

AMATH 563 Homework 2

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Abstract

The work presented here is motivated by material covered in AMATH 563 Inferring Structure of Complex Systems regarding the applications of Dynamic Mode Decomposition and Sparse Regression for dynamical system model discovery. In many instances governing equations for the dynamics of a system are unknown therefor requiring data driven model discovery. Dynamic Mode Decomposition (DMD) seeks to describe the time evolution of recorded variables through linear mapping from one time step to the next. This provides a suitable estimation of the dynamics of the system in the linear case and for small time windows. However, it is often the case that more complex (i.e. nonlinear) variable interactions drive the dynamics in the observed data. In this case, using sparse regression in conjunction with a model term library allows for fitting nonlinear models to the data. This approach is termed the sparse identification of nonlinear dynamics (SINDy) algorithm and leverages the assumption that most dynamical systems have dynamics with only a few active terms. DMD and SINDy are implemented here in the context of hare and lynx population modelling. DMD is also used to illustrate the dynamics of a Belousov-Zhabotinsky chemical oscillator from video pixel data. Together, DMD and model term selection with sparse regression represent important approaches that address the central challenge of discovering dynamical systems models from data.

1 Introduction and Overview

Identifying governing equations of dynamical systems is a main focus of many science and engineering fields. Future state prediction, design and optimization, estimation and control, and physical understanding are outcomes that result from modelling the interactions that underlie system dynamics. DMD and SINDy are recent developments in data-driven dynamical systems modelling that seek to accomplish this goal. In the work presented here both standard DMD, DMD with a sliding window algorithm, and DMD with time-delay embedding are explored to model the population dynamics of a lynx and hare predator-prey relationship from biennial pelt data running from 1845 to 1903. In an effort to better capture nonlinear and multi-scale behavior inherent to this system SINDy is also employed to identify coefficients for a library of model terms. Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and Kullback–Leibler divergence are used to compare the how well the different modelling approaches fit the data. Lastly, DMD is employed to extract the dynamics of a Belousov-Zhabotinsky chemical oscillator from video pixel data. Standard, windowed, and DMD with time-delay embedding are used to model the spatial and temporal dynamics of the chemical oscillator.

2 Theoretical Background

2.1 Dynamic Mode Decomposition (DMD)

DMD is based on proper orthogonal decomposition (POD), and utilizes the singular value decomposition (SVD) such that dimensionality reduction can be achieved. DMD differs from SVD/POD in that instead of yielding top modes based on spatial correlation and singular value size, DMD finds modes that are spatially correlated and also have the same linear behavior in time. This temporal constraint on the modes is not present in SVD/POD thus obfuscating the time evolution of the top modes. In this way, DMD serves to reduce dimensionality and elucidate temporal information. In practice, DMD can be understood as seeking

to identify the linear dynamical system that best describes how the data transitions from one time step to the next. This is accomplished by first collecting pairs of state descriptions for sequential time steps. These snapshot pairs are arranged into two data matrices (Brunton 2019):

$$\mathbf{X} = \begin{bmatrix} | & | & \cdots & | \\ \mathbf{x}(t_1) & \mathbf{x}(t_2) & \cdots & \mathbf{x}(t_m) \\ | & | & \cdots & | \end{bmatrix} \quad (1)$$

$$\mathbf{X}' = \begin{bmatrix} | & | & \cdots & | \\ \mathbf{x}(t'_1) & \mathbf{x}(t'_2) & \cdots & \mathbf{x}(t'_m) \\ | & | & \cdots & | \end{bmatrix} \quad (2)$$

The pairs of time sequential state descriptions are denoted $x(t_k)$ and $x(t'_k)$ where $t'_k = t_k \Delta t$. Next these data matrices are used in the context of an optimization problem to find a linear operator \mathbf{A} that maps \mathbf{X} to \mathbf{X}' (i.e $\mathbf{X}' \approx \mathbf{A}\mathbf{X}$). The operator \mathbf{A} that is the best fit operator is defined as (Brunton 2019):

$$\mathbf{A} = \arg \min_A (\|\mathbf{X}' - \mathbf{A}\mathbf{X}\|_F) = \mathbf{X}'\mathbf{X}^\dagger \quad (3)$$

In practice the operator \mathbf{A} is found by first computing the SVD of \mathbf{X} and performing a rank reduction based on the top ranked SVD modes. This rank reduced SVD of \mathbf{X} allows for the pseudoinverse to be computed and subsequently the best fit linear operator \mathbf{A} . The rank reduced version of \mathbf{A} is generated by projecting onto the POD modes of the matrix \mathbf{U} of the rank reduced SVD. This rank reduced version of \mathbf{A} has the same eigenvalues as the full matrix and as such can be used in place of a \mathbf{A} for computing the DMD modes. These modes are achieved by first taking the spectral decomposition of this rank reduced version of \mathbf{A} denoted as $\tilde{\mathbf{A}}$ (Brunton 2019).

$$\tilde{\mathbf{A}}\mathbf{W} = \mathbf{W}\mathbf{\Omega} \quad (4)$$

$\mathbf{\Omega}$ is a diagonal matrix containing the eigenvalues $\tilde{\mathbf{A}}$ which are also the eigenvalues of the full rank matrix \mathbf{A} and are referred to as the DMD eigenvalues. \mathbf{W} contains an eigenvector of $\tilde{\mathbf{A}}$ in each column. These eigenvectors are important because they are used to construct the DMD modes $\mathbf{\Phi}$ (Brunton 2019).

$$\mathbf{\Phi} = \mathbf{X}'\tilde{\mathbf{V}}\tilde{\mathbf{\Sigma}}^{-1}\mathbf{\Omega} \quad (5)$$

These DMD modes and eigenvalues can then be used to expand the current system state (Brunton 2019).

$$\mathbf{x}_k = \sum_{j=1}^r \phi_j \lambda_j^{k-1} b_j = \mathbf{\Phi}\mathbf{\Lambda}^{k-1}\mathbf{b} \quad \text{where: } \mathbf{b} = \mathbf{\Phi}^\dagger \mathbf{x}_1 \quad (6)$$

It is often useful to rewrite his spectral expansion in continuous time where the continuous time eigenvalues are: $\omega = \frac{\log(\lambda)}{\Delta t}$. The system state expansion then becomes (Brunton 2019):

$$\mathbf{x}(t) = \sum_{j=1}^r \phi_j e^{\omega_j t} b_j = \mathbf{\Phi} \exp(\mathbf{\Omega} t) \mathbf{b} \quad (7)$$

2.1.1 Time-Delay Embedding

The aim of time-delay embedding, also termed delay-coordinate embedding, is to use of time delays to construct a feature space for geometrical reconstruction of non-linear dynamical systems (Pan and Duraisamy 2019). This approach is justified by the Takens embedding theorem which states that by using a delay-coordinate map, one can construct a diffeomorphic shadow manifold from univariate observations of the original system (Brunton 2019, Pan and Duraisamy 2019). In the dynamical systems context explored here, time delays are leveraged in higher order or Hankel Dynamic Mode Decomposition. Eigen-time-delay coordinates are obtained from a time-series of a single system measurement $x(t)$ by taking the SVD of the

Hankel matrix (Brunton 2019):

$$\mathbf{H} = \begin{bmatrix} x(t_1) & x(t_2) & \dots & x(t_{m_c}) \\ x(t_2) & x(t_3) & \dots & x(t_{m_c+1}) \\ \vdots & \vdots & \ddots & \vdots \\ x(t_{m_0}) & x(t_{m_0+1}) & \dots & x(t_m) \end{bmatrix} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^* \quad (8)$$

The columns of \mathbf{H} are well-approximated by the first r columns of \mathbf{U} which form what is termed a Koopman invariant subspace (Brunton 2019). The first r columns of \mathbf{V} provide a time series of the magnitude of each of the columns of $\mathbf{U}\mathbf{\Sigma}$ in the data. By plotting the first three columns of \mathbf{V} , an embedded attractor is obtained. This connection between eigen-time-delay coordinates and the Koopman operator motivates a linear regression model on the variables in \mathbf{V} . Thus, Dynamic Mode Decomposition of the Hankel matrix can serve to find the best fit linear operator that describes the time dynamics of the system. The DMD modes of the Hankel matrix are associated with a fixed oscillation frequency and decay/growth rate and are approximations of the modes of the Koopman operator thus providing a global linear representation (Brunton 2019).

2.2 Sparse Identification of of Nonlinear Dynamics (SINDy)

Identifying nonlinear parameters of a model from data is a challenge that cannot be addressed by linearization methods such as DMD. Extracting nonlinear structure from data is challenging because there are many possible mathematical combinations of model terms. Sparse identification of nonlinear dynamics (SINDy) attempts to circumvent this challenge by assuming that dynamical systems have dynamics described by right hand side functions with few terms. In practice this is accomplished by first constructing a function library of functions that depend on the measured system variables. A linear map is then fit to this library to predict the derivatives of the system parameters measured in time. To find this mapping generally requires solving an overdetermined system of equations as there will be more state variable measurements in time than there will be model terms. Therefore this presents as an optimization problem where imposing sparsity promoting regularization can solve for the simplest mapping (i.e. fewest model terms) from state space to the time rate of change of each state variable. Common regularizations selected for this purpose are least absolute shrinkage and selection operator (lasso) regression or least squares regression with iterative coefficient thresholding.

2.3 Model Performance Metrics

In order to assess the degree to which the implemented modelling methods fit the data of interest, three metrics are employed: Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and Kullback–Leibler divergence.

2.3.1 Kullback–Leibler divergence

Given two data distributions f and g , KL divergence is the measure of how much information is lost when using distribution g to estimate f (Brunton 2019).

$$I(f, g) = \int f(\mathbf{X}, \beta) \log \left[\frac{f(\mathbf{X}, \beta)}{g(\mathbf{X}, \mu)} \right] \quad (9)$$

2.3.2 Akaike Information Criterion (AIC)

KL divergence cannot always be computed in practice as it requires complete statistical knowledge of the true model and of all the parameters in the proposed model being compared (Brunton 2019). Akaike Information Criterion (AIC) seeks resolve this issue by estimating KL divergence based on the empirical log-likelihood function at its maximum point (Brunton 2019).

$$AIC = 2K - 2\log [\mathcal{L}(\hat{\mu}|\mathbf{x})] \quad (10)$$

K is the number of parameters, $\hat{\mu}$ is an estimate of the best fit parameters and \mathbf{x} is the data being fit (Brunton 2019). Of note is that AIC penalizes model complexity by including $2K$ which will grow as the number of terms of the fit model increases.

2.3.3 Bayesian Information Criterion (BIC)

BIC differs from AIC only in the strength of the penalization on non-parsimonious models.

$$BIC = \log(n)K - 2\log[\mathcal{L}(\hat{\mu}|\mathbf{x})] \quad (11)$$

Here n is the number of data points. The rationale for this is to ensure that, if the true model is included in a set of other proposed models, it will be selected as the best model. Using AIC does not always guarantee this due to the large penalty on model complexity that does not depend on the sample size n (Brunton 2019).

