# ESTIMATING THE DIMENSION OF A MANIFOLD AND FINDING LOCAL CHARTS ON IT BY USING NONLINEAR SINGULAR VALUE DECOMPOSITION 

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#### Abstract

In this paper we propose a method of using nonlinear generalization of Singular Value Decomposition (SVD) to arrive at an upper bound for the dimension of a manifold which is embedded in some $R^{N}$. We have assumed that the data about its co-ordinates is available. We would also assume that there exists at least one small neighborhood with sufficient number of data points. Given these conditions, we show a method to compute the dimension of a manifold. We begin by looking at the simple case when the manifold is in the form of a lower dimensional affine subspace. In this case, we show that the well known technique of SVD can be used to (i) calculate the dimension of the manifold and (ii) to get the equations which define the subspace. For the more general case, we have applied a nonlinear generalization of the SVD (i) to search for an upper bound for the dimension of the manifold and (ii) to find the equations for the local charts of the manifold. We have included a brief discussion about how this method would be highly useful in the context of the Takens' embedding which is used in the analysis of a time series data from a dynamical system. We show a specific problem that has recently been found out when applying this method. One very effective solution is to develop a model which is based on local charts and for this purpose a good estimate of the underlying dimension of an embedded data is required.


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## 1. Introduction

In this paper we show a method to compute the dimension of a manifold and to find equations for its charts. Here, we illustrate it by an example of a simple geometrical object. The main application of this method, however, could be in the context of an analysis of a dynamical system from observed data, which has been embedded in some $R^{N}$ using a method known as the Takens' delay embedding [1]. A companion paper about ECG data analysis uses the results of this paper in this context [2].

In the case of a geometrical object, let us assume that the manifold has already been embedded in some $R^{N}$ and the data about its co-ordinates is available. We would also assume that there exists at least one small neighborhood with sufficient number of data points. For the case of dynamical systems, this requires the existence of a property known as Recurrence [3].

In what follows, section 2 describes how the technique of singular value decomposition can be used to find the dimension of a manifold when the manifold is an affine subspace. Section 2.1 discusses a numerical example of finding the dimension when an unknown subspace is embedded in $R^{4}$. Section 3 generalizes the method for a realistic case when the manifold is not a linear subspace. Section 3.1 shows a numerical example of finding the equation for a local neighborhood on a manifold using the co-ordinate data of möbius strip. The paper ends with a brief discussion of how the method can be useful in some of the problems involving the modeling and the stability analysis of dynamical systems from time series data.

## 2. The Case of an M-dimensional Subspace embedded in $R^{N}$ WHERE $N>M$

In this section and the next one, we are going to look at a manifold that has already been embedded in $R^{N}$, and the coordinates of a large number of points which belong to this manifold are available as a numerical data. In these two sections we will discuss how to implement a numerical technique to investigate if the data belongs to a manifold which might have a dimension less than $N$. First, in this section we will look at a relatively simpler case when the manifold is an affine subspace of $R^{N}$. In the next section we would look at a more general case of an $M$ dimensional manifold embedded in $R^{N}$. In any case, given the data it would always be worthwhile to first check if an affine subspace is an adequate description of the manifold under consideration.

Our first step to check for the possibility of the existence of an affine subspace is to locate the centroid of the data and reset it as a new origin. Trivially if the data belonged to an affine subspace this centroid would also belong to the same subspace. Further, if we were now to set the centroid as the new origin, we would get a linear vector subspace if and only if the original data belonged to an affine subspace.

This reduces our investigation to see if the modified data belongs to a linear subspace. In practice a numerical technique of Singular Value Decomposition (SVD) is quite suited to do this task.

The Singular Value decomposition (SVD) is based on a theorem that says that any matrix $B$ of size $(P \times N)$; (where $P \geq N$, usually $P \gg N$ is better for a noisy data) can be decomposed into three matrices as follows: $U$, a column orthogonal matrix of size $(P \times N)$; W, a diagonal square matrix of size $(N \times N)$ and $V$, an orthogonal square matrix of size $(N \times N)$; such that,

$$
\begin{equation*}
B=U W V^{T} \tag{2.1}
\end{equation*}
$$

where $V^{T}$ represents transpose of the matrix $V$. The diagonal entries of W are called the singular values.

