PyDMD - Python Dynamic Mode Decomposition

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1 Introduction

PyDMD - Python Dynamic Mode Decomposition [4] is a Python package that uses Dynamic Mode Decomposition for a data-driven model simplification based on spatiotemporal coherent structures.
Dynamic Mode Decomposition (DMD) is a model reduction algorithm developed by Schmid [15]. Since then has emerged as a powerful tool for analyzing the dynamics of nonlinear systems. DMD relies only on the high-fidelity measurements, like experimental data and numerical simulations, so it is an equation-free algorithm. Its popularity is also due to the fact that it does not make any assumptions about the underlying system. See Kutz [9] for a comprehensive overview of the algorithm and its connections to the Koopman-operator analysis, initiated in Koopman [8], along with examples in computational fluid dynamics.
In the last years many variants arose, such as multiresolution DMD [10], compressed DMD [5], DMD with control [13], forward backward DMD, sparsity promoting DMD to choose dynamically important DMD modes [7], and higher order DMD [11] among others, in order to deal with noisy data, big dataset, or spurius data for example.
In the **PyDMD** package we implemented in Python the majority of the variants mentioned above with a user friendly interface. We also provide many tutorials that show all the characteristics of the software, ranging from the basic use case to the most sofisticated one allowed by the package.
The research in the field is growing both in computational fluid dynamic and in structural mechanics, due to the equation-free nature of the model. We cite among others, applications in the framework of shape optimization in naval engineering [2, 16, 3]. For numerical non-intrusive pipelines for applied sciences and industrial application we cite [14, 17].

2 Main features

The main important features of the **PyDMD** package are the following:

- Thoroughly documented, with an easily accessible online documentation.
- Modular package easily integrable into existing computational pipelines.
- Fast learning rate due to the simplicity of the code design inspired by `scikit-learn`.
- No external dependencies. It uses only standard and well spread Python packages.
- Written following the Python programming best practices.
- Open source software, distributed via GitHub. This ensures an easy contributing procedure and issue tracking.
- A permissive free software license (MIT License), with an excellent license compatibility.
- A vast amount of tutorials.

3 Installation

PyDMD requires requires `numpy`, `scipy`, `matplotlib`, `future`, `sphinx` (for local documentation) and `nose` (for local test). The code is compatible with Python 2.7 and Python 3.6. It can be installed using `pip` or directly from the source code.
Mac and Linux users can install pre-built binary packages using `pip`. To install the package just type:

```
pip install pydmd
```

To uninstall the package:

```
pip uninstall pydmd
```

It is also possible to install the package locally, after cloning it, for example during the developing stage of new features, with

```
git clone https://github.com/mathLab/PyDMD
python setup.py install
```

or, in alternative, to install the lastest version on the master branch on GitHub use the following command

```
pip install git+https://github.com/mathLab/PyDMD.git
```

4 Documentation

PyDMD uses `sphinx` for code documentation. You can view the documentation online here: `https://mathlab.github.io/PyDMD/`. To build the html version of the docs locally simply type the following from within the pydmd folder:

```
cd docs
make html
```

The generated html can be found in `docs/build/html`. Open up the `index.html` file you find there to browse the documentation.

5 Testing

We are using Travis CI for continuous intergration testing for Mac and Linux platforms and for Python 2.7 and 3.6. You can check out the current status here: `https://travis-ci.org/mathLab/PyDMD`.
To run tests locally (`nose` is required):

```
python test.py
```

6 Tutorials

We are going to present the main features of the software following some of the tutorials available online. First we introduce mathematically the algorithm, then in the following subsections we start with the basic usage of the classical DMD, then we introduce more advanced options we can pass to the base class, and finally we show how to use the DMD variants we implemented. All the tutorials can be found online in the GitHub repository at `https://github.com/mathLab/PyDMD/tree/master/tutorials`

6.1 Mathematical formulation

The dynamic mode decomposition is a powerful method that allows the approximation of complex nonlinear systems as the combination of low-rank structures evolve linearly in time. These structures, called *modes*, and their time evolution, called *dynamics*, come from the decomposition, based on the singular value decomposition (SVD), of the output data of the studied system. Relying only on the high-fidelity measurements (experimental data, numerical simulations), the DMD has the big benefit of being an equation-free algorithm, and it does not make assumptions about the underlying system. Due to the complex systems simplification through the dynamics modes, this method gives us the possibility to

- better understand the model thanks to the analysis of the low-rank spatiotemporal features extracted, as we are going to show in Section 6.2;
- accurately reconstruct the temporal evolution of the system and a short-time future estimation.