3 Algorithm Implementation and Development

3.1 Canadian Lynx and Snowshoe Hare Population Modelling

1. Transcribe and import data. Interpolate to generate more data points.
2. Construct the data snapshot pair matrices for DMD
3. Perform DMD, compute continuous time eigenvalues and subsequently the DMD model time dynamics
4. Plot the DMD model time dynamics alongside the raw population data.
5. Repeat DMD for a sliding window across the population data. Plot DMD model time dynamics.
6. Construct Hankel matrices for each variable (Lynx and Hare). Layer the rows of these individual Hankel matrices in an alternating fashion to generate overall system Hankel matrix.
7. Compute SVD of Hankel matrix. Plot energy per SVD mode.
8. Perform DMD on Hankel matrix, compute continuous time eigenvalues and subsequently the DMD model time dynamics.
9. Plot the time-delay embedded DMD model time dynamics alongside the raw population data.
10. Construct Lotka-Volterra model ($\dot{x} = (b - py)x$ and $\dot{y} = (rx - d)y$) term library
11. Compute derivative of raw population data.
12. Perform least squares regression with thresholding to determine best fit Lotka-Volterra model term coefficients
13. Construct model term libraries of higher order polynomial and sinusoidal terms.
14. Perform least squares regression with thresholding to determine best fit model term coefficients for these libraries.
15. Calculate Kullback–Leibler divergence, AIC, and BIC for each model: standard DMD, sliding window DMD, DMD with time-delay embedding, and the Lotka-Volterra model and other model term libraries fit with sparse regression.

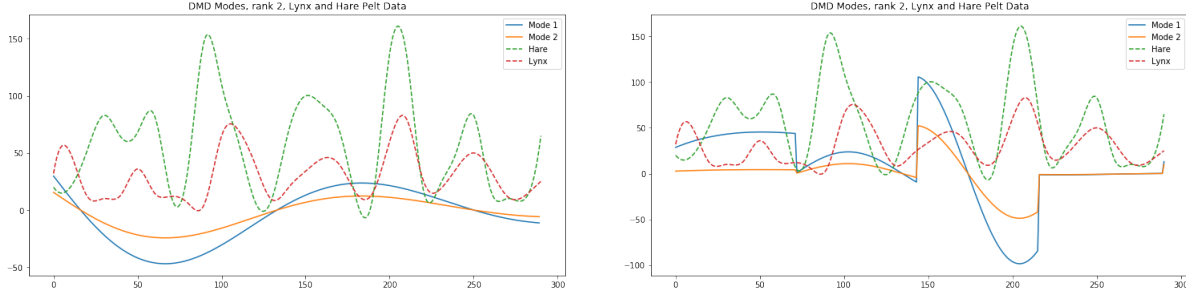


Figure 1: (Left) Plot of the DMD predicted Hare and Lynx population values. (Right) Plot of the DMD predicted Hare and Lynx population values using a sliding window with width of 72 data points.

3.2 Belousov-Zhabotinsky Chemical Oscillator Modelling

1. Import Belousov-Zhabotinsky chemical oscillator movie data
2. Flatten each image frame into single array, concatenate all frames together to form the data matrix. Min/Max normalize the data matrix.
3. Construct the data snapshot pair matrices for DMD
4. Perform DMD, compute continuous time eigenvalues and subsequently the DMD model time dynamics
5. Plot the DMD model time dynamics alongside the raw population data.
6. Construct Hankel matrix matrices in an alternating fashion to generate overall system Hankel matrix.
7. Compute SVD of Hankel matrix. Plot energy per SVD mode.
8. Perform DMD on Hankel matrix, compute continuous time eigenvalues and subsequently the DMD model time dynamics.

4 Computational Results

4.1 Canadian Lynx and Snowshoe Hare Population Modelling

The methods employed here are largely DMD based approaches and fitting model term libraries to the population data with sparse regression. Results for standard DMD and DMD on sliding windows across the data are shown in Figure 1. Resulting predictions from a DMD model with time-delay embedding are shown in Figure 2. Fitting the Lotka-Volterra model ($\dot{x} = (b - py)x$ and $\dot{y} = (rx - d)y$) library to the data with sparse regression resulted in model parameter estimates of : $b = 0.23$, $p = 0$, $r = 0$, and $d = 0.23$ (Figure 3). Model predictions for polynomial and sinusoidal model term libraries are depicted in Figure 3 and Figure 10. Kullback-Leibler divergence, AIC, and BIC for each model are tabulated in Table 1.

4.2 Belousov-Zhabotinsky Chemical Oscillator Modelling

The top DMD modes resulting from DMD being performed on the flattened movie frame pixel data are shown in Figure 6. Resulting predictions of the time dynamics for the top DMD modes from a DMD model with time-delay embedding are shown in Figure 7.

5 Summary and Conclusions

5.1 Canadian Lynx and Snowshoe Hare Population Modelling

Standard DMD using only a single time-delay to predict the time evolution of system dynamics produced qualitatively poor hare and lynx population predictions. Introducing a sliding window technique improved

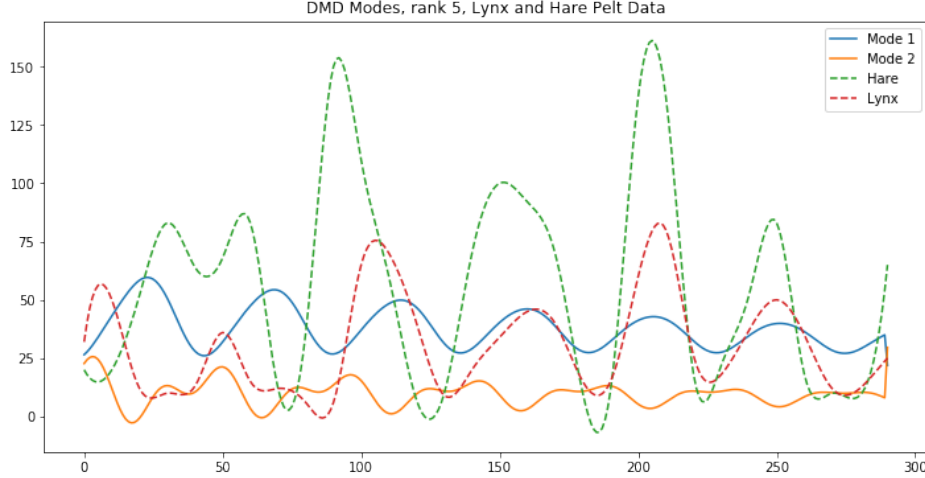


Figure 2: Time-delay DMD Hare and Lynx population predicted values.

Model	AIC	BIC	KL-Divergence
DMD	65.438210	62.824505	inf
Sliding DMD	65.290537	62.676832	inf
Time Delay DMD	61.528248	58.914542	inf
Lotka-Volterra	66.528297	63.914592	0.269209
Polynomial Order 3	61.724015	59.110309	0.013239
Polynomial Order 4 + Sinusoids	60.553052	57.939346	0.016766
Polynomial Order 4 + Sinusoids Polynomial Order 2	62.283924	59.670219	0.002573
Polynomial Order 4 + Sinusoids Polynomial Order 2	63.220951	60.607246	0.000272

Table 1: Table of model performance metrics.

the qualitative fit slightly, but did not markedly improve the DMD model predictions. Using time delay embedding to generate a Hankel matrix for DMD yielded a similarly poor model. Based on the number of SVD modes of the Hankel matrix of significant energy, it is likely there are latent variables driving the system dynamics. Several rank truncations were tested, and the rank 5 Hankel matrix truncation was found to produce the best model. Model term libraries were successfully constructed for the Lotka-Volterra, polynomial, and sinusoidal models. Sparse regression on these model libraries yielded estimates of the Lotka-Volterra parameters and produced superior population models compared to the DMD methods. The best model library used polynomials of order 4 and sinusoids up to order 2 (e.g. $\sin(x^2)$, $\sin(y^2)$, $\sin(xy)$).

5.2 Belousov-Zhabotinsky Chemical Oscillator Modelling

DMD analysis was successful in extracting top DMD modes describing fundamental dynamics of the Belousov-Zhabotinsky Chemical Oscillator. DMD with time-delay embedding resulted in a seemingly accurate depiction of a damped oscillator (Figure 7).

References

- Brunton, Steven L. (Steven Lee) (2019). *Data-driven science and engineering : machine learning, dynamical systems, and control*. Cambridge, United Kingdom ; New York, NY: Cambridge University Press. ISBN: 9781108422093.
- Pan, Shaowu and Karthik Duraisamy (2019). “On the Structure of Time-delay Embedding in Linear Models of Non-linear Dynamical Systems”. In:

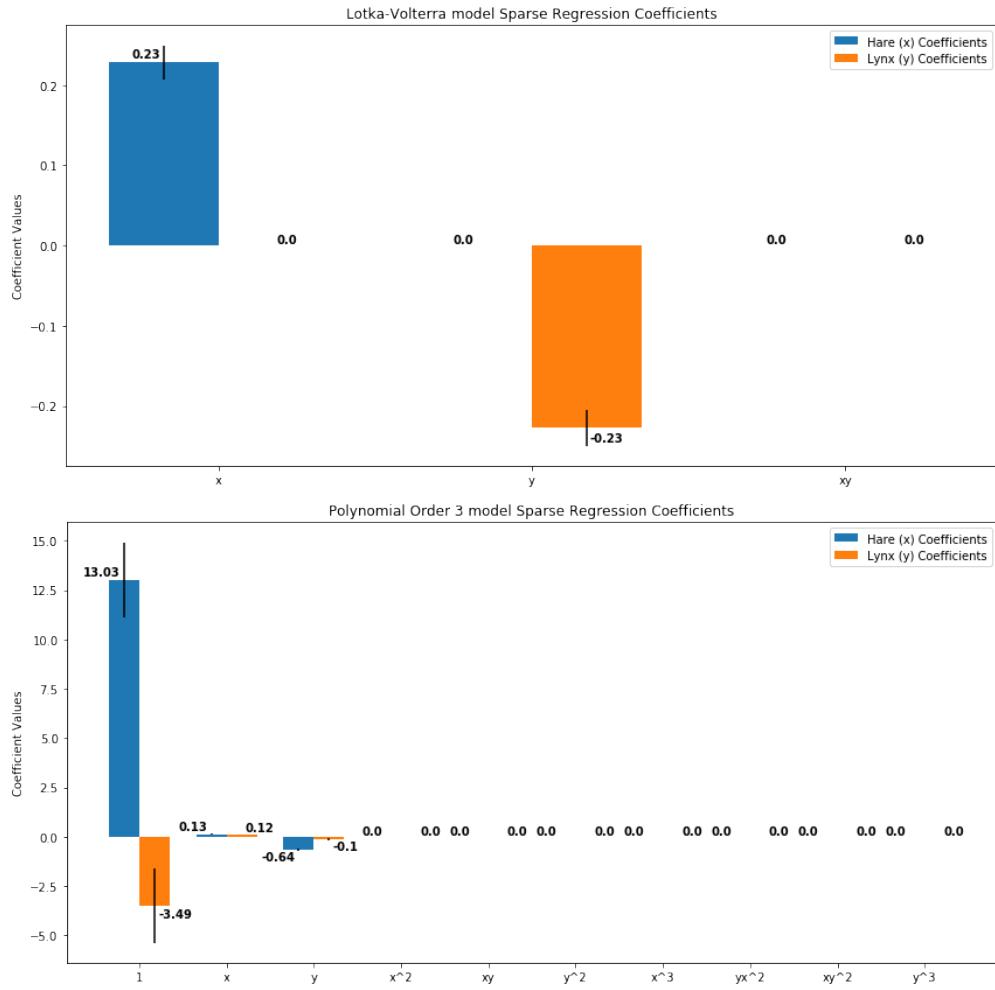


Figure 3: The coefficients for Lotka-Volterra and polynomial order 3 model term library sparse regression model. X axis values indicate the model terms. The Y axis represents the size of the coefficient. The color scale indicates which population dynamics (Hare or Lynx) the coefficient contributes to.