To use this tool, we construct a matrix $D$ whose rows represent various data points and the columns correspond to various coordinates. Thus the entry in the $i^{\text {th }}$ row and $j^{\text {th }}$ column would be the value of the $j^{\text {th }}$ co-ordinate of the $i^{t h}$ data point. So that if $x_{1}, x_{2}, \ldots x_{N}$ are the variables representing the $N$ coordinates, $D_{i, j}$ would be the value of $x_{j}$ at $i^{t h}$ observation point.

The $n^{\text {th }}$ coordinate of the centroid of all the data points represented by $D$ is given by,

$$
\begin{equation*}
d_{n}=\frac{1}{P} \sum_{p=1}^{P} D_{p, n} \quad \text { for } \mathrm{n}=1,2 \ldots \mathrm{~N} \tag{2.2}
\end{equation*}
$$

Therefore to set the centroid as origin we create a new matrix $A$ such that,

$$
\begin{equation*}
A_{p, n}=D_{p, n}-d_{n} \quad \text { for all } \mathrm{p} \tag{2.3}
\end{equation*}
$$

Using the result of SVD given in Eq. 2.1 we can now prove two simple theorems. For these theorems, the matrices $W$ and $V$ are assumed to have been computed from the given data matrix using readily available procedures [5].

Theorem 2.1. If the $S V D$ of the matrix $A$ defined above gives $Q$ singular values which are zero then there exists an $N-Q$ dimensional affine subspace on which the data resides and the equations defining the subspace are given as follows,

$$
\begin{equation*}
\sum_{n=1}^{N} V_{n, q}\left(Z_{n}-d_{n}\right)=0 ; \quad \text { for } \mathrm{q}=(\mathrm{N}-\mathrm{Q}+1) \ldots \mathrm{N} \tag{2.4}
\end{equation*}
$$

where, $V$ is the orthogonal matrix we got after SVD. Z represents the co-ordinates of $R^{N}$ and $d_{n}$ is the centroid of the data points.

Theorem 2.2. If the matrix $A$ defined above, represents a collection of points which lie on a linear subspace of codimension $Q$ which is defined by $Q$ independent linear algebraic homogenous equations, then the SVD of $A$ will have at least $Q$ singular values which are zero.

We begin with the proof of the Theorem 2.1 in the main text of this paper. Theorem 2.2 is proved in the Appendix.

Proof (Theorem 2.1):
Singular value decomposition of matrix $A$,

$$
\begin{equation*}
A=U W V^{T} \tag{2.5}
\end{equation*}
$$

By post multiplying Eq. 2.5 by V we get,

$$
\begin{equation*}
A V=U W \tag{2.6}
\end{equation*}
$$

Upon transposing,

$$
\begin{equation*}
V^{T} A^{T}=W U^{T} \tag{2.7}
\end{equation*}
$$

Note: $W^{T}=W$ as $W$ is a diagonal square matrix.
Expanding, for any column $p$ we get,

$$
\begin{equation*}
\sum_{n=1}^{N} V_{m, n}^{T} A_{n, p}^{T}=\sum_{n=1}^{N} W_{m, n} U_{n, p}^{T} \tag{2.8}
\end{equation*}
$$

If we define $Y_{n}(p)=A_{n, p}^{T}+d_{n}$ for all $p ; Y(p)$ would be the original data vector at $p^{t h}$ data point. Therefore, using Eq. 2.8 we find that, if we have $Q$ singular values going to zero; all the data vectors (from the original data, before the correction for centroid was applied) will fit the following equation:

$$
\begin{equation*}
\sum_{n=1}^{N} V_{n, q}\left(Z_{n}-d_{n}\right)=0 \quad \text { for } \mathrm{q}=(\mathrm{N}-\mathrm{Q}+1) \ldots \mathrm{N} \tag{2.9}
\end{equation*}
$$

$Z$ is in $R^{N}$ and the above set of equations represent the governing equations for an $N-Q$ dimensional affine subspace of $R^{N}$.
2.1. Numerical Example of a linear subspace. We started with 100 samples each of two random variables $g 1$ and $g 2$. Both were selected using a program to find uniform random numbers in the interval $[0,1]$. From each of these pairs, coordinates for points in $R^{4}$ were selected by using linear transformations. These coordinates became the column entries of the $A$ matrix. The first column of this matrix, representing a coordinate $S 1$ consisted of $0.2 g 1+0.4 g 2$; second column $S 2$ consisted
of $0.3 g 1+0.5 g 2$; third column $S 3$ consisted of $0.5 g 1+0.6 g 2$; and the last column $S 4$ consisted of $0.7 g 1+0.1 g 2$. Singular values of the data matrix $A$ (after the removal of the column means $d_{n}$ ) were,