The basic idea behind DMD is to approximate the evolution of the complex system with a linear operator $\mathbf{A}$ such that $x_{k+1} = \mathbf{A}x_k$, where $x_k \in \mathbb{R}^n$ is the vector representing the state of the system at time k. We underline that the state vectors are equispaced in time. To obtain the minimum approximation error across all these *snapshots*, it is possible to arrange them in two matrices as following:

$$\mathbf{X} = \begin{bmatrix} x_1^1 & x_2^1 & \cdots & x_{m-1}^1 \\ x_1^2 & x_2^2 & \cdots & x_{m-1}^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_1^n & x_2^n & \cdots & x_{m-1}^n \end{bmatrix}, \qquad \mathbf{Y} = \begin{bmatrix} x_2^1 & x_3^1 & \cdots & x_m^1 \\ x_2^2 & x_3^2 & \cdots & x_m^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_2^n & x_3^n & \cdots & x_m^n \end{bmatrix}. \tag{1}$$

In this way, each column of $\mathbf{Y}$ contains the state vector at the next timestep of the one in the corresponding $\mathbf{X}$ column.
We underline that the snapshots are sampling the evolution of a nonlinear system and we are looking for a linear operator. Thus, we want to find $\mathbf{A}$ such that $\mathbf{Y} \approx \mathbf{AX}$. The best-fit $\mathbf{A}$ matrix is given by $\mathbf{A} = \mathbf{YX}^\dagger$, where the symbol † denotes the Moore-Penrose pseudo-inverse.
Since the snapshots x_i represent the state of the system, we assume they are high dimensional: hence the matrix $\mathbf{A}$ has n^2 elements (supposing the dimension n of a snapshot is larger than the number of snapshots m) and it is difficult to decompose or to handle. The DMD algorithm projects the data onto a low-rank subspace defined by the proper orthogonal decomposition (POD) modes, then computes the low-dimensional operator $\tilde{\mathbf{A}}$; finally this operator is used to reconstruct the leading nonzero eigenvalues and eigenvectors of the full-dimensional operator $\mathbf{A}$ without ever explicitly computing $\mathbf{A}$.
First, we compute the truncated SVD of the matrix $\mathbf{X}$:

$$\mathbf{X} \approx \mathbf{U}_r \mathbf{\Sigma}_r \mathbf{V}_r^*, \tag{2}$$

where $\mathbf{U}_r \in \mathbb{C}^{n\times r}$, $\mathbf{\Sigma}_r \in \mathbb{C}^{r\times r}$ and $\mathbf{V}_r \in \mathbb{C}^{m\times r}$. Here r is the rank of the reduced SVD approximation and * denotes the conjugate transpose. The columns of $\mathbf{U}_r$ are orthonormal and they are the first r POD modes, so we can use the matrix $\mathbf{U}_r$ to build the low-dimensional operator $\tilde{\mathbf{A}}$. Recalling the definition of $\mathbf{A}$ and the decomposition of $\mathbf{X}$ we obtain

$$\tilde{\mathbf{A}} = \mathbf{U}_r^* \mathbf{Y} \mathbf{V}_r \mathbf{\Sigma}_r^{-1}. \tag{3}$$