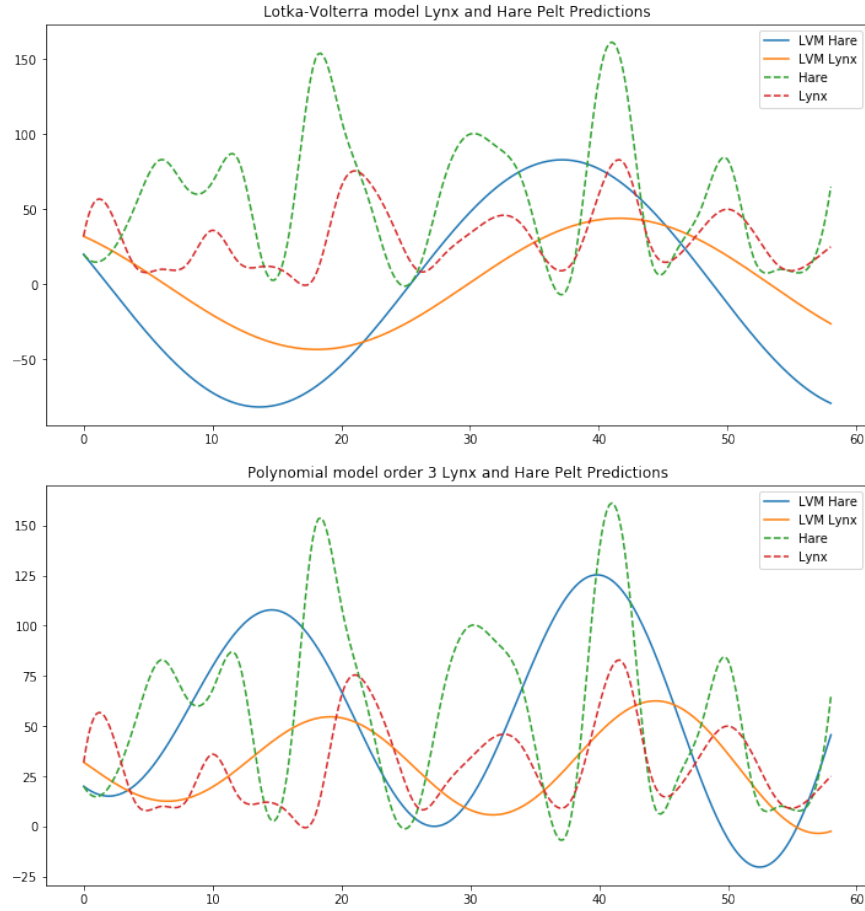


Figure 4: The predicted population values for each fit model. X axis indicates time. The Y axis represents the population size in number of pelts (thousands). The color scale indicates the specific species population (Hare or Lynx).

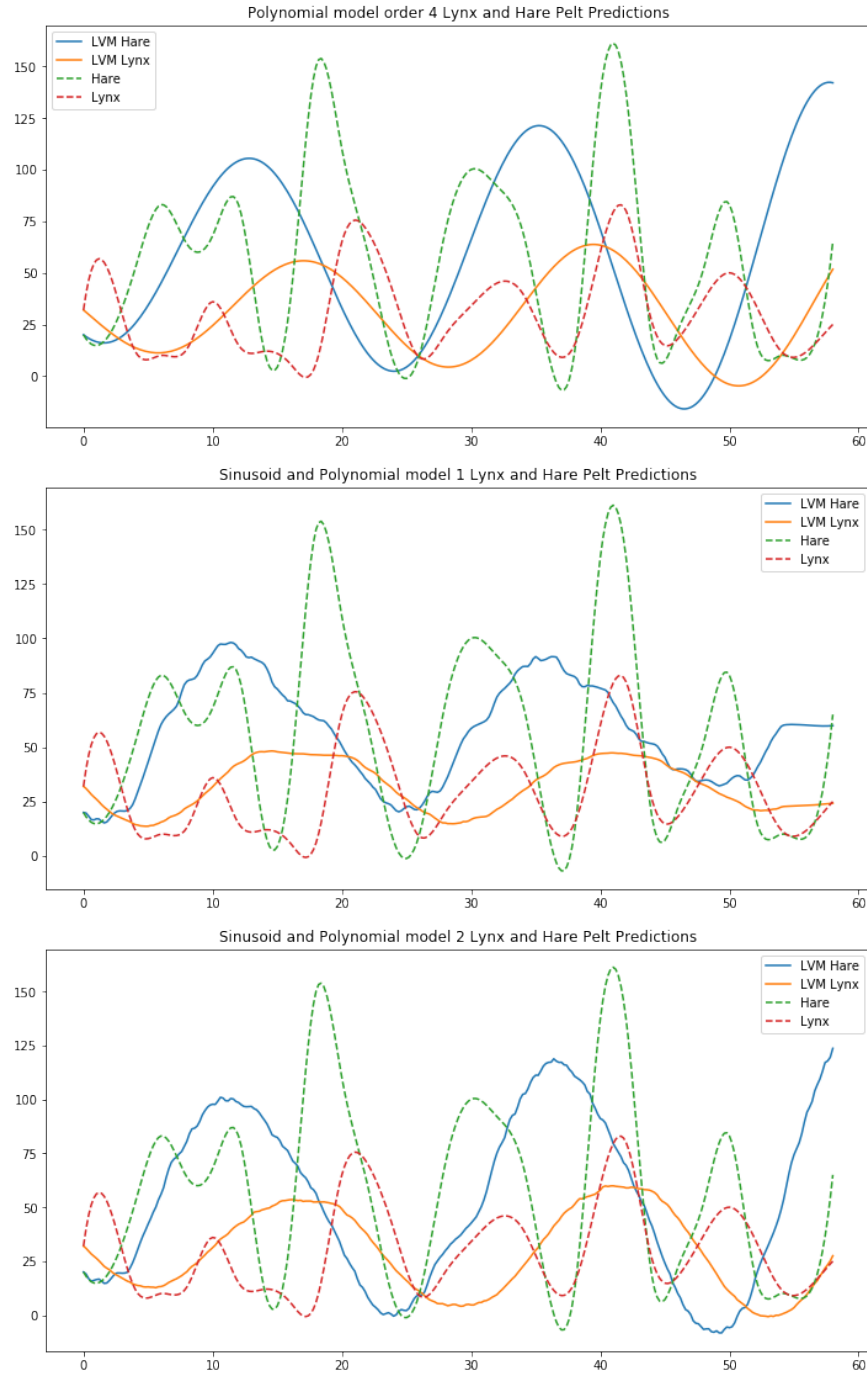


Figure 5: The predicted population values for each fit model. X axis indicates time. The Y axis represents the population size in number of pelts (thousands). The color scale indicates the specific species population (Hare or Lynx).

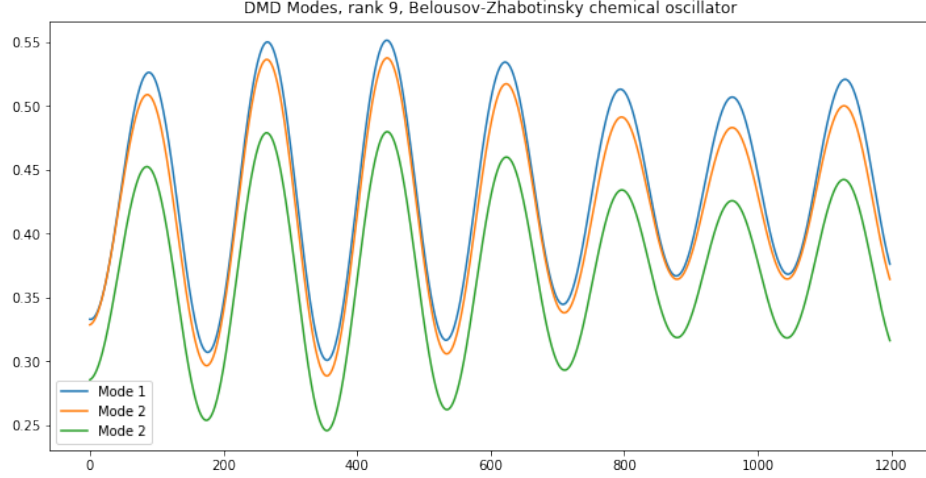


Figure 6: Top 3 DMD modes for the Belousov-Zhabotinsky Chemical Oscillator data matrix.

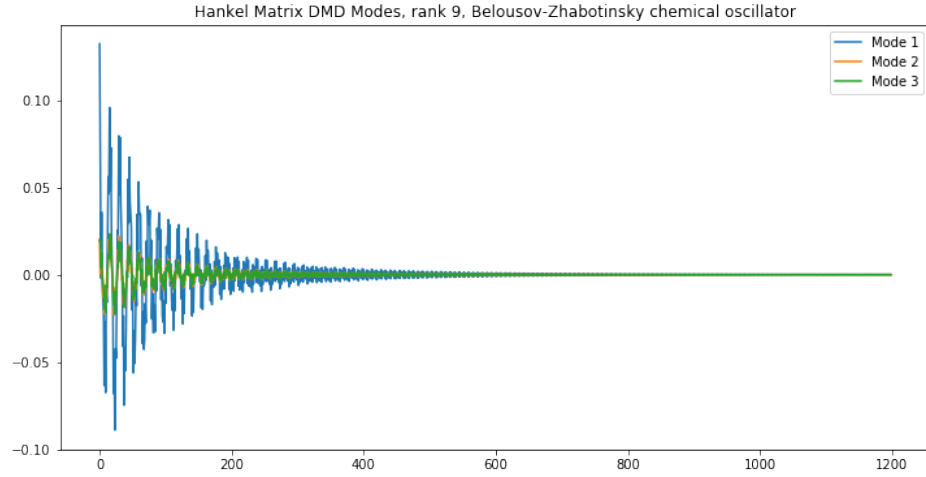


Figure 7: Time-delay DMD Belousov-Zhabotinsky Chemical Oscillator predicted time dynamics for top three DMD modes.

Appendix A Python Functions

- `numpy.linalg.lstsq(a, b, rcond='warn')`
Return the least-squares solution to a linear matrix equation. Solves the equation $Ax = b$ by computing a vector x that minimizes the squared Euclidean 2-norm $\|b - Ax\|_2^2$. The equation may be under-, well-, or over-determined (i.e., the number of linearly independent rows of a can be less than, equal to, or greater than its number of linearly independent columns). If A is square and of full rank, then x (but for round-off error) is the “exact” solution of the equation.
- `sklearn.preprocessing.MinMaxScaler(feature_range=(0, 1) copy=True)`
Transform features by scaling each feature to a given range. This estimator scales and translates each feature individually such that it is in the given range on the training set, e.g. between zero and one.

Appendix B Supplemental Figures

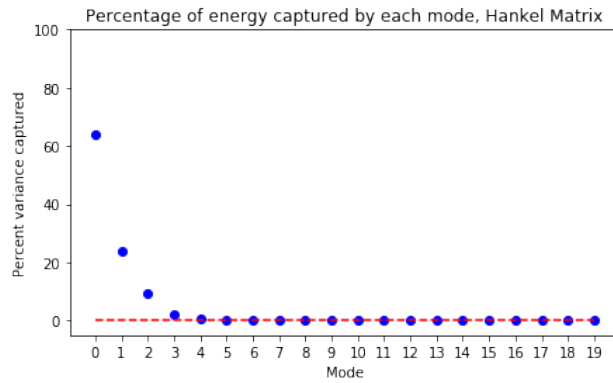


Figure 8: Energy of top SVD modes for the Hare and Lynx Hankel matrix.

