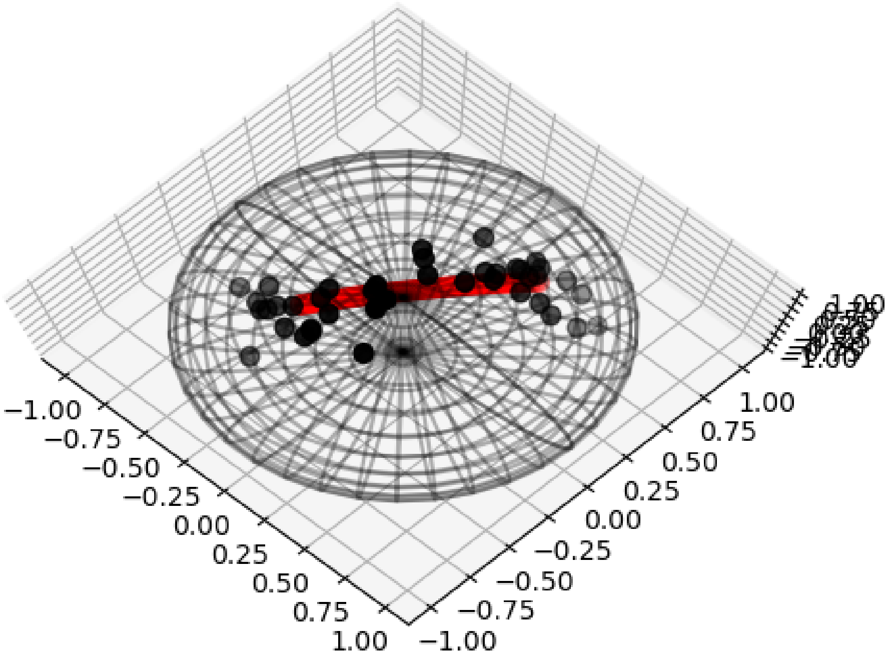


Figure 5.2: Principal Flow on Toy Data, $\mathbb{R}^3$

the s curve on the sphere.

5.1.2 With Noise

Next, gaussian noise was added to the S-shaped data on the sphere to create a noisy dataset. Then we fitted a principal flow to this noisy data.


−1.00
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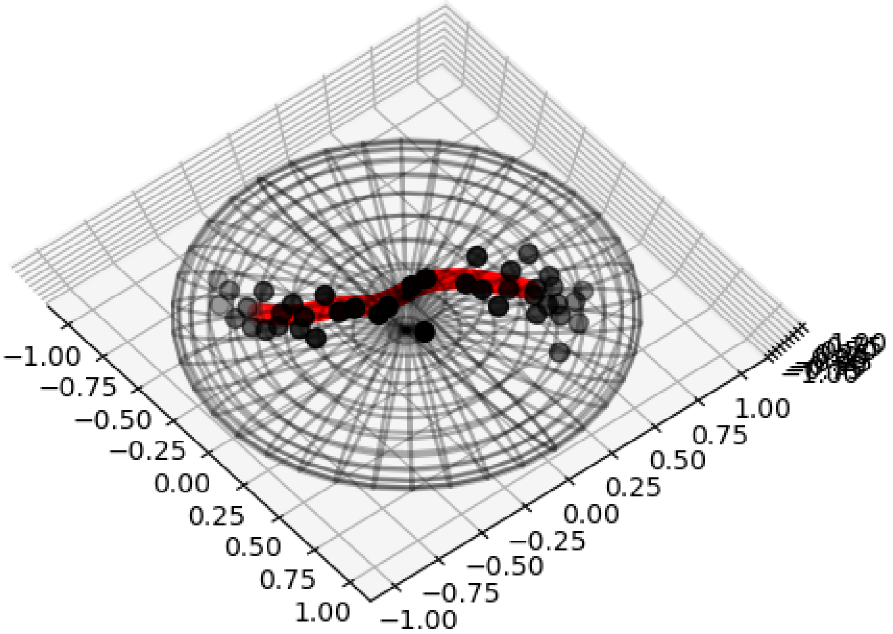
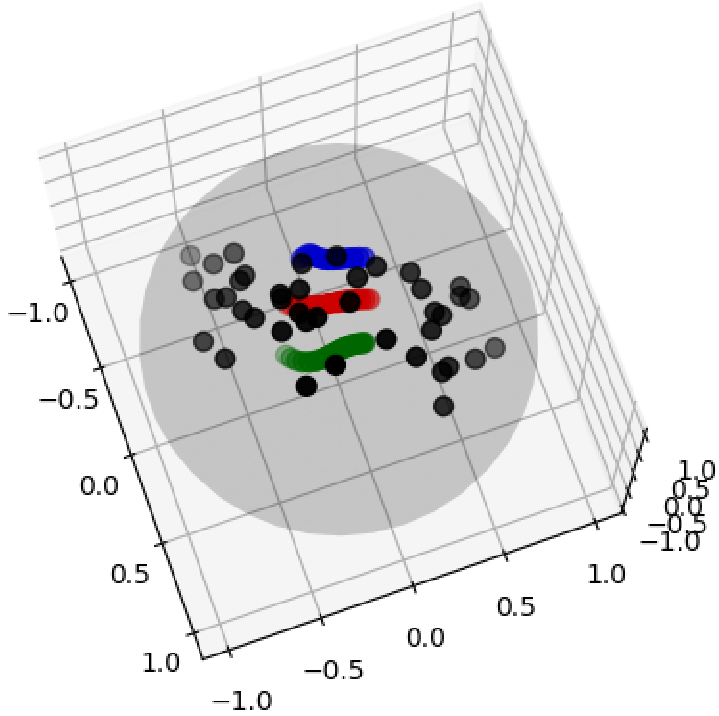