Avoiding the explicit calculation of the high-dimensional operator $\mathbf{A}$, we obtain the matrix $\tilde{\mathbf{A}} \in \mathbb{C}^{r\times r}$ that defines the linear evolution of the low-dimensional model as $\tilde{x}_{k+1} = \tilde{\mathbf{A}}\tilde{x}_k$, where $\tilde{x}_k$ is the low-rank approximated state. It is possible reconstruct the high-dimensional state x_k as $x_k = \mathbf{U}_r \tilde{x}_k$.
Thanks to the eigendecomposition of $\tilde{\mathbf{A}}$

$$\tilde{\mathbf{A}}\mathbf{W} = \mathbf{W}\mathbf{\Lambda} \tag{4}$$

we can reconstruct the eigenvectors and eigenvalues of the matrix $\mathbf{A}$: in particular the eigenvectors can be computed in two ways:

- the eigenvectors of $\mathbf{A}$ are reconstructed by projecting the low-rank approximation $\mathbf{W}$ on the high-dimensional space: $\mathbf{\Phi} = \mathbf{U}_r\mathbf{W}$. We call the eigenvectors computed in this way the *projected* dynamic mode decomposition (DMD) modes.
- the so called *exact* DMD modes, the real eigenvectors of $\mathbf{A}$, are instead the columns of $\mathbf{\Phi} = \mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{W}$.

To demonstrate the relation between the exact DMD modes and the eigenvectors of the matrix $\tilde{\mathbf{A}}$, we recall the eigendecomposition of the high-dimensional operator and the definitions $\mathbf{A} = \mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{U}_r^*$ and $\tilde{\mathbf{A}} = \mathbf{U}_r^*\mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}$:

$$\begin{aligned}
\mathbf{A}\mathbf{\Phi} &= \mathbf{\Phi}\mathbf{\Lambda}\\
\mathbf{A}\mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{W} &= \mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{W}\mathbf{\Lambda}\\
\mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{U}_r^*\mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{W} &= \mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{W}\mathbf{\Lambda}\\
\mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}\tilde{\mathbf{A}}\mathbf{W} &= \mathbf{Y}\mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{W}\mathbf{\Lambda}\\
\tilde{\mathbf{A}}\mathbf{W} &= \mathbf{W}\mathbf{\Lambda}.
\end{aligned} \tag{5}$$

This also proves that the eigenvalues obtained from the decomposition of $\tilde{\mathbf{A}}$ coincide with the eigenvalues of $\mathbf{A}$. These eigenvalues $\mathbf{\Lambda} = \begin{bmatrix}\lambda_0 & \lambda_1 & \dots & \lambda_r\end{bmatrix}$ with $\lambda_i \in \mathbb{C}$ for $i = 0, 1, \dots, r$, contain growth/decay rates and frequencies of the corresponding DMD modes.
We use the eigendecomposition to rewrite the definition of the linear operator:

$$\begin{aligned}
\mathbf{Y} &\approx \mathbf{A}\mathbf{X}\\
&\approx \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\dagger\mathbf{X}\\
&\approx \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\dagger\begin{bmatrix}\mathbf{x}_0 & \mathbf{x}_1 & \mathbf{x}_2 & \dots & \mathbf{x}_r\end{bmatrix}\\
&\approx \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\dagger\begin{bmatrix}\mathbf{x}_0 & \mathbf{A}\mathbf{x}_0 & \mathbf{A}^2\mathbf{x}_0 & \dots & \mathbf{A}^{r-1}\mathbf{x}_0\end{bmatrix}\\
&\approx \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\dagger\begin{bmatrix}\mathbf{x}_0 & \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\dagger\mathbf{x}_0 & \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\dagger\mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\dagger\mathbf{x}_0 & \dots & (\mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\dagger)^{r-1}\mathbf{x}_0\end{bmatrix}\\
&\approx \mathbf{\Phi}\mathbf{\Lambda}\begin{bmatrix}\mathbf{b} & \mathbf{\Lambda}\mathbf{b} & \mathbf{\Lambda}^2\mathbf{b} & \dots & \mathbf{\Lambda}^{r-1}\mathbf{b}\end{bmatrix}\\
&\approx \mathbf{\Phi}\begin{bmatrix}\mathbf{\Lambda} & \mathbf{\Lambda}^2 & \dots & \mathbf{\Lambda}^r\end{bmatrix}\mathbf{b}
\end{aligned} \tag{6}$$