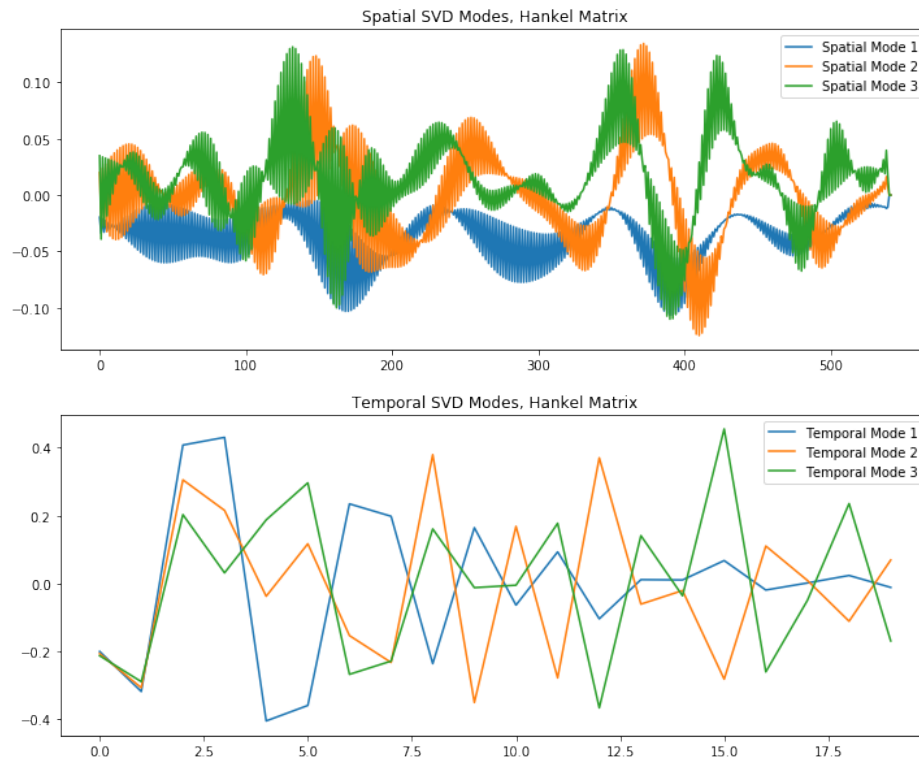


Figure 9: Spatial and temporal SVD modes for time-delayed Hare and Lynx population data.

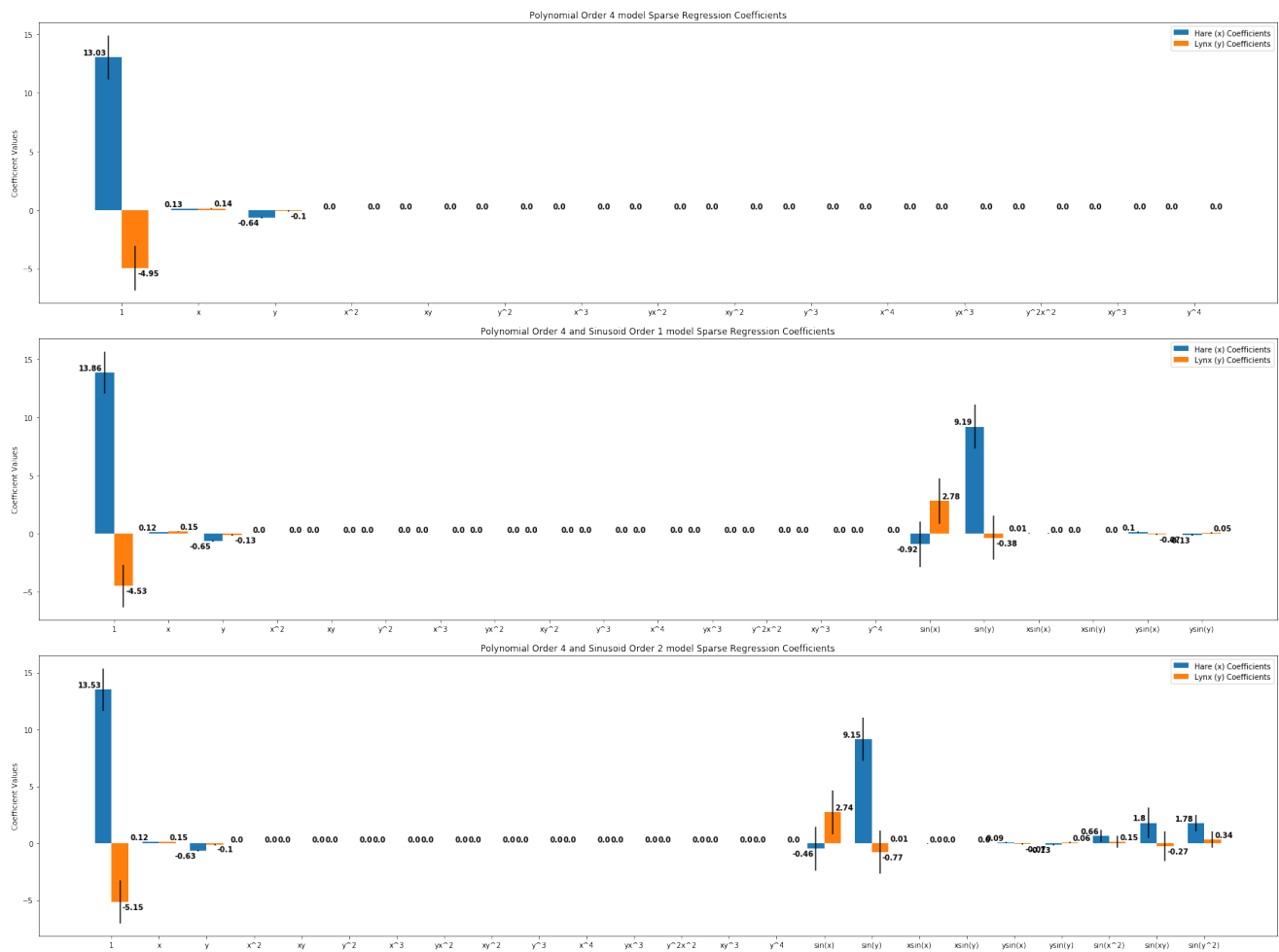


Figure 10: The coefficients for larger model term library sparse regression models. X axis values indicate the model terms. The Y axis represents the size of the coefficient. The color scale indicates which population dynamics (Hare or Lynx) the coefficient contributes to.

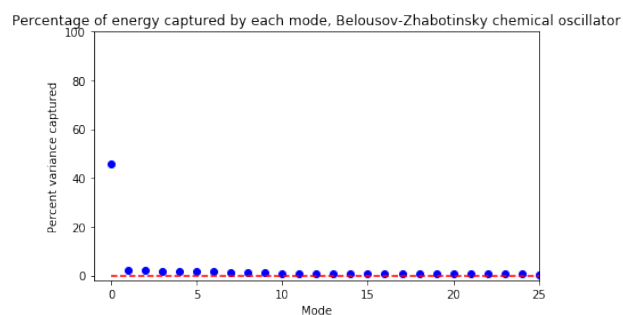


Figure 11: Energy of top SVD modes for the Belousov-Zhabotinsky Chemical Oscillator data matrix.

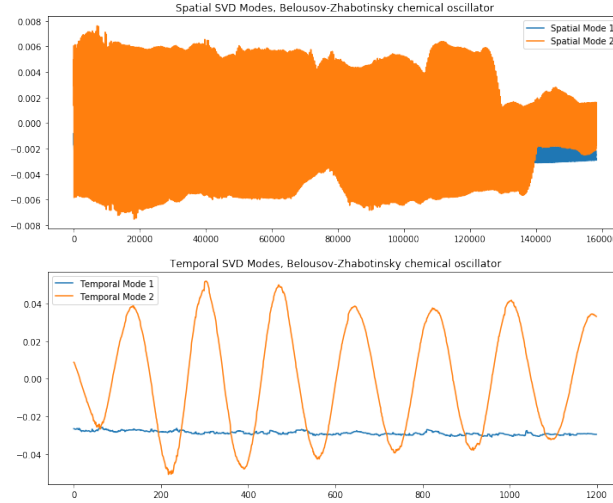


Figure 12: Temporal and spatial SVD modes for the Belousov-Zhabotinsky Chemical Oscillator data matrix.

Appendix C Python Code

```
#!/usr/bin/env python
# coding: utf-8

# In[50]:

from urllib.request import urlretrieve
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from scipy.interpolate import interp1d
from scipy import linalg
from scipy.linalg import hankel
from sklearn.model_selection import KFold
import h5py
from sklearn.preprocessing import MinMaxScaler
import matplotlib.cm as cm
import matplotlib.ticker as plticker
from matplotlib.patches import Patch
from tqdm.notebook import tqdm
from matplotlib import rcParams

# In[3]:

# Notebook functions
'''DMD function takes in X and Xprime which are numpy arrays with measurements along the x axis and time along the y
(i.e each column is a time point with the measurements for that time point down the columns). Each column in X and
is related to the same column in Xprime as those two columns represent a pair of snapshots of the state of a system
as it evolves in time. This means X and Xprime are constructed such that for a given column in X, the same column in
Xprime contains the measurements for the very next time shot of the system. DMD seeks to find the best mapping
possible between these pairs of snapshots that best advances snapshot measurements forward in time. DMD also takes
in a integer value r that stands for rank and indicates how many of the top SVD modes are kept of X for DMD. DMD returns
Phi, Lambda, and b. Lambda is a diagonal matrix of the eigen values of the matrix Atilde produced by DMD on the
rank reduced X data. Phi is a matrix of the high-dimensional DMD modes which are eigenvectors of the high-dimensional
A matrix corresponding to the eigenvalues in Lambda. lastly, b contains the DMD mode amplitudes.'''
def DMD(X,Xprime,r):
    U,Sigma,VT = np.linalg.svd(X,full_matrices=0) # Step 1
    Ur = U[:,0:r]
    Sigmar = np.diag(Sigma[0:r])
    VTr = VT[0:r,:]
    Atilde = np.linalg.solve(Sigmar.T,(Ur.T @ Xprime @ VTr.T).T) # Step 2
    Lambda, W = np.linalg.eig(Atilde) # Step 3
    Lambda = np.diag(Lambda)

    Phi = Xprime @ np.linalg.solve(Sigmar.T,VTr).T @ W # Step 4
    alpha1 = Sigmar @ VTr[:,0]
    b = np.linalg.solve(W @ Lambda,alpha1)
```

```

    return Phi, Lambda, b

'''Constructs model term library for the model terms of the Lotka-Volterra model.'''
def makeLVM(data):
    n = data.shape[0] #number of time points recorded for each variable x, y of data
    nVars = 2 #number of variables in the Lotka-Volterra model
    out = np.zeros((n,1)) #initialize matrix to hold function library

    # poly order 1, x & y
    for i in range(nVars):
        out = np.append(out, data[:,i].reshape((data.shape[0],1)), axis=1) #append x and y data as first two columns of library
    # poly order 2, xy
    for i in range(nVars):
        for j in range(i + 1, nVars):
            out = np.append(out, (data[:,i]*data[:,j]).reshape((data.shape[0],1)), axis=1) #append xy data as third column

    out = out[:,1:] #discard first column of zeros from initialized function library
    return out

'''Function to perform least squares regression with thresholding. The threshold value
below which coefficients are zeroed out is controlled by the input lamb.'''
def sparsifyDynamics(Theta, dXdt, lamb, n):
    Xi = np.linalg.lstsq(Theta, dXdt, rcond=None)[0] # Initial guess: Least-squares

    for k in range(10):
        smallinds = np.abs(Xi) < lamb # Find small coefficients
        Xi[smallinds] = 0 # and threshold
        for ind in range(n): # n is state dimension
            biginds = smallinds[:,ind] == 0
            # Regress dynamics onto remaining terms to find sparse Xi
            Xi[biginds, ind] = np.linalg.lstsq(Theta[:,biginds], dXdt[:,ind], rcond=None)[0]

    return Xi

'''
Calculates KL divergence of two distributions. p and p_m are normalized probability distribution.
'''
def kl_divergence(p, p_m):
    return np.sum(p * np.log(p / p_m))

'''
Calculates AIC score for a given model. Takes in array of model predictions and array of true values.
k is an integer value indicating the number of parameters.
'''
def AIC(model, data, k):
    n = len(data)
    RSS = np.linalg.norm(model-data)**2
    sigma2 = RSS / n
    logL = - n * np.log(2*np.pi) / 2 - n * np.log(sigma2) - n / 2
    return 2*k - 2*logL

'''
Calculate BIC score for a given model. Takes in array of model predictions and array of true values.
k is an integer value indicating the number of parameters.
'''
def BIC(model, data, k):
    n = len(data)
    RSS = np.linalg.norm(model-data)**2
    sigma2 = RSS / n
    logL = - n * np.log(2*np.pi) / 2 - n * np.log(sigma2) - n / 2
    return np.log(n) * k - 2 * logL

'''
Constructs model term library for sparse regression. Takes in an array containing the
data for the measured system parameters. Polynomial order and types of sinusoid functions
to include are controllable. Returns array where each column contains values for specific
model terms at each measured time point.
'''
def poolData(yin, nVars, polyorder, sinusoid=False, sinusoid2=False):
    n = yin.shape[0]
    yout = np.zeros((n,1))

    # poly order 0
    yout[:,0] = np.ones(n)

    # poly order 1
    for i in range(nVars):
        yout = np.append(yout, yin[:,i].reshape((yin.shape[0],1)), axis=1)