$$
\left[\begin{array}{c}
3.29739 \\
1.32848 \\
0 \\
0
\end{array}\right]
$$

And the $V$ matrix was,

$$
\left[\begin{array}{cccc}
-0.35101 & -0.33214 & -0.87549 & 0 \\
-0.46934 & -0.34316 & 0.31836 & -0.74874 \\
-0.64884 & -0.21017 & 0.33987 & 0.64756 \\
-0.48531 & 0.85308 & -0.12906 & -0.14165
\end{array}\right]
$$

and the mean vector $d$ was,
$\left[\begin{array}{c}0.2925 \\ 0.39093 \\ 0.53994 \\ 0.40198\end{array}\right]$.

Expanding Eq.2.9 using the last 2 columns of this $V$ matrix we get

$$
\begin{align*}
& \sum_{n=1}^{4} V_{n, 3}\left(Z_{n}-d_{n}\right)=0  \tag{2.10}\\
& \sum_{n=1}^{4} V_{n, 4}\left(Z_{n}-d_{n}\right)=0 \tag{2.11}
\end{align*}
$$

Now we can find 2 final equations in terms of $(S 1, S 2, S 3, S 4)$ corresponding to the last two zero singular values. Those equations are:

$$
-0.74874(S 2-0.39093)+0.64756(S 3-0.53994)-0.14165(S 4-0.40198)=
$$ 0 and

$$
\begin{aligned}
& -0.87549(S 1-0.2925)+0.31836(S 2-0.39093)+0.33987(S 3-0.53994)- \\
& 0.12906(S 4-0.40198)=0 .
\end{aligned}
$$

We re-write these equations to get the coordinates $S 1$ and $S 2$ in terms of $S 3$ and $S 4$ as follows,

$$
\begin{align*}
& S 1=0.7027 S 3-0.07862 S 4-0.05531 . \\
& S 2=0.86487 S 3-0.18918 S 4-0.00001 \tag{2.12}
\end{align*}
$$

Now consider a new space $R^{2}$ given by co-ordinates $(T 1, T 2)$ where $T 1=S 3, T 2=S 4$. We get the following diffeomorphisms defining the local chart co-ordinates:

$$
\left[\begin{array}{c}
S 1  \tag{2.13}\\
S 2 \\
S 3 \\
S 4
\end{array}\right]=\left[\begin{array}{cc}
0.7027 & -0.07862 \\
0.86487 & -0.18918 \\
1 & 0 \\
0 & 1
\end{array}\right] \cdot\left[\begin{array}{c}
T 1 \\
T 2
\end{array}\right]+\left[\begin{array}{c}
-0.05531 \\
-0.00001 \\
0 \\
0
\end{array}\right]
$$

and the inverse is,

$$
\left[\begin{array}{l}
T 1  \tag{2.14}\\
T 2
\end{array}\right]=\left[\begin{array}{llll}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{array}\right] \cdot\left[\begin{array}{l}
S 1 \\
S 2 \\
S 3 \\
S 4
\end{array}\right]
$$

Thus we can see that T1 and T2 define local coordinates of a two dimensional manifold which contains the data. (In this simple case they also turn out to be the global co-ordinates.) This creates an upper bound on the dimension of the manifold as 2 . (This is only an upper bound because there may be a submanifold which contains the data.)

## 3. Finding nonlinear equations from data using NONLINEAR SVD

The method which we discussed in section 2 , using the conventional method of SVD may not work for many of the practical cases for the reason that the data may not be confined to a linear subspace. For such situations, the SVD procedure can still be used with one modification, which is to augment the data matrix by additional columns generated from a set of trial nonlinear functions $f_{k}\left(x_{1}, x_{2}, \ldots x_{N}\right)$ of the N variables [4]. To see this modified procedure, we recall that every row of the original data matrix $D$ consisted of the observed values of the N co-ordinates. Now if we denote the $k^{t h}$ trial function by $f_{k}\left(x_{1}, x_{2}, \ldots x_{N}\right)$, the augmented matrix $E$ can be represented as,

$$
\begin{aligned}
E_{p, n} & =D_{p, n} ; \quad \text { for } \mathrm{n}=1,2 \ldots \mathrm{~N} \\
E_{p, N+k} & =f_{k}\left(D_{p, 1}, D_{p, 2}, \ldots D_{p, N}\right) ; \quad \text { for } \mathrm{k}=1,2 \ldots \mathrm{~K} .
\end{aligned}
$$