where $\mathbf{b}$ refers to the amplitudes of the first snapshot such that $\mathbf{b} = \mathbf{\Phi}^\dagger\mathbf{x}_0$. Thus, it is possible to approximate the state of the system at the generic time $t_k = k\Delta t$ by computing $\mathbf{x}_k = \mathbf{\Phi}\mathbf{\Lambda}^k\mathbf{b}$.

6.2 How to use the standard algorithm

In the following tutorial, we apply the standard DMD to a very simple system in order to show the capabilities of the algorithm and the package interface. We create the input data by summing the following two functions

$$\begin{aligned}
f_1(x,t) &= \operatorname{sech}(x+3)\exp(i2.3t),\\
f_2(x,t) &= 2\operatorname{sech}(x)\tanh(x)\exp(i2.8t).
\end{aligned} \tag{7}$$

and we import the **PyDMD** environment and in particular the `DMD` class using the code below.

```python
import matplotlib.pyplot as plt
import numpy as np

from pydmd import DMD
```

```python
def f1(x,t):
    return 1./np.cosh(x+3)*np.exp(2.3j*t)

def f2(x,t):
    return 2./np.cosh(x)*np.tanh(x)*np.exp(2.8j*t)

x = np.linspace(-5, 5, 128)
t = np.linspace(0, 4*np.pi, 256)
xgrid, tgrid = np.meshgrid(x, t)

X1 = f1(xgrid, tgrid)
X2 = f2(xgrid, tgrid)
X = X1 + X2
```

Now we have the temporal snapshots in the input matrix rows: we can easily create a new DMD instance and exploit it in order to compute the decomposition on the data. Since the snapshots must be arranged by columns, in this case we need to transpose the matrix.

```python
dmd = DMD(svd_rank=2)
dmd.fit(X.T)
```

The `dmd` object contains the principal information about the decomposition:

- the attribute `modes` is a 2D numpy array where the columns are the low-rank structures individuated;
- the attribute `dynamics` is a 2D numpy array where the rows refer to the time evolution of each mode;
- the attribute `eigs` refers to the eigenvalues of the low dimensional operator;
- the attribute `reconstructed_data` refers to the approximated system evolution.

We are able to easily visualise the eigenvalues using the method `plot_eigs` or plotting the modes and the dynamics thanks to `matplotlib` library, as shown in Figure 1.

```python
for mode in dmd.modes.T:
    plt.plot(x, mode.real)
    plt.title('Modes')
plt.show()

for dynamic in dmd.dynamics:
    plt.plot(t, dynamic.real)
    plt.title('Dynamics')
plt.show()
```

Finally, we can reconstruct the original dataset as the product of modes and dynamics. In Figure 2 we plot the evolution of each mode to emphasize their similarity with the input functions and we plot the reconstructed data.

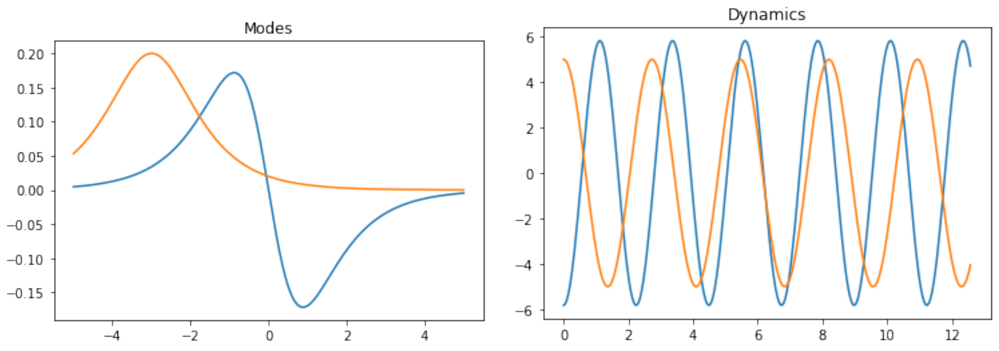


Figure 1: The DMD modes and the corresponding dynamics.