```

```

# poly order 2
if polyorder >= 2:
    for i in range(nVars):
        for j in range(i, nVars):
            yout = np.append(yout, (yin[:, i] * yin[:, j]).reshape((yin.shape[0], 1)), axis=1)

# poly order 3
if polyorder >= 3:
    for i in range(nVars):
        for j in range(i, nVars):
            for k in range(j, nVars):
                yout = np.append(yout, (yin[:, i] * yin[:, j] * yin[:, k]).reshape((yin.shape[0], 1)), axis=1)

# poly order 4
if polyorder >= 4:
    for i in range(nVars):
        for j in range(i, nVars):
            for k in range(j, nVars):
                for l in range(k, nVars):
                    yout = np.append(yout, (yin[:, i] * yin[:, j] * yin[:, k] * yin[:, l]).reshape((yin.shape[0], 1)), axis=1)

#sin
if sinusoid == True:
    #sin(x), sin(y)...
    for i in range(nVars):
        yout = np.append(yout, np.sin(yin[:, i]).reshape((yin.shape[0], 1)), axis=1)

    #xsin(x), xsin(y), ysin(x)..etc.
    for i in range(nVars):
        for j in range(nVars):
            yout = np.append(yout, (yin[:, i] * np.sin(yin[:, j])).reshape((yin.shape[0], 1)), axis=1)

    if sinusoid2 == True:
        #sin(x^2) sin(xy) sin(y^2)
        for i in range(nVars):
            for j in range(i, nVars):
                yout = np.append(yout, np.sin(yin[:, i] * yin[:, j]).reshape((yin.shape[0], 1)), axis=1)

return yout
'''Helper function to label bar plots with values'''
def autolabel(rects, xpos='center'):
    """
    Attach a text label above each bar in *rects*, displaying its height.

    *xpos* indicates which side to place the text w.r.t. the center of
    the bar. It can be one of the following {'center', 'right', 'left'}.
    """

    ha = {'center': 'center', 'right': 'left', 'left': 'right'}
    offset = {'center': 0, 'right': 1, 'left': -1}

    for rect in rects:
        height = round(rect.get_height(), 2)
        if np.sign(height) == -1:
            ax.annotate('{}' .format(height),
                        xy=(rect.get_x() + rect.get_width() / 2, height),
                        xytext=(offset[xpos]*3, np.sign(height)*12), # use 3 points offset
                        weight='bold',
                        textcoords="offset points", # in both directions
                        ha=ha[xpos], va='bottom')
        else:
            ax.annotate('{}' .format(height),
                        xy=(rect.get_x() + rect.get_width() / 2, height),
                        xytext=(offset[xpos]*3, np.sign(height)), # use 3 points offset
                        weight='bold',
                        textcoords="offset points", # in both directions
                        ha=ha[xpos], va='bottom')

# In[103]:

#load in Lynx and Hare pelt data
names = ['Year', 'Hare', 'Lynx'] #header names for dataframe
df = pd.read_csv('LynxHareData.txt', header=None, names=names, delim_whitespace=True) #read in txt file with data
years = df[['Year']].to_numpy()
data = np.transpose(df[['Hare', 'Lynx']].to_numpy()) #for DMD need data at each time point in columns
last_year = df['Year'].iloc[len(df) - 1]
first_year = df['Year'].iloc[0]
dt = (last_year - first_year) / (len(df) - 1)

t = np.arange(0, 2*(len(years)), 2) #create time array starting from 1 in steps of 2 for 30 iterations

```

```

interp = interp1d(t, data, kind='cubic',axis=1)#interpolate to generate more data points

# evaluate interpolation on a finer mesh
scale = 10
t_fine = np.linspace(0,58,30*scale-(scale-1))
dt_interp = t_fine[1] - t_fine[0]
data_interp = interp(t_fine)
m, n = data_interp.shape

X1 = data_interp[:,0:n-2]#all columns starting from first column up to the penultimate
X2 = data_interp[:,1:n-1]#all columns starting from second column up to the last column

#Plot percentage of variance captured by differnt modes
U,Sig,VT = linalg.svd(data_interp, full_matrices=False)
V = np.transpose(VT)
f, ax1 = plt.subplots(1, 1, figsize=(7, 4))
ax1.plot((Sig/ sum(Sig)) * 100, 'bo')
ax1.set_title('Percentage of energy captured by each mode, Lynx and Hare Pelt Data')
ax1.set_ylabel('Percent variance captured')
ax1.set_xlabel('Mode')
ax1.set_ylim(( 0, 100))
ax1.set_xticks([0, 1])

#Plot
f, [ax1, ax2] = plt.subplots(2, 1, figsize=(12, 10))
ax1.plot(np.real(U[:, 0]), label='Spatial Mode 1')
ax1.plot(np.real(U[:, 1]), label='Spatial Mode 2')
ax1.set_title('Spatial SVD Modes, Lynx and Hare Pelt Data')
ax1.legend()
ax2.plot(np.real(V[:,0]), label='Temporal Mode 1')
ax2.plot(np.real(V[:,1]), label='Temporal Mode 2')
ax2.set_title('Temporal SVD Modes, Lynx and Hare Pelt Data')
ax2.legend()

# In[104]:

r1 = 1
r2 = 2
Phi_fr, Lambda_fr, b_fr = DMD(X1, X2, r2)#no rank truncation DMD
Phi_r1, Lambda_r1, b_r1 = DMD(X1, X2, r1)#rank 1 truncation DMD

omega_fr = np.log(np.diag(Lambda_fr)) / dt_interp#the continuous eigenvalues full rank DMD
omega_r1 = np.log(np.diag(Lambda_r1)) / dt_interp#the continuous eigenvalues rank 1 DMD

#calculate time dynamics for full rank DMD
time_dynamics_fr = np.empty((r2, len(t_fine) - 1))#initialize time dynamics array
for i in range(0, len(t_fine) - 1):
    time_dynamics_fr[:, i] = b_fr*np.exp(omega_fr*t_fine[i])
X_DMD_fr = np.matmul(Phi_fr, time_dynamics_fr)
#calculate time dynamics for rank 1 DMD
time_dynamics_r1 = np.zeros((r1, len(t_fine) - 1))
for i in range(0, len(t_fine) - 1):
    time_dynamics_r1[:, i] = b_r1*np.exp(omega_r1*t_fine[i])
X_DMD_r1 = np.matmul(Phi_r1, time_dynamics_r1)

#compare the SVD modes to the DMD modes.. DMD says find the modes such that the modes in time are exactly oscillatory
#Plot SVD and DMD modes full rank
f, [ax1, ax2] = plt.subplots(2, 1, figsize=(12, 10))
ax1.plot(np.real(U[:, 0]), label='SVD Mode 1')
ax1.plot(np.real(U[:, 1]), label='SVD Mode 2')
ax1.plot(np.real(Phi_fr[:, 0]), '--', label='DMD Mode 1')
ax1.plot(np.real(Phi_fr[:, 1]), '--',label='DMD Mode 2')
ax1.set_title('Spatial SVD and DMD Modes, rank 2 (full), Lynx and Hare Pelt Data')
ax1.legend()
ax2.plot(np.real(V[:,0]), label='SVD Mode 1')
ax2.plot(np.real(V[:,1]), label='SVD Mode 2')
ax2.plot(np.real(np.transpose(time_dynamics_fr[:, 0]), '--', label='DMD Mode 1')
ax2.plot(np.real(np.transpose(time_dynamics_fr[:, 1]), '--', label='DMD Mode 2')
ax2.set_title('Temporal SVD and DMD Modes, rank 2, Lynx and Hare Pelt Data')
ax2.legend()

#Plot SVD and DMD modes rank 1
f, [ax1, ax2] = plt.subplots(2, 1, figsize=(12, 10))
ax1.plot(U[:, 0], label='SVD Spatial Mode 1')
ax1.plot(Phi_r1[:, 0], '--', label='DMD Spatial Mode 1')
ax1.set_title('Spatial SVD and DMD Modes, rank 1, Lynx and Hare Pelt Data')
ax1.legend()

```



```

ax2.plot(V[:, 0], label='SVD Temporal Mode 1')
ax2.plot(np.transpose(time_dynamics_r1)[: ,0], '--', label='DMD Temporal Mode 1')
ax2.set_title('Temporal SVD and DMD Modes, Lynx and Hare Pelt Data')
ax2.legend()

# In[105]:

#DMD combined modes for entire data set, prediction is terrible
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.real(X_DMD_fr[0, :]), label='Mode 1')
ax1.plot(np.real(X_DMD_fr[1, :]), label='Mode 2')
ax1.plot(data_interp[0, :], '--', label='Hare')
ax1.plot(data_interp[1, :], '--', label='Lynx')
ax1.set_title('DMD Modes, rank 2, Lynx and Hare Pelt Data')
ax1.legend()

#Phase
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(data_interp[0, :], data_interp[1, :])
ax1.set_title('Lynx and Hare Pelt Data Phase Portrait')
ax1.set_xlabel('Lynx Pelts (E3)')
ax1.set_ylabel('Hare Pelts (E3)')

# In[106]:

#Try sliding window method, build prediction in chunks
res = 72#how many time points to include per DMD fit
r = 2
X_DMD_total = np.empty((r2, len(t_fine)))
j = 0
start = 0
while (j + res) < len(t_fine) - 1:
    t_chunk = t_fine[j:j+2*res]#make time vector running from chunk start to 2x the time resolution
    X1 = data_interp[:,j:(j + res) - 1]#all columns starting from first column up to the penultimate
    X2 = data_interp[:,(j + 1):(j + res)]#all columns starting from second column up to the last column
    Phi, Lambda, b = DMD(X1, X2, r)#no rank truncation DMD
    omega = np.log(np.diag(Lambda)) / dt_interp#the continuous eigenvalues full rank DMD

    #calculate time dynamics for full rank DMD
    time_dynamics = np.empty((r, len(t_chunk)))#initialize time dynamics array
    for i in range(0, len(t_chunk) - 1):
        time_dynamics[:, i] = b*np.exp(omega*t_chunk[i])
    X_DMD = np.matmul(Phi, time_dynamics)
    X_DMD_total[:, j:(j + 2*res)] = X_DMD
    start = start + res + 1
    j = j + res

#DMD combined modes for entire data set, prediction is terrible
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.real(X_DMD_total[0, :]), label='Mode 1')
ax1.plot(np.real(X_DMD_total[1, :]), label='Mode 2')
ax1.plot(data_interp[0, :], '--', label='Hare')
ax1.plot(data_interp[1, :], '--', label='Lynx')
ax1.set_title('DMD Modes, rank 2, Lynx and Hare Pelt Data')
ax1.legend()

# In[107]:

#Make hankel matrices for each variable (Lynx and Hare)
width = 20
rows = len(t_fine) - width#how many sliding windows of specified width can fit within sampled length of time
x1_h = np.empty((rows,width))#initialize Hare hankel
x2_h = np.empty((rows,width))#initialize Lynx hankel
start = 0
j = 0
for i in range(0, rows):
    for j in range(start, (start+width)):
        x1_h[i, (j - i)%width] = data_interp[0,j]
        x2_h[i, (j - i)%width] = data_interp[1,j]
    start = start + 1#reset index to 1 more than the beginning of the window

H = np.empty((2*rows, width))
for i in range(0, rows - 1):
    H[2*i, :] = x1_h[i, :]

