Dynamic mode decomposition as an analysis tool for time-dependent partial differential equations

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Abstract—The time-dependent fields obtained by solving partial differential equations in two and more dimensions quickly overwhelm the analytical capabilities of the human brain. A meaningful insight into the temporal behaviour can be obtained by using scalar reductions, which, however, come with a loss of spatial detail. Dynamic Mode Decomposition is a data-driven analysis method that solves this problem by identifying oscillating spatial structures and their corresponding frequencies. This paper presents the algorithm and provides a physical interpretation of the results by applying the decomposition method to a series of increasingly complex examples.

Keywords—dynamic mode decomposition; data-driven analysis; wave equation; non-Newtonian natural convection

I. INTRODUCTION

Humans possess a remarkable ability for pattern recognition that is however still quickly overwhelmed when analysing complex systems. When dealing with time series of two or three dimensional field snapshots, as is common in e.g. hydrodynamics, we are often forced to use reductions that decrease complexity and provide an approachable insight into the system’s behaviour. An example of such reduction when dealing with natural convection is tracking the ratio between heat convection and conduction, also known as the Nusselt number, on a significant boundary. The Nusselt number provides us with a scalar value that reflects the behaviour in our system. Analysing time series of such values can provide insight on whether the system is stable, oscillatory or maybe even chaotic, with Fourier analysis available as a potent tool to extract the characteristic frequencies reflected in the chosen reduction. No matter how good the reduction is we still lose the majority of the spatial detail which is often important for understanding the dynamics.

Spatial structure of the analysed system is required for good understanding of the dynamics, which is especially important when dealing with engineering challenges like the airflow around aircraft structures. A common approach to identifying important spatial structures in analysed fields is modal decomposition, with Proper Orthogonal Decomposition (POD) proposed for hydrodynamics by Lumley in 1967, and its variations as one of the most widely used techniques. POD is a decomposition technique that identifies orthogonal modes that best represent the dataset and provides an ordering based on their importance.

Modes obtained with POD provide information about energetically important parts of the system but are completely oblivious to the temporal behaviour meaning that the results of the decomposition would stay the same even if analysis was performed on reordered snapshots. Dynamic mode decomposition (DMD) was proposed by Schmid in a 2008 talk and the subsequent paper in 2010 as a technique that joins the spatial aspects of POD and temporal aspects of Fourier transform. DMD identifies characteristic frequencies, corresponding spatial structures and whether they amplify, decay or remain constant through the sampled timespan. The method was initially proposed for hydrodynamics but has since found other applications including infectious disease spread and computer vision as it is completely data-driven and independent of the underlying dynamics.

This paper introduces the DMD algorithm and interpretation in Sec. II demonstrates the results on vibrating membrane examples in Sec. III and concludes with the decomposition applied to a more interesting case of oscillatory non-Newtonian natural convection in Sec. IV.

II. DYNAMIC MODE DECOMPOSITION

A. Interpretation

The DMD algorithm is based on finding eigenvalues $\lambda$ and eigenvectors $\varphi$ of the linear mapping represented by the matrix $A$

$$v_{i+1} = Av_i,$$  \hspace{1cm} (1)

that connects the subsequent states $v_i$ and $v_{i+1}$ of the analysed system. As such the algorithm is completely independent of the governing equations that drive the underlying dynamics and can be applied to any experimental or simulated data.

1 Also known as principal component analysis (PCA) and various other names in different fields.

2 Optimal in $L_2$ sense that corresponds to energy when decomposing flow field.
The linear nature of eigendecomposition does not preclude us from analysing non-linear systems as the dynamics of any such system can be expressed with an infinite-dimensional linear Koopman operator \([9]\) with the DMD providing a good approximation of it’s eigendecomposition as long as the quality and quantity of input data is sufficient \([10]\).

DMD eigenvalues \(\lambda\) provide information about the temporal behaviour of the spatial structure described in the eigenvector. Eigenvalues are complex numbers with the mode’s angular frequency information contained in the argument

\[
\nu_i = \frac{\arg(\lambda_i)}{2\pi \Delta t},
\]

with sampling interval \(\Delta t\) providing scaling to the output, that is otherwise unaffected by the frequency of data snapshot sampling. The magnitude of eigenvalues provides information about changes in mode’s strength, with \(|\lambda| > 1\) for amplifying and \(|\lambda| < 1\) for decaying modes.

The linear combination of DMD modes calculated from real valued input data has to be real valued, which can be satisfied either by real eigenvalues/eigenvectors or complex-conjugate pairs of complex eigenvalues/eigenvectors. Real eigenvalues represent modes with frequency 0. At least one such background mode with frequency 0 and eigenvalue magnitude of 1 is present whenever the decomposed data has non-zero average but multiple such real-valued growing/decaying non-oscillatory modes can appear. Complex conjugate pairs represent oscillating modes and can be treated as a single mode and will be in most of the later visualisations.

### B. Algorithm

The algorithm for exact DMD proposed by Tu \([11]\) starts by taking subsequent snapshots \(v_i\) of analysed fields separated by \(\Delta t\). Uniformly sampled snapshots simplify calculation and frequency interpretation but are not explicitly required for DMD. Snapshots are flattened from their arbitrary shape into vectors with length \(M\) and arranged as columns in a matrix

\[
V_i^N = \begin{bmatrix} v_i & v_{i+1} & \cdots & v_N \end{bmatrix},
\]

with \(N\) denoting the number of snapshots. The number of data points in a snapshot \(M\) is usually much larger than the number of snapshots \(N\), leading to tall and narrow matrices \(V_i^N\) that can be exploited to efficiently calculate the eigendecomposition of the large \(M \times M\) matrix \(A\).