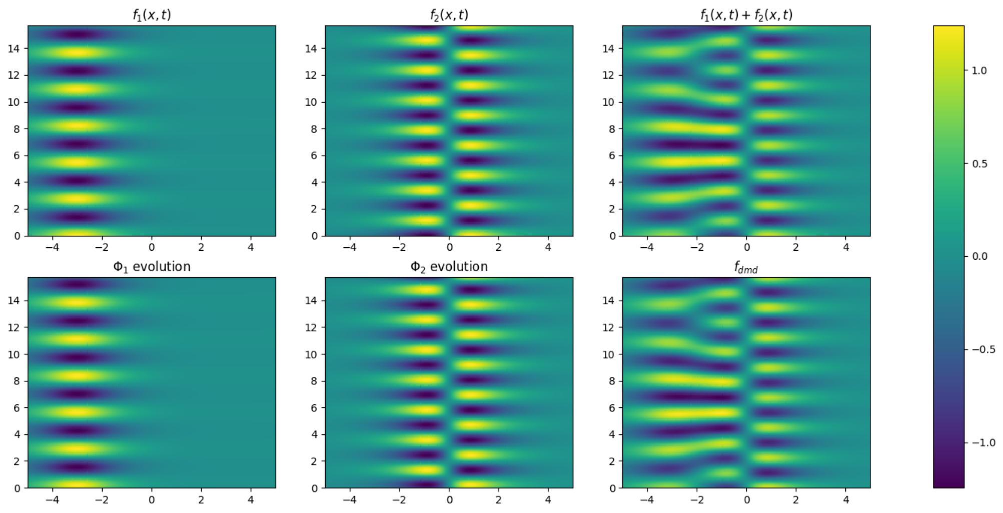


Figure 2: The application of the DMD algorithm on the toy dataset: the evolving system is simulated summing f_1 and f_2; the two dynamics coincide with these functions and the target dynamical system is faithfully reconstructed.

6.3 More advanced options

We create the dataset with an hyperbolic secant with damped oscillations as in the following formula:

$$f(x, y, t) = \operatorname{sech}(x)\operatorname{sech}(y)2.4i^{-t} + r \tag{8}$$

where r is a random noise term sampled from a normal (Gaussian) distribution, $r \sim \mathcal{N}(\mu, \sigma^2)$, with mean $\mu = 0$ and variance $\sigma = 0.4$. In Figure 3 the 16 equispaced snapshots for $t \in [0, 6]$ generated with the code below.

```python
x1 = np.linspace(-3, 3, 80)
x2 = np.linspace(-3, 3, 80)
x1grid, x2grid = np.meshgrid(x1, x2)

time = np.linspace(0, 6, 16)

data = [2/np.cosh(x1grid)/np.cosh(x2grid)*(1.2j**-t) for t in time]
noise = [np.random.normal(0.0, 0.4, size=x1grid.shape) for t in time]

snapshots = [d+n for d,n in zip(data, noise)]

fig = plt.figure(figsize=(18,12))
for id_subplot, snapshot in enumerate(snapshots, start=1):
    plt.subplot(4, 4, id_subplot)
    plt.pcolor(x1grid, x2grid, snapshot.real, vmin=-1, vmax=1)
```