This is equivalent to embedding the $N$ dimensional system in a higher dimension $N+K$. Though the system is nonlinear in $N$ dimensions, it happens many times that the system is linear in the higher dimension $N+K$, if the choice of trial functions is successful. (The choice of trial functions are often arbitrary based on trial and error. Often the trial functions are polynomial combinations of the variables. At times the physical situation of the problem might suggest some specific choice of trial functions). Thus, in $N+K$ dimensional space we hope that the system will confine to an affine subspace.

Following the same idea used in section 2 for constructing the matrix $A$ from the matrix $D$, we now construct a matrix $F$ from the matrix $E$ by removing the column averages. In addition to the previously calculated mean vector $d$ (given Eq. 2.2) we also define a mean vector $g$ for the additional columns as,

$$
\begin{equation*}
g_{k}=\frac{1}{P} \sum_{p=1}^{P} E_{p, N+k} \quad \text { for } \mathrm{k}=1,2 \ldots \mathrm{~K} \tag{3.1}
\end{equation*}
$$

Now the modified $F$ matrix is given by,

$$
\begin{align*}
F_{p, n} & =E_{p, n}-d_{n} ; \quad \text { for } \mathrm{n}=1,2 \ldots \mathrm{~N}  \tag{3.2}\\
F_{p, N+k} & =E_{p, N+k}-g_{k} ; \quad \text { for } \mathrm{k}=1,2 \ldots \mathrm{~K} . \tag{3.3}
\end{align*}
$$

Now, if that the SVD of this $F$ matrix gives $Q$ singular values that are zero, we would once again get $Q$ equations using a slightly modified formula in the extended $N+K$ dimensional space,

$$
\begin{equation*}
\sum_{n=1}^{N+K} V_{n, q} F_{n, q}^{T}=0 ; \quad \text { for } \mathrm{q}=(\mathrm{N}-\mathrm{Q}+1) \ldots \mathrm{N} . \tag{3.4}
\end{equation*}
$$

However, using the known set of nonlinear equations we can see that the data vectors will obey the following equation at all the points, if the singular values are exactly zero.

$$
\begin{equation*}
\sum_{n=1}^{N} V_{n, q}\left(Z_{n}-d_{n}\right)+\sum_{k=N}^{N+K} V_{n, q}\left(f_{k}-g_{k}\right)=0 \tag{3.5}
\end{equation*}
$$

for $q$ ranging from $(N-Q+1)$ to $N . V$ is now an orthogonal matrix that has dimension $(N+K) \times(N+K)$.

As in the linear case, if we have $Q$ equations in Eq. 3.5 we conclude that we have a manifold of at the most $N-Q$ dimension.
3.1. Numerical example: Möbius Strip embedded in $R^{3}$. Consider the data generated on a möbius strip that is represented by the following parametrization,

$$
\begin{align*}
& x(u, v)=\left(1+v \cdot \cos \frac{u}{2}\right) \cos (u) \\
& y(u, v)=\left(1+v \cdot \cos \frac{u}{2}\right) \sin (u)  \tag{3.6}\\
& z(u, v)=v \cdot \sin (u)
\end{align*}
$$



Figure 1. Möbius Strip projected to $R^{2}$
where $0 \leq u<2 \pi$ and $-0.3 \leq v \leq 0.3$. The parameter $u$ runs around the strip while $v$ moves from one edge to the other. Its projection in $R^{2}$ can be seen in Figure. 1

Assume that we have generated data in the form of co-ordinates $(x, y, z)$ in $R^{3}$ using the set of equations given by Eq. 3.6. Given the data we wish to find a small neighborhood in the manifold where sufficient number of data points are available. This neighborhood data will be thus a small subset of the whole data. We use this subset to see if there is any relationship that exists between the co-ordinates.