```

```

H[2*i + 1, :] = x2_h[i, :]

u,s,vh = np.linalg.svd(H) # take SVD

f, ax1 = plt.subplots(1, 1, figsize=(7, 4))
xticks = np.arange(len(s)).tolist()
ax1.set_title('Percentage of energy captured by each mode, Hankel Matrix')
ax1.set_ylabel('Percent variance captured')
ax1.set_xlabel('Mode')
ax1.set_ylim((-5, 100))
ax1.set_xticks(xticks)
ax1.plot((s/ sum(s)) * 100, 'bo')
ax1.plot(np.arange(len(s)), np.zeros(len(s)), 'r--');

#Plot u (eigen vectors of time delay embedding, dominant correlation structure in space)
#and v vectors to show the dominant correlated structures in time.
f, [ax1, ax2] = plt.subplots(2, 1, figsize=(12, 10))
ax1.plot(np.real(u[:, 0]), label='Spatial Mode 1')
ax1.plot(np.real(u[:, 1]), label='Spatial Mode 2')
ax1.plot(np.real(u[:, 2]), label='Spatial Mode 3')
ax1.set_title('Spatial SVD Modes, Hankel Matrix')
ax1.legend()
ax2.plot(np.real(vh[:,0]), label='Temporal Mode 1')
ax2.plot(np.real(vh[:,1]), label='Temporal Mode 2')
ax2.plot(np.real(vh[:,2]), label='Temporal Mode 3')
ax2.set_title('Temporal SVD Modes, Hankel Matrix')
ax2.legend()

# In[108]:

#DMD on Hankel matrix (rank 5)
Phi_H, Lambda_H, b_H = DMD(H[:,0:width - 1], H[:, 1:width], 5)#rank 5 truncation DMD

omega_H = np.log(np.diag(Lambda_H)) / 0.2#the continuous eigenvalues full rank DMD

#calculate time dynamics for full rank DMD
time_dynamics_H = np.empty((5, len(t_fine)))#initialize time dynamics array
for i in range(0, len(t_fine) - 1):
    time_dynamics_H[:, i] = b_H*np.exp(omega_H*t_fine[i])
X_DMD_H = np.matmul(Phi_H, time_dynamics_H)

#DMD combined modes for entire data set, prediction is terrible
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.real(X_DMD_H[0, :]), label='Mode 1')
ax1.plot(np.real(X_DMD_H[1, :]), label='Mode 2')
ax1.plot(data_interp[0, :], '--', label='Hare')
ax1.plot(data_interp[1, :], '--', label='Lynx')
ax1.set_title('DMD Modes, rank 5, Lynx and Hare Pelt Data')
ax1.legend()

# In[109]:

'''
Lotka-Volterra model:  $\dot{x} = (b - py)x = bx - pyx$  and  $\dot{y} = (rx - d)y = rxy - dy$ 
Use the data to fit values of b, p, r and d.
Use sparse regression where the library functions for dx/dt are [x, xy] and y [y, xy].
So, the only parameters to get really are just b, p, r, d
'''

dh = np.gradient(data_interp[0], dt_interp)#derivative of hare data (x variable)
dl = np.gradient(data_interp[1], dt_interp)#derivative of lynx data (y variable)
deriv = np.transpose(np.array([dh, dl]))#concatenate derivatives first col dHare/dt, second col dLynx/dt
A = makeLVM(np.transpose(data_interp))# Make function library for Lotka-Volterra model fit
lamb = 0.025 # sparsification knob lambda
cv_folds = 5#number of cross validation folds
kf = KFold(n_splits = cv_folds, random_state = 17, shuffle = True)#initialize KFold for iterative cross validation
Xcv = np.zeros((A.shape[1],2,cv_folds))#for storing cross validation of least squares thresholding coeffs 3 coeffs (x, y, xy)x 2 variables (x, y) x
cv_i = 0
for train_index, test_index in kf.split(A):
    Xcv[:, :, cv_i] = sparsifyDynamics(A[train_index, :], deriv[train_index, :], lamb, 2)#least squares thresholding to fit model library to derivative
    cv_i = cv_i + 1

Xcv_LVM = np.average(Xcv,axis=2)#average of model coefficients
vals_LVM = A@Xcv_LVM

```

```

# In[110]:

#kf = KFold(n_splits = cv_folds, random_state = 17, shuffle = True)#initialize KFold for iterative cross validation
A_h = A[:, [0, 2]]
Xcv_h = np.zeros((A_h.shape[1],cv_folds))#for storing cross validation of least squares thresholding coeffs 3 coeffs (x, y, xy)x 2 variables (x, y)
cv_i = 0

for train_index, test_index in kf.split(A_h):
    Xcv_h[:,cv_i] = sparsifyDynamics(A_h[train_index,:],deriv[train_index,0],lamb,0)#least squares thresholding to fit model library to derivative
    cv_i = cv_i + 1

Xcv_h = np.insert(Xcv_h, 1, 0, axis=0)
Xcv_h_LVM = np.average(Xcv_h,axis=1)#average of model coefficients
vals_h_LVM = A@Xcv_h_LVM

A_l = A[:, [1, 2]]
Xcv_l = np.zeros((A_l.shape[1],cv_folds))#for storing cross validation of least squares thresholding coeffs 3 coeffs (x, y, xy)x 2 variables (x, y)
cv_i = 0

for train_index, test_index in kf.split(A_l):
    Xcv_l[:,cv_i] = sparsifyDynamics(A_l[train_index,:],deriv[train_index,1],lamb,0)#least squares thresholding to fit model library to derivative
    cv_i = cv_i + 1
Xcv_l = np.insert(Xcv_l, 0, 0, axis=0)
Xcv_l_LVM = np.average(Xcv_l,axis=1)#average of model coefficients
vals_l_LVM = A@Xcv_l_LVM

# In[111]:

#Plot fit model parameter values
hare_vals = (np.average(Xcv_h[0,:], axis=0), np.average(Xcv_h[1,:], axis=0), np.average(Xcv_h[2,:], axis=0))
lynx_vals = (np.average(Xcv_l[0,:], axis=0), np.average(Xcv_l[1,:], axis=0), np.average(Xcv_l[2,:], axis=0))
hare_std = (np.std(Xcv_h[0,:], axis=0), np.std(Xcv_h[1,:], axis=0), np.std(Xcv_h[2,:], axis=0))
lynx_std = (np.std(Xcv_l[0,:], axis=0), np.std(Xcv_l[1,:], axis=0), np.std(Xcv_l[2,:], axis=0))
ind = np.arange(len(hare_vals)) # the x locations for the groups
width = 0.35 # the width of the bars

fig, ax = plt.subplots(1, 1, figsize=(12, 6))
rects1 = ax.bar(ind - width/2, hare_vals, width, yerr=hare_std,
                label='Hare (x) Coefficients')
rects2 = ax.bar(ind + width/2, lynx_vals, width, yerr=lynx_std,
                label='Lynx (y) Coefficients')

# Add some text for labels, title and custom x-axis tick labels, etc.
ax.set_ylabel('Coefficient Values')
ax.set_title('Lotka-Volterra model Sparse Regression Coefficients')
ax.set_xticks(ind)
ax.set_xticklabels(('x', 'y', 'xy'))
ax.legend()

autolabel(rects1, "left")
autolabel(rects2, "right")

fig.tight_layout()

plt.show()

# In[112]:

#polynomial non-linear sparse regression model fit
A = poolData(np.transpose(data_interp),2,3)# Make function library for polynomial
lamb = 0.025 # sparsification knob lambda
cv_folds = 5#number of cross validation folds
kf = KFold(n_splits = cv_folds, random_state = 17, shuffle = True)#initialize KFold for iterative cross validation
Xcv = np.zeros((A.shape[1],2,cv_folds))#for storing cross validation of least squares thresholding coeffs 3 coeffs (x, y, xy)x 2 variables (x, y)
cv_i = 0
for train_index, test_index in kf.split(A):
    Xcv[:,cv_i] = sparsifyDynamics(A[train_index,:],deriv[train_index,:],lamb,2)#least squares thresholding to fit model library to derivative
    cv_i = cv_i + 1

Xcv_poly = np.average(Xcv,axis=2)#average of model coefficients
vals_poly = A@Xcv_poly

#Plot fit model parameter values
hare_vals = []
lynx_vals = []
hare_std = []