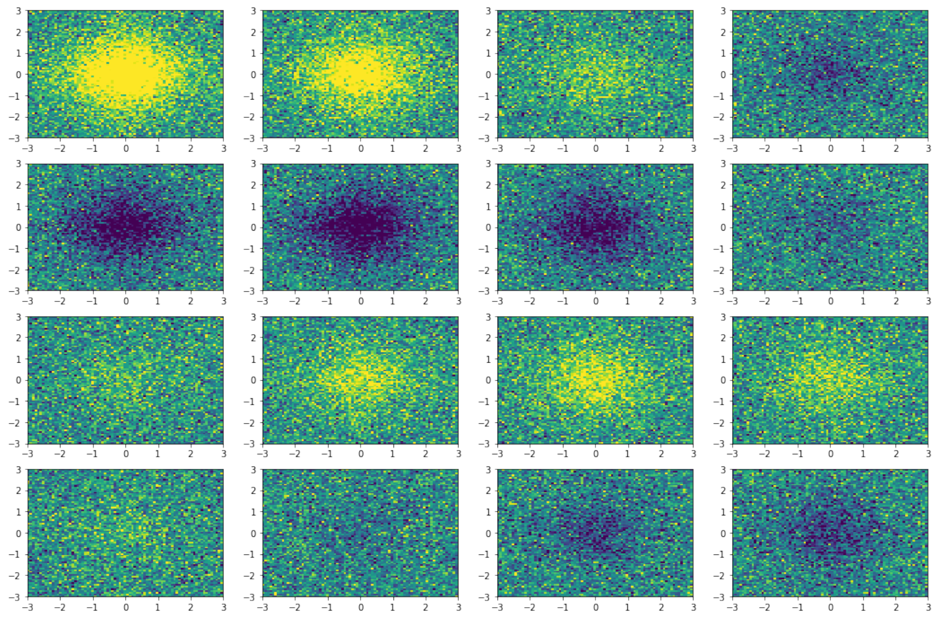


Figure 3: Snapshots state of the dynamical system.

Alright, now it is time to apply the DMD to the collected data. First, we create a new `DMD` instance.

```python
dmd = DMD(svd_rank=1, tlsq_rank=2, exact=True, opt=True)
```

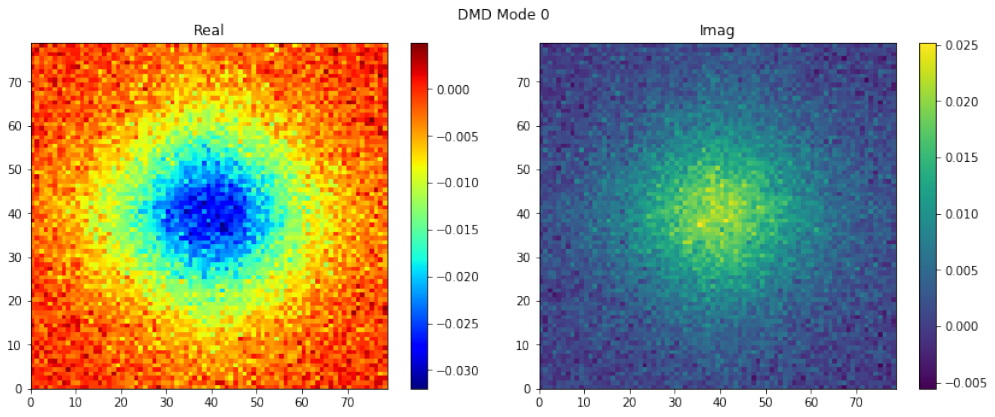
We note there are four optional parameters:

- `svd_rank`: since the dynamic mode decomposition relies on singular value decomposition, we can specify the number of the largest singular values used to approximate the input data. It is also possible to set it to 0 and the algorithm will calculate for you the optimal rank truncation [6]. Moreover it accepts non-integer values between 0 and 1, indicating the percentage of spectral energy you want to retain with the truncation, for instance 0.8 means to retain at least 80% of the cumulative energy of the singular values, starting from the greatest.

- `tlsq_rank`: using the total least square, it is possible to perform a linear regression in order to remove the noise on the data; because this regression is based again on the singular value decomposition, this parameter indicates how many singular values are used.
- `exact`: boolean flag that allows to choose between the exact modes or the projected one (see Subsection 6.1).
- `opt`: boolean flag that allows to choose between the standard version and the optimized one. If true the optimal amplitudes of the DMD modes are computed by minimizing the error between the time evolution and all the original snapshots [7]. If false the amplitudes are computed using only the initial condition, that is the first snapshot.