We can see that the principal flow obtained seems to follow the new pattern of variation in the data: from the more dense cloud of points on the left, to the curve of the points in the center to the other dense cloud of points on the right.

5.1.3 Boundary Flow with Noise



5.2 Real World Data

5.2.1 MNIST

5.2.2 Fashion MNIST

5.2.3 Olivetti faces

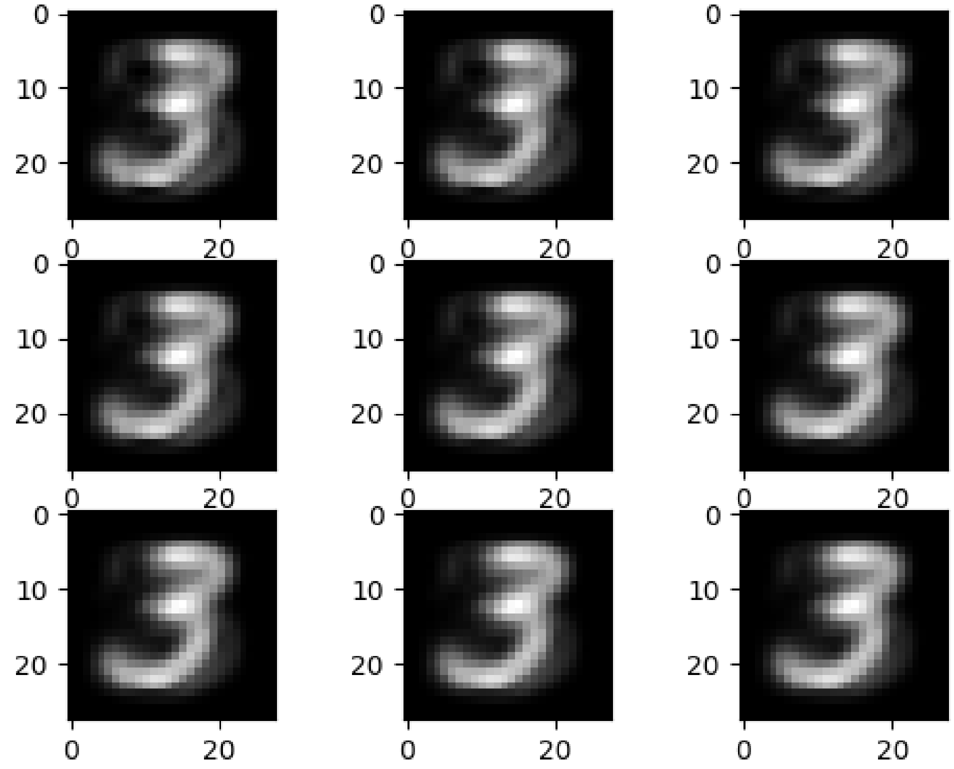


Figure 5.3: MNIST Flow, part 1

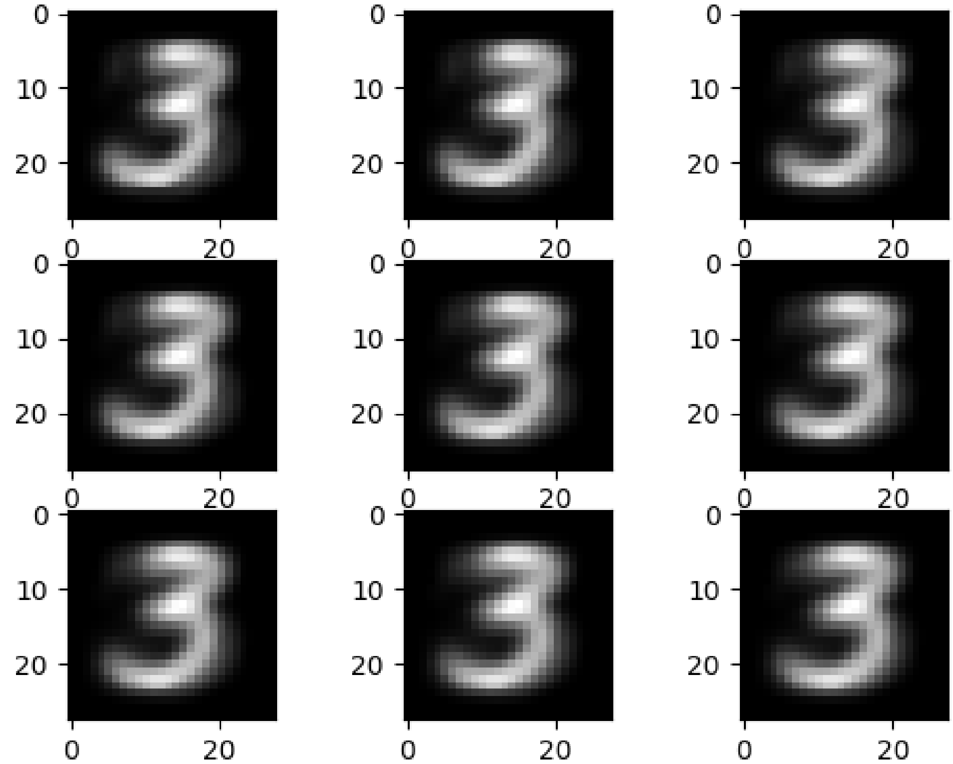


Figure 5.4: MNIST Flow, part 2