```

```

lynx_std = []
for i in range(0, Xcv.shape[0]):#for all coefficients
    hare_vals.append(np.average(Xcv[i,0:], axis=0))
    lynx_vals.append(np.average(Xcv[i,1:], axis=0))
    hare_std.append(np.std(Xcv[i,0:], axis=0))
    lynx_std.append(np.std(Xcv[i,0:], axis=0))

ind = np.arange(len(hare_vals)) # the x locations for the groups
width = 0.35 # the width of the bars

fig, ax = plt.subplots(1, 1, figsize=(12, 6))
rects1 = ax.bar(ind - width/2, hare_vals, width, yerr=hare_std,
                label='Hare (x) Coefficients')
rects2 = ax.bar(ind + width/2, lynx_vals, width, yerr=lynx_std,
                label='Lynx (y) Coefficients')

# Add some text for labels, title and custom x-axis tick labels, etc.
ax.set_ylabel('Coefficient Values')
ax.set_title('Polynomial Order 3 model Sparse Regression Coefficients')
ax.set_xticks(ind)
ax.set_xticklabels(('1', 'x', 'y', 'x^2', 'xy', 'y^2', 'x^3', 'yx^2', 'xy^2', 'y^3'))
ax.legend()
autolabel(rects1, "left")
autolabel(rects2, "right")

fig.tight_layout()

plt.show()

# In[113]:

#try sparse regression with sinusoids in pool data library
A = poolData(np.transpose(data_interp),2,4,True)# Make function library for sin 1
lamb = 0.05 # sparsification knob lambda
cv_folds = 5#number of cross validation folds
kf = KFold(n_splits = cv_folds, random_state = 17, shuffle = True)#initialize KFold for iterative cross validation
Xcv = np.zeros((A.shape[1],2,cv_folds))#for storing cross validation of least squares thresholding coeffs 3 coeffs (x, y, xy)x 2 variables (x, y) x
cv_i = 0
for train_index, test_index in kf.split(A):
    Xcv[:, :, cv_i] = sparsifyDynamics(A[train_index, :], deriv[train_index, :], lamb, 2)#least squares thresholding to fit model library to derivative
    cv_i = cv_i + 1

Xcv_sin1 = np.average(Xcv,axis=2)#average of model coefficients
vals_sin1 = A@Xcv_sin1#apply model

#Plot fit model parameter values
hare_vals = []
lynx_vals = []
hare_std = []
lynx_std = []
for i in range(0, Xcv.shape[0]):#for all coefficients
    hare_vals.append(np.average(Xcv[i,0:], axis=0))
    lynx_vals.append(np.average(Xcv[i,1:], axis=0))
    hare_std.append(np.std(Xcv[i,0:], axis=0))
    lynx_std.append(np.std(Xcv[i,0:], axis=0))

ind = np.arange(len(hare_vals)) # the x locations for the groups
width = 0.35 # the width of the bars

fig, ax = plt.subplots(1, 1, figsize=(24, 6))
rects1 = ax.bar(ind - width/2, hare_vals, width, yerr=hare_std,
                label='Hare (x) Coefficients')
rects2 = ax.bar(ind + width/2, lynx_vals, width, yerr=lynx_std,
                label='Lynx (y) Coefficients')

# Add some text for labels, title and custom x-axis tick labels, etc.
ax.set_ylabel('Coefficient Values')
ax.set_title('Polynomial Order 4 and Sinusoid Order 1 model Sparse Regression Coefficients')
ax.set_xticks(ind)
ax.set_xticklabels(('1', 'x', 'y', 'x^2', 'xy', 'y^2', 'x^3', 'yx^2', 'xy^2',
                    'y^3', 'x^4', 'yx^3', 'y^2x^2', 'xy^3', 'y^4',
                    'sin(x)', 'sin(y)', 'xsin(x)', 'xsin(y)', 'ysin(x)', 'ysin(y)'))

ax.legend()
autolabel(rects1, "left")
autolabel(rects2, "right")

fig.tight_layout()

#plt.show()

```

```

# In[114]:

#try with sinusoids of (sin(xy), sin(yx^2), sin(xy^2)) in pool data library
A = poolData(np.transpose(data_interp),2,4,True,True)# Make function library for sin2
lamb = 0.05 # sparsification knob lambda
cv_folds = 5#number of cross validation folds
kf = KFold(n_splits = cv_folds, random_state = 17, shuffle = True)#initialize KFold for iterative cross validation
Xcv = np.zeros((A.shape[1],2,cv_folds))#for storing cross validation of least squares thresholding coeffs 3 coeffs (x, y, xy)x 2 variables (x, y) x
cv_i = 0
for train_index, test_index in kf.split(A):
    Xcv[:, :, cv_i] = sparsifyDynamics(A[train_index, :], deriv[train_index, :], lamb, 2)#least squares thresholding to fit model library to derivative
    cv_i = cv_i + 1

Xcv_sin2 = np.average(Xcv, axis=2)#average of model coefficients
vals_sin2 = A@Xcv_sin2

#Plot fit model parameter values
hare_vals = []
lynx_vals = []
hare_std = []
lynx_std = []
for i in range(0, Xcv.shape[0]):#for all coefficients
    hare_vals.append(np.average(Xcv[i, 0, :], axis=0))
    lynx_vals.append(np.average(Xcv[i, 1, :], axis=0))
    hare_std.append(np.std(Xcv[i, 0, :], axis=0))
    lynx_std.append(np.std(Xcv[i, 1, :], axis=0))

ind = np.arange(len(hare_vals)) # the x locations for the groups
width = 0.35 # the width of the bars

fig, ax = plt.subplots(1, 1, figsize=(24, 6))
rects1 = ax.bar(ind - width/2, hare_vals, width, yerr=hare_std,
                label='Hare (x) Coefficients')
rects2 = ax.bar(ind + width/2, lynx_vals, width, yerr=lynx_std,
                label='Lynx (y) Coefficients')

# Add some text for labels, title and custom x-axis tick labels, etc.
ax.set_ylabel('Coefficient Values')
ax.set_title('Polynomial Order 4 and Sinusoid Order 2 model Sparse Regression Coefficients')
ax.set_xticks(ind)
ax.set_xticklabels(('1', 'x', 'y', 'x^2', 'xy', 'y^2', 'x^3', 'yx^2', 'xy^2',
                    'y^3', 'x^4', 'yx^3', 'y^2x^2', 'xy^3', 'y^4', 'sin(x)', 'sin(y)',
                    'xsin(x)', 'xsin(y)', 'ysin(x)', 'ysin(y)',
                    'sin(x^2)', 'sin(xy)', 'sin(y^2)'))

ax.legend()
autolabel(rects1, "left")
autolabel(rects2, "right")

fig.tight_layout()

plt.show()

# In[115]:

#try 4th degree polynomial
A = poolData(np.transpose(data_interp),2,4)# Make function library for sin2
lamb = 0.05 # sparsification knob lambda
cv_folds = 5#number of cross validation folds
kf = KFold(n_splits = cv_folds, random_state = 17, shuffle = True)#initialize KFold for iterative cross validation
Xcv = np.zeros((A.shape[1],2,cv_folds))#for storing cross validation of least squares thresholding coeffs 3 coeffs (x, y, xy)x 2 variables (x, y) x
cv_i = 0
for train_index, test_index in kf.split(A):
    Xcv[:, :, cv_i] = sparsifyDynamics(A[train_index, :], deriv[train_index, :], lamb, 2)#least squares thresholding to fit model library to derivative
    cv_i = cv_i + 1

Xcv_p4 = np.average(Xcv, axis=2)#average of model coefficients
vals_p4 = A@Xcv_p4

#Plot fit model parameter values
hare_vals = []
lynx_vals = []
hare_std = []
lynx_std = []
for i in range(0, Xcv.shape[0]):#for all coefficients
    hare_vals.append(np.average(Xcv[i, 0, :], axis=0))
    lynx_vals.append(np.average(Xcv[i, 1, :], axis=0))

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hare_std.append(np.std(Xcv[i,0:], axis=0))
lynx_std.append(np.std(Xcv[i,0:], axis=0))

ind = np.arange(len(hare_vals)) # the x locations for the groups
width = 0.35 # the width of the bars

fig, ax = plt.subplots(1, 1, figsize=(24, 6))
rects1 = ax.bar(ind - width/2, hare_vals, width, yerr=hare_std,
                label='Hare (x) Coefficients')
rects2 = ax.bar(ind + width/2, lynx_vals, width, yerr=lynx_std,
                label='Lynx (y) Coefficients')

# Add some text for labels, title and custom x-axis tick labels, etc.
ax.set_ylabel('Coefficient Values')
ax.set_title('Polynomial Order 4 model Sparse Regression Coefficients')
ax.set_xticks(ind)
ax.set_xticklabels(('1', 'x', 'y', 'x^2', 'xy', 'y^2', 'x^3', 'yx^2', 'xy^2',
                  'y^3', 'x^4', 'yx^3', 'y^2x^2', 'xy^3', 'y^4'))

ax.legend()
autolabel(rects1, "left")
autolabel(rects2, "right")

fig.tight_layout()

plt.show()

# In[116]:

'''Compute AIC, BIC, KL Divergence for DMD, Time delay DMD, Lotka-Volterra model, Non-linear poly order 3,
Non-linear poly order 3 with simple sinusoids, and Non-linear poly order 3 with sinusoids'''
from scipy import integrate

'''y is 2D array with each column corresponding to a variable, rows the time points'''
def rhs_LVM(t, y):
    coeffs = Xcv_LVM
    var1 = np.where(abs(coeffs[:,0])>0)
    var2 = np.where(abs(coeffs[:,1])>0)
    A = np.transpose(makeLVM(y.reshape(1, -1))).flatten()# Make function library for Lotka-Volterra model fit
    return np.array([sum(A[var1]*np.transpose(coeffs[var1, 0]).flatten()), sum(A[var2]*np.transpose(coeffs[var2, 1]).flatten())])
def rhs_poly(t, y):
    coeffs = Xcv_poly
    var1 = np.where(abs(coeffs[:,0])>0)
    var2 = np.where(abs(coeffs[:,1])>0)
    A = np.transpose(poolData(y.reshape(1, -1),2,3)).flatten()# Make function library for polynomial
    return np.array([sum(A[var1]*np.transpose(coeffs[var1, 0]).flatten()), sum(A[var2]*np.transpose(coeffs[var2, 1]).flatten())])
def rhs_sin1(t, y):
    coeffs = Xcv_sin1
    var1 = np.where(abs(coeffs[:,0])>0)
    var2 = np.where(abs(coeffs[:,1])>0)
    A = np.transpose(poolData(y.reshape(1, -1),2,4,True)).flatten()# Make function library for sin 1
    return np.array([sum(A[var1]*np.transpose(coeffs[var1, 0]).flatten()), sum(A[var2]*np.transpose(coeffs[var2, 1]).flatten())])
def rhs_sin2(t, y):
    coeffs = Xcv_sin2
    var1 = np.where(abs(coeffs[:,0])>0)
    var2 = np.where(abs(coeffs[:,1])>0)
    A = np.transpose(poolData(y.reshape(1, -1),2,4,True,True)).flatten()# Make function library for sin2
    return np.array([sum(A[var1]*np.transpose(coeffs[var1, 0]).flatten()), sum(A[var2]*np.transpose(coeffs[var2, 1]).flatten())])
def rhs_p4(t, y):
    coeffs = Xcv_p4
    var1 = np.where(abs(coeffs[:,0])>0)
    var2 = np.where(abs(coeffs[:,1])>0)
    A = np.transpose(poolData(y.reshape(1, -1),2,4,True,True)).flatten()# Make function library for sin2
    return np.array([sum(A[var1]*np.transpose(coeffs[var1, 0]).flatten()), sum(A[var2]*np.transpose(coeffs[var2, 1]).flatten())])

y0 = data_interp[:,0]#initial values for hare and lynx populations
model0 = integrate.solve_ivp(rhs_LVM,[0,58],y0,method='RK45',t_eval=t_fine)
model1 = integrate.solve_ivp(rhs_poly,[0,58],y0,method='RK45',t_eval=t_fine)
model2 = integrate.solve_ivp(rhs_sin1,[0,58],y0,method='RK45',t_eval=t_fine)
model3 = integrate.solve_ivp(rhs_sin2,[0,58],y0,method='RK45',t_eval=t_fine)
model4 = integrate.solve_ivp(rhs_p4,[0,58],y0,method='RK45',t_eval=t_fine)

#plot the integrated values of Lotka-Volterra model
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.linspace(0,58,len(model0.y[0,:])), model0.y[0,:], label='LVM Hare')
ax1.plot(np.linspace(0,58,len(model0.y[1,:])), model0.y[1,:], label='LVM Lynx')
ax1.plot(t_fine, data_interp[0, :], '--', label='Hare')
ax1.plot(t_fine, data_interp[1, :], '--', label='Lynx')
ax1.set_title('Lotka-Volterra model Lynx and Hare Pelt Predictions')
ax1.legend()