Identification of a neighborhood based on the property of Recurrence: A point in state space is said to be recurrent if the time series generated by the system keeps on visiting the neighborhood of the point [3]. We identify a neighborhood for some recurrent point as follows: we start with some initial point $\left(x_{0}, y_{0}, z_{0}\right)$ and record its evolution in the state space. For the neighborhood of a reference point, the Euler metric - L2 norm (square root of sum of squared distances between vectors) of the reference point with respect to all its neighbors is defined to be less than some threshold value $\Delta$. For finding a small neighborhood of a particular point $\left(x_{p}, y_{p}, z_{p}\right)$ we measured the distance of all the vectors with
respect to the reference recurrent point in the state space. For the numerical simulation explained below $(0.7,0,0)$ was chosen as the reference point. The threshold $\Delta$ was set as 0.032 . As the trajectory approaches the neighborhood with a distance less than $\Delta$, they were considered as the members of the neighborhood.

We collect the data belonging to the neighborhood into a matrix $D$. $D$ has a dimension $P \times 3$, where $P$ is the number of data points in the neighborhood. Create the matrix $A$ from matrix $D$ by removing the column averages of the data points from $D$ as shown in Eq. 2.3. For the specific neighborhood we have selected, the singular values of $A$ matrix were,

$$
\left[\begin{array}{c}
0.352 \\
0.01 \\
2.286 \times 10^{-5}
\end{array}\right]
$$

The low third value is encouraging but to improve the accuracy, we embedded the co-ordinates in $R^{9}$ (from $R^{3}$ ) by using nonlinear trial functions of the $x, y, z$ co-ordinates of the data points (for this particular demonstration we have limited the columns to just the quadratics). We created the extended data matrix $E$ from $D$ matrix by augmenting the trial functions $x^{2}, y^{2}, z^{2}, x y, x z, y z$ to the $D$ matrix. Now the $E$ matrix can be denoted as,

$$
E=\left[\begin{array}{lllllllll}
x & y & z & x^{2} & y^{2} & z^{2} & x y & x z & y z
\end{array}\right] .
$$

Note that $E$ has dimension $P \times 9$ where $P$ is the number of data points in the neighborhood. Next step is to generate the matrix $F$ from $E$ by removing the mean vector $d$ and $g$ from $E$ as explained in Eq. 3.2 and 3.3. The mean vector $d$ was,

$$
\left[\begin{array}{c}
0.694 \\
0.086 \\
-0.018
\end{array}\right],
$$

and the mean vector $g$ was,

$$
\left[\begin{array}{c}
0.481 \\
0.01 \\
4.667 \times 10^{-4} \\
0.059 \\
-0.013 \\
-2.172 \times 10^{-3}
\end{array}\right]
$$

We did the SVD of $F$ matrix and the singular values were,

$$
\left[\begin{array}{c}
0.43287 \\
0.024 \\
4.02788 \times 10^{-4} \\
8.31511 \times 10^{-6} \\
2.43449 \times 10^{-8} \\
1.28177 \times 10^{-10} \\
2.19759 \times 10^{-12} \\
9.08467 \times 10^{-14} \\
0
\end{array}\right] .
$$

Note that the $9^{\text {th }}$ singular value is zero. Using the Eq. 3.5, we get a relationship between the coordinates as,

$$
\begin{equation*}
\sum_{n=1}^{3} V_{n, 9}\left(Z_{n}-d_{n}\right)+\sum_{k=4}^{9} V_{n, 9}\left(f_{k}-g_{k}\right)=0 \tag{3.7}
\end{equation*}
$$

Expanding this we get an equation for the local neighborhood on manifold as,

$$
\begin{aligned}
& 0.05\left(x-d_{1}\right)+\left(1.185 \times 10^{-4}\right)\left(y-d_{2}\right)+\left(4.378 \times 10^{-4}\right)\left(z-d_{3}\right)+ \\
& 0.334\left(x^{2}-g_{1}\right)+0.319\left(y^{2}-g_{2}\right)-0.855\left(z^{2}-g_{3}\right)+\left(5.139 \times 10^{-5}\right)(x y- \\
& \left.g_{4}\right)-\left(4.046 \times 10^{-4}\right)\left(x z-g_{5}\right)-0.231\left(y z-g_{6}\right)=0 .
\end{aligned}
$$

Substituting the mean values we get the exact equation for the manifold as, $0.05 x+\left(1.185 \times 10^{-4}\right) y+\left(4.378 \times 10^{-4}\right) z+0.334 x^{2}+0.319 y^{2}-$ $0.855 z^{2}+\left(5.139 \times 10^{-5}\right) x y-\left(4.046 \times 10^{-4}\right) x z-0.231 y z-0.198=0$.