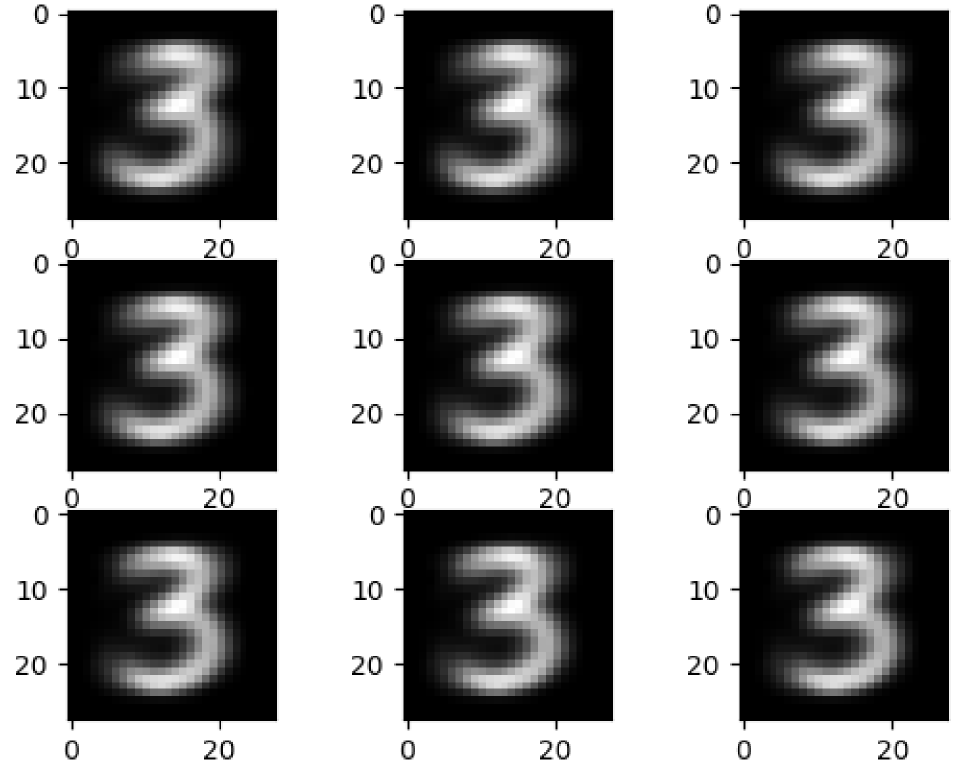


Figure 5.5: MNIST Flow, part 3

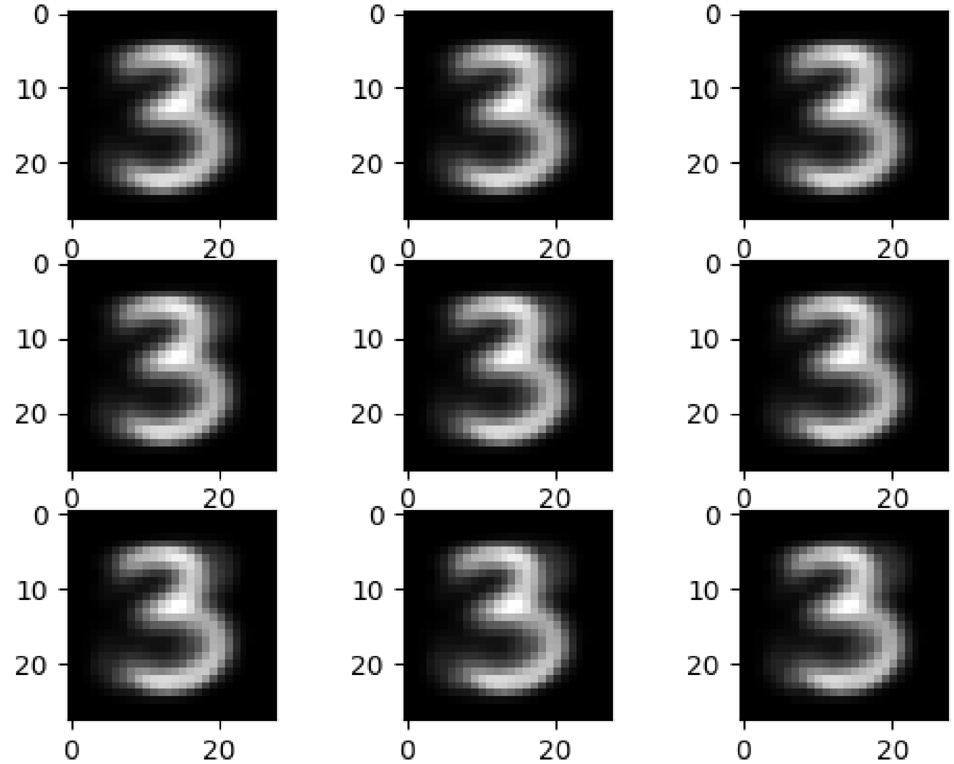


Figure 5.6: MNIST Flow, part 4

Future Directions

What open questions can we investigate further?

Chapter 6

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