```

```

#plot the integrated values of polynomial library fit
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.linspace(0,58,len(model1.y[0,:])), model1.y[0,:], label='LVM Hare')
ax1.plot(np.linspace(0,58,len(model1.y[0,:])), model1.y[1,:], label='LVM Lynx')
ax1.plot(t_fine, data_interp[0, :], '--', label='Hare')
ax1.plot(t_fine, data_interp[1, :], '--', label='Lynx')
ax1.set_title('Polynomial model order 3 Lynx and Hare Pelt Predictions')
ax1.legend()

#plot the integrated values of polynomial order 4 library fit
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.linspace(0,58,len(model4.y[0,:])), model4.y[0,:], label='LVM Hare')
ax1.plot(np.linspace(0,58,len(model4.y[0,:])), model4.y[1,:], label='LVM Lynx')
ax1.plot(t_fine, data_interp[0, :], '--', label='Hare')
ax1.plot(t_fine, data_interp[1, :], '--', label='Lynx')
ax1.set_title('Polynomial model order 4 Lynx and Hare Pelt Predictions')
ax1.legend()

#plot the integrated values of sinusoid library fit 1
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.linspace(0,58,len(model2.y[0,:])), model2.y[0,:], label='LVM Hare')
ax1.plot(np.linspace(0,58,len(model2.y[0,:])), model2.y[1,:], label='LVM Lynx')
ax1.plot(t_fine, data_interp[0, :], '--', label='Hare')
ax1.plot(t_fine, data_interp[1, :], '--', label='Lynx')
ax1.set_title('Sinusoid and Polynomial model 1 Lynx and Hare Pelt Predictions')
ax1.legend()

#plot the integrated values of sinusoid library fit 2
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.linspace(0,58,len(model3.y[0,:])), model3.y[0,:], label='LVM Hare')
ax1.plot(np.linspace(0,58,len(model3.y[0,:])), model3.y[1,:], label='LVM Lynx')
ax1.plot(t_fine, data_interp[0, :], '--', label='Hare')
ax1.plot(t_fine, data_interp[1, :], '--', label='Lynx')
ax1.set_title('Sinusoid and Polynomial model 2 Lynx and Hare Pelt Predictions')
ax1.legend()

# In[117]:

#AIC BIC KL Div
all_models = [X_DMD_fr, X_DMD_total, X_DMD_H[0:2, :], model0.y
               , model1.y, model4.y, model2.y, model3.y]
models = ['DMD', 'Sliding DMD', 'Time Delay DMD', 'Lotka-Volterra', 'Polynomial Order 3',
          'Polynomial Order 4', 'Polynomial Order 4 + Sinusoids Polynomial Order 1',
          'Polynomial Order 4 + Sinusoids Polynomial Order 2']
aic = np.zeros(len(models))
bic = np.zeros(len(models))
kl_div = np.zeros(len(models))
k = 2
for i in range(0, len(models)):
    if models[i] == 'DMD':
        data = data_interp[:, :290]
    else:
        data = data_interp
    model = all_models[i]
    aic[i] = AIC(model, data, k)
    bic[i] = BIC(model, data, k)

#For KL Divergence 1) histogram of data w/ each bin = a population count and
#height of bin = number of data points in interpolated time series that has
#that population count. 2) Normalize histogram to get probability distribution
center = np.average(data, axis=1)
pd_data = np.histogram2d(data[0], data[1], [[-np.inf, center[0], np.inf], [-np.inf, center[1], np.inf]])[0]
pd_model = np.histogram2d(model[0], model[1], [[-np.inf, center[0], np.inf], [-np.inf, center[1], np.inf]])[0]
#Normalize probability distributions
pd_data /= np.sum(pd_data)
pd_model /= np.sum(pd_model)
# compute KL divergence
kl_div[i] = kl_divergence(pd_data, pd_model)

df = pd.DataFrame({'Model': models, "AIC": aic, "BIC": bic, "KL-Divergence": kl_div})
display(df)

# In[4]:

'''
Download the data set BZ.mat (which is a snippet from a Belousov-Zhabotinsky chemical oscillator movie { check them out on youtube).
1. get the data: download from the course website (It is next to HW 2)
2. See what you can do with the data (i.e. repeat the first two steps above)
'''
file = h5py.File('BZ.mat', 'r')

```

```

data = np.array(file.get('BZ_tensor'))
[r,c,d] = data.shape
dt = 0.2#guess of movie dt
t = np.arange(0, r*0.2, 0.2)#time range of movie
data_flat = np.transpose(data.reshape(data.shape[0], -1))#each column is a time point

# train the normalization
scaler = MinMaxScaler()
scaler = scaler.fit(data_flat)
#print('Min: %f, Max: %f' % (scaler.data_min_, scaler.data_max_))
# normalize the dataset and print the first 5 rows
data_flat = scaler.transform(data_flat)

n = data_flat.shape[1]
X1 = data_flat[:,0:n-2]#all columns starting from first column up to the penultimate
X2 = data_flat[:,1:n-1]#all columns starting from second column up to the last column

#Plot percentage of variance captured by differnt modes
U,Sig,VT = linalg.svd(data_flat, full_matrices=False)
V = np.transpose(VT)
f, ax1 = plt.subplots(1, 1, figsize=(7, 4))
ax1.plot((Sig/ sum(Sig)) * 100, 'bo')
ax1.plot(np.zeros((len(Sig))), 'r--')
ax1.set_title('Percentage of energy captured by each mode, Belousov-Zhabotinsky chemical oscillator')
ax1.set_ylabel('Percent variance captured')
ax1.set_xlabel('Mode')
ax1.set_ylim((-2, 100))
ax1.set_xlim((-1, 25))

#Plot
f, [ax1, ax2] = plt.subplots(2, 1, figsize=(12, 10))
ax1.plot(np.real(U[:, 0]), label='Spatial Mode 1')
ax1.plot(np.real(U[:, 1]), label='Spatial Mode 2')
ax1.set_title('Spatial SVD Modes, Belousov-Zhabotinsky chemical oscillator')
ax1.legend()
ax2.plot(np.real(V[:,0]), label='Temporal Mode 1')
ax2.plot(np.real(V[:,1]), label='Temporal Mode 2')
ax2.set_title('Temporal SVD Modes, Belousov-Zhabotinsky chemical oscillator')
ax2.legend()

# In[5]:

rank = 5#rank 9 truncation
Phi, Lambda, b = DMD(X1, X2, rank)#no rank truncation DMD

omega = np.log(np.diag(Lambda)) / dt#the continuous eigenvalues full rank DMD

#calculate time dynamics for full rank DMD
time_dynamics = np.empty((rank, r - 1))#intialize time dynamics array
for i in range(0, r - 1):
    time_dynamics[:, i] = b*np.exp(omega*t[i])
X_DMD_BZ = np.matmul(Phi, time_dynamics)

#compare the SVD modes to the DMD modes.. DMD says find the modes such that the modes in time are exactly oscillatory
#Plot SVD and DMD modes full rank
f, [ax1, ax2] = plt.subplots(2, 1, figsize=(12, 10))
ax1.plot(np.real(Phi[:, 0]), '--', label='DMD Mode 1')
ax1.plot(np.real(Phi[:, 1]), '--', label='DMD Mode 2')
ax1.set_title('Spatial SVD and DMD Modes, rank 9, Belousov-Zhabotinsky chemical oscillator')
ax1.legend()
ax2.plot(np.real(V[:,0]), label='SVD Mode 1')
ax2.plot(np.real(V[:,1]), label='SVD Mode 2')
ax2.plot(np.real(np.transpose(time_dynamics[:, 0]), '--', label='DMD Mode 1')
ax2.plot(np.real(np.transpose(time_dynamics[:, 1]), '--', label='DMD Mode 2')
ax2.set_title('Temporal SVD and DMD Modes, rank 9, Belousov-Zhabotinsky chemical oscillator')
ax2.legend()

#DMD combined modes for entire data set, prediction is terrible
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.real(X_DMD_BZ[0, :]), label='Mode 1')
ax1.plot(np.real(X_DMD_BZ[1, :]), label='Mode 2')
ax1.plot(np.real(X_DMD_BZ[2, :]), label='Mode 2')
ax1.set_title('DMD Modes, rank 9, Belousov-Zhabotinsky chemical oscillator')
ax1.legend()

# In[41]:

```



```

#get low rank approximation of data matrix
r = 20
Ar = np.zeros((r, 1200))
for i in range(r):
    Ar[i,:] = Sig[i] * U[i]* VT[i]

# In[43]:

#Make hankel matrices for each variable
width = 500
rows = len(t) - width + 1#how many sliding windows of specified width can fit within sampled length of time
H = np.empty((r*rows, width))
start = 0
j = 0
i = 1
while i < (rows + 1):
    print("Progress {:.21%}".format(i / (rows+1)), end="\r")#print progress
    for k in range(0, Ar.shape[0]):
        for j in range(start, (start+width)):
            H[i*k, (j - i)%width] = Ar[k,j]

    start = start + 1#reset index to 1 more than the beginning of the window
    i = i + 1#reset Hankel matrix row index holder to next set of time delay arrays

u,s,vh = np.linalg.svd(H)# take SVD

f, ax1 = plt.subplots(1, 1, figsize=(7, 4))
xticks = np.arange(len(s)).tolist()
ax1.set_title('Percentage of energy captured by each mode, Hankel Matrix')
ax1.set_ylabel('Percent variance captured')
ax1.set_xlabel('Mode')
ax1.set_ylim((-5, 100))
ax1.set_xticks(xticks)
ax1.plot((s/ sum(s)) * 100, 'bo')
ax1.plot(np.arange(len(s)), np.zeros(len(s)), 'r--');

#Plot u (eigen vectors of time delay embedding, dominant correlation structure in space)
#and v vectors to show the dominant correlated structures in time.
f, [ax1, ax2] = plt.subplots(2, 1, figsize=(12, 10))
ax1.plot(np.real(u[:, 0]), label='Spatial Mode 1')
ax1.plot(np.real(u[:, 1]), label='Spatial Mode 2')
ax1.plot(np.real(u[:, 2]), label='Spatial Mode 3')
ax1.set_title('Spatial SVD Modes, Hankel Matrix')
ax1.legend()
ax2.plot(np.real(vh[:,0]), label='Temporal Mode 1')
ax2.plot(np.real(vh[:,1]), label='Temporal Mode 2')
ax2.plot(np.real(vh[:,2]), label='Temporal Mode 3')
ax2.set_title('Temporal SVD Modes, Hankel Matrix')
ax2.legend()

# In[49]:

#DMD on Hankel matrix (rank 4)
r = 9
Phi_BZ_H, Lambda_BZ_H, b_BZ_H = DMD(H[:,0:width - 1], H[:, 1:width], r)#rank 4 truncation DMD

omega_BZ_H = np.log(np.diag(Lambda_BZ_H)) / dt#the continuous eigenvalues full rank DMD

#calculate time dynamics for full rank DMD
time_dynamics_BZ_H = np.empty((r, len(t)))#intialize time dynamics array
for i in range(0, len(t) - 1):
    time_dynamics_BZ_H[:, i] = b_BZ_H*np.exp(omega_BZ_H*t[i])
X_DMD_BZ_H = np.matmul(Phi_BZ_H, time_dynamics_BZ_H)

#Hankel Matrix DMD modes
f, ax1 = plt.subplots(1, 1, figsize=(12, 6))
ax1.plot(np.real(X_DMD_BZ_H[0, :1199]), label='Mode 1')
ax1.plot(np.real(X_DMD_BZ_H[1, :1199]), label='Mode 2')
ax1.plot(np.real(X_DMD_BZ_H[2, :1199]), label='Mode 3')
ax1.set_title('Hankel Matrix DMD Modes, rank 9, Belousov-Zhabotinsky chemical oscillator')
ax1.legend()

```