This equation implies that the manifold is at the most 2 dimensional. We can now choose $y$ and $z$ co-ordinates and create a chart that goes from $(y, z)$ to $(x, y, z)$. Using the above equation, for every point $(y, z)$ we can get a quadratic equation of the form $\left(\alpha x+\beta x^{2}+\gamma\right)=0$ for the neighborhood on the manifold where,

$$
\begin{align*}
& \alpha=0.05+\left(5.139 \times 10^{-5}\right) y-\left(4.046 \times 10^{-4}\right) z  \tag{3.8}\\
& \beta=0.334
\end{align*}
$$

$\gamma=\left(1.185 \times 10^{-4}\right) y+\left(4.378 \times 10^{-4}\right) z+0.319 y^{2}-0.855 z^{2}-0.231 y z-0.198$.
Solution of this quadratic equation gives a prediction for the $x$ data. Fig. 2. shows a comparison between predicted and original $x$ data.


Figure 2. The upper figure shows the $x$ data and its prediction xpred; the error between the data and its prediction is shown in the lower figure.

## 4. Possible application to dynamical systems

We find that the methods reported here have an interesting application to nonlinear dynamics. This is because it offers a solution to a specific problem that arises in the analysis of time series data generated by some unknown dynamical system. It is quite common in such cases to embed
the data some high dimensional $R^{N}$ using Takens' embedding, using delayed coordinates (refer Appendix C). Takens' Delay embedding theorem gives the conditions under which a dynamical system can be reconstructed from a time series generated by it [1]. The reconstruction is diffeomorphic to the original dynamics and it preserves the properties of the dynamical system and it does not change under smooth coordinate changes. To be sure of the embedding, the minimum embedding dimension $m$ is $(2 d+1)$ where $d$ is the dimension of the manifold on which the dynamics resides. This has been improved somewhat to the criterion that says the embedding dimension should be $(>2 h)$, where $h$ is the box counting dimension.

It has been a common practice to use such embedded data to model the dynamical system. However, there is problem that we have recently found [6] in using this approach which is particularly serious if we use such a model to predict the stability of the original system. The problem is that if the data is actually generated by a non-linear dynamical system of dimension $d$, and if the data were to be free of noise it would occupy a $d$ dimensional submanifold in the embedded space. But if the data were to be noisy, we would now have a very large number of competing dynamical systems which agree on the $d$ dimensions but disagree on the $m-d$ dimensions. Therefore, in some of these $m-d$ dimensions the system might be asymptotically unstable, while the original system was quite stable.

The best way to resolve this problem is to carry out the modeling using an atlas and develop local charts in $d$ dimension itself if we can find the dimension and charts from the numerical data. We have shown in a companion paper [2] that this can be done.

## 5. Appendix A: Proof of Theorem 2.2

The Q linear algebraic homogeneous equations can always be written as,

$$
\begin{equation*}
G Z=0 \tag{5.1}
\end{equation*}
$$

where G is $Q \times N$ constant matrix of maximal rank $Q$, and $Z$ is a column vector of dimension $N$ representing the co-ordinates in $R^{N}$.

Now consider the transpose of the data matrix A. Each of the columns of $A^{T}$ represents a vector which will also belong to the subspace governed by the Eq. 5.1. Recall the SVD of matrix $A$,

$$
\begin{equation*}
A=U W V^{T} \tag{5.2}
\end{equation*}
$$

By post multiplying Eq. 5.2 by V we get,

$$
\begin{equation*}
A V=U W \tag{5.3}
\end{equation*}
$$

Upon transposing,

$$
\begin{equation*}
V^{T} A^{T}=W U^{T} \tag{5.4}
\end{equation*}
$$

Now if we denote any of the columns of $A^{T}$ by $X$ and the corresponding column of the $U^{T}$ by $u$,

$$
\begin{gather*}
V^{T} x=W u  \tag{5.5}\\
x=V W u . \tag{5.6}
\end{gather*}
$$

But $x$ lies on the subspace defined by $G Z=0$.
Substituting Eq. 5.6 in Eq. 5.1 we get,

$$
\begin{equation*}
G V W u=0 \tag{5.7}
\end{equation*}
$$

$u$ is the equivalent co-ordinates of the data points in the $U$ matrix. Since Eq. 5.7 has to be true for all $u$,

$$
\begin{equation*}
G V W=0 . \tag{5.8}
\end{equation*}
$$

Consider the matrix product $M=G V . G$ has rank $Q$ and $V$ being an orthogonal matrix is of full rank $N$ which is higher than $Q$. Now by using the Sylvester's inequality for the product of two matrices [7], rank of the product $G V$ is at least $Q+N-N=Q$. In fact, we know that it is $Q$ because G has only $Q$ rows.