The snapshot matrix \(V_i^N\) needs to have a sufficient\(^3\) rank to describe the dynamics. Rank deficiency issues usually appear when dealing with standing waves \([10], [12]\) that cause a linear dependency between snapshots in columns of \(V_i^N\) and can be solved by stacking subsequent snapshots

\[
V_i^N = \begin{bmatrix} v_i & v_{i+1} & \cdots & v_{N-m} \\
v_{i+1} & v_{i+2} & \cdots & v_{N-m+1} \\
\vdots & \vdots & \ddots & \vdots \\
v_{i+m} & v_{i+m+1} & \cdots & v_N \end{bmatrix},
\]

and can be deduced from either the unitary eigenvectors or the eigenvalues that carry temporal data. This deficiency is bypassed ensuring \(\text{rank}(V_i^N) \geq m\) at the cost of effectively larger system, and only using the first \(M\) values from the now larger DMD eigenvectors. Time shift augmentation can also help with noisy data or in cases where snapshots are small \([12]\).

For simplicity we continue our discussion with the notation from Eq. \((5)\), apply the relationship from Eq. \((1)\) to the matrix

\[
V_i^N = [Av_0 \quad Av_1 \quad \cdots \quad Av_{N-1}] = AV_0^{N-1},
\]

and perform the compact singular value decomposition (SVD) on the data matrix

\[
V_0^{N-1} = USW^\dagger.
\]
by calculating the projection coefficients for expressing the measured datasets in terms of DMD eigenvectors

$$\mathbf{v}(t) = \sum_k \varphi_k \mathbf{b}_k(t).$$

(10)

As the relative importance of eigenvectors in an oscillating dataset changes with time it is best to calculate their importance for all available snapshots expressed in matrix form as

$$\mathbf{V}_0^{N-1} = \Phi \mathbf{B},$$

(11)

with eigenvectors collected in columns of matrix $\Phi = [\varphi_0 \varphi_1 \cdots \varphi_r]$ and coefficients corresponding to datasets in $\mathbf{V}_0^{N-1}$ collected as columns in matrix $\mathbf{B} = [\mathbf{b}_0 \mathbf{b}_1 \cdots \mathbf{b}_{N-1}]$. The complex number $B_{ij}$ corresponds to the projection coefficient of the $i$-th eigenvector for the $j$-th data sample. Columns of $\mathbf{B}$ can be thus interpreted as the time evolution of mode importance that can be condensed into a single value by calculating the average value. We use the mode power ($P$)

$$P_i = \frac{1}{N} \sum_{j=0}^{N-1} |B_{ij}|$$

(12)

to rank the calculated modes.

An efficient algorithm for calculating $\mathbf{B}$ has also been proposed by Tu et al. [10]. The algorithm avoids additional computation beyond calculating the left eigenvectors $\mathbf{Z}$ during the eigendecomposition of $\mathbf{A}$ by expressing the matrix as

$$\mathbf{B} = \mathbf{Z}^\dagger \mathbf{S} \mathbf{W}^\dagger.$$  

(13)

III. VibRATING MEMBRANE

A. Numerical model

We demonstrate the DMD algorithm with a damped wave equation on a 2D square membrane. This case is convenient as it still allows for comparison against known analytic results but is closer to possible real world applications. We are solving the wave equation

$$\frac{\partial^2 \mathbf{h}}{\partial t^2} = c^2 \nabla^2 \mathbf{h} - \gamma \frac{\partial \mathbf{h}}{\partial t},$$

(14)

with $c$ denoting the velocity of wave propagation and $\gamma$ the damping factor, on a square domain $\Omega = \{(x,y) : x, y \in [0,1]\}$ with Dirichlet boundary condition $h_{\partial \Omega} = 0$. A constant velocity $c = 1$ is used for all of the presented examples.

We start the dynamics with a Gaussian initial condition with $\sigma = 0.1$ and amplitude of 1 placed at an arbitrarily chosen position $(0.3, 0.4)$ to simulate an impact against the membrane. We would like to show that DMD identifies eigenmodes for the membrane and analyse how damping might affect the accuracy.

B. Analytic solution

We can obtain an analytic solution for the partial differential equation (14) by using the separation of variables. For now we ignore damping as it is not relevant for the eigenstate spatial configuration. The solution is a linear combination of modes defined with two integer quantization indices $m,n \geq 1$. Analytical eigenfrequencies and eigenvectors are expressed in terms of $m$ and $n$

$$\nu = \frac{c}{2} \sqrt{m^2 + n^2},$$

$$h(x,y,m,n) = \sin(m\pi x) \sin(n\pi y),$$

(15)

(16)

with eigenvectors shown in Figure 1. Only one eigenvector is shown for the degenerate frequencies.

C. Results

The partial differential equation is solved numerically for different damping rates using the meshless RBF-FD [13] method implemented with the Medusa [14] C++ library. A subset of system state snapshots for the 0 damping case that that we use in DMD is shown in the right graphs of Figure 2. The dynamics are disordered due to the non-symmetric position of the