Then using a well known code design, borrowed from `scikit-learn` [12, 1], with the `fit` method it is possible to compute the DMD modes, given the original snapshots. Now we can plot the 2D modes easily with `plot_modes_2D`, it is that simple!

```
dmd.fit(snapshots)
dmd.plot_modes_2D(figsize=(12,5))
```



We have everything to compute the reconstructed snapshots using the DMD mode we have computed. The approximated system is similar to the original one and, moreover, the noise is greatly reduced.

```
fig = plt.figure(figsize=(18,12))
for id_subplot, snapshot in enumerate(dmd.reconstructed_data.T, start=1):
    plt.subplot(4, 4, id_subplot)
    plt.pcolor(x1grid, x2grid, snapshot.reshape(x1grid.shape).real, vmin=-1, vmax=1)
```

We can also manipulate the interval between the approximated states and extend the temporal window where the data is reconstructed thanks to DMD. Let us make the DMD delta time a quarter of the original and extend the temporal window to $[0, 3t_{\mathrm{org}}]$, where t_{org} indicates the time when the last snapshot was caught.

```
dmd.dmd_time['dt'] *= .25
dmd.dmd_time['tend'] *= 3
```

If we recalculate the reconstructed data with this new timeframe we obtain the video you can find at: `https://github.com/mathLab/PyDMD/blob/master/readme/dmd-example.gif`

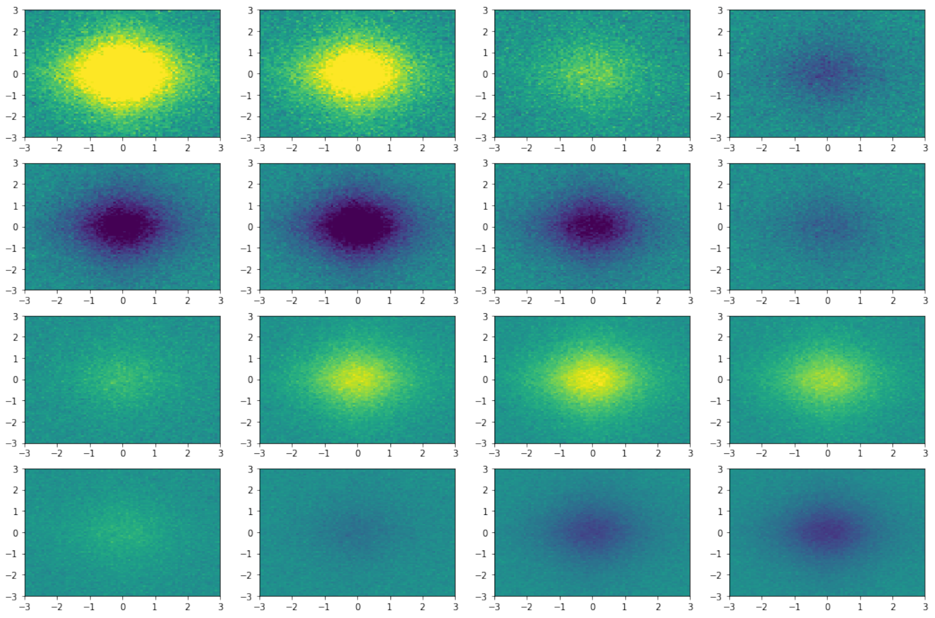


Figure 4: Snapshots state reconstructed by the DMD algorithm.

6.4 DMD variants use cases

PyDMD allows to use many variants of the standard DMD algorithm: the multi-resolution dynamic mode decomposition (mrDMD), the forward/backward DMD, the DMD with control (DMDc), the compressed DMD, and the high order dynamic mode decomposition (HODMD). For all these implementations we refer to the folder `tutorials` within the package repository, accessible at `https://github.com/mathLab/PyDMD/tree/master/pydmd`, where there is a tutorial for each one of them.

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