Now consider the product of $M$ with $W$ and let the rank of $W$ be $R$. Again by using the same inequality, the rank of $M W$ is at least $Q+R-N$. But we know that it is zero, because of Eq. 5.8. This implies that the rank of $W$ is at the most $N-Q$. Since $W$ is a diagonal matrix, it means that at least $Q$ of the diagonal elements, the singular values must be zero. This proves the theorem 2.2 for the linear subspace.

## 6. Appendix B: A verification of using the procedure OF NONLINEAR SVD TO FIND EXPLICIT NONLINEAR EQUATIONS FOR CHARTS ON THE MANIFOLD

Consider $X$ data, 100 random numbers selected from a uniform noise distribution in the interval $[0,1]$. Generate $Y$ data from $X$ using a quadratic equation of the form $Y=a X+b X^{2}+c$; where the coefficients were $a=2, b=3, c=1.5$. Now the goal is to predict $a, b, c$ from the data $X, Y$ using the procedure of nonlinear SVD. The procedure to determine the coefficients of a quadratic equation are explained below.
step1: Create a data matrix $D$ with columns $X, X^{2}, Y$.
step2: Remove the means $\bar{X}, \bar{X}^{2}, \bar{Y}$ from the columns $X, X^{2}, Y$ to create a matrix $A$ with columns $x 1, x 2, x 3$, where $x 1=X-\bar{X}, x 2=X^{2}-$ $\bar{X}^{2}, x 3=Y-\bar{Y}$. Record the means: $\bar{X}=0.50593, \bar{X}^{2}=0.33601, \bar{Y}=$ 3.51989
step3: Do the SVD of A matrix. The singular values of the $A$ matrix in this case were,

$$
\left[\begin{array}{c}
14.62048 \\
0.52504 \\
1.21589 \times 10^{-15}
\end{array}\right]
$$

And the third column of the $V$ matrix were,

$$
\left[\begin{array}{c}
0.53452 \\
0.80178 \\
-0.26726
\end{array}\right]
$$

The $3^{r d}$ singular value can be considered to be zero because of the rounding error.
step4: Using the Eq. 3.5, get a relationship between the third column of $V$ matrix and the coordinates $x 1, x 2, x 3$ as,

$$
\begin{gathered}
0.53452 x 1+0.80178 x 2-0.26726 x 3=0 \\
x 3=\frac{0.53452}{0.26726} x 1+\frac{0.80178}{0.26726} x 2 \\
x 3=2 x 1+3 x 2
\end{gathered}
$$

Substitute for the actual data coordinates,

Hence the parameters of the quadratic equation are recovered.

## 7. Appendix C: Takens Delay Embedding

The standard Takens embedding (also known as delay embedding) is a method of reconstruction of the state space with time delayed data segments (known as the embedding vectors) [1]. A typical embedding vector $e_{i} \in R^{m}$ is the $m$ dimensional embedding vector generated from the given time series of $\{d\}=d_{1}, d_{2} \ldots d_{n}$, where $d_{i} \in R$ as follows.

$$
\begin{aligned}
e_{1} & =\left(d_{1} d_{2} \ldots d_{m}\right) \\
e_{2} & =\left(d_{2} d_{3} \ldots d_{m+1}\right) \\
& \ldots \\
e_{i} & =\left(d_{i} d_{i+1} \ldots d_{m+i}\right)
\end{aligned}
$$

The collection $\left\{e_{i}\right\} \in R^{m}$ is a delay embedding of the given data $\{d\}$. A matrix $E$, created from $k$ such embedding vectors represents the delay embedding

$$
E=\left[\begin{array}{c}
\left(e_{1}\right)  \tag{7.1}\\
\left(e_{2}\right) \\
\cdots \\
\cdots \\
\left(e^{k}\right)
\end{array}\right]=\left[\begin{array}{cccc}
d_{1} & d_{2} & \cdots & d_{m} \\
d_{2} & d_{3} & \cdots & d_{m+1} \\
& & \cdots & d_{m+k}
\end{array}\right] .
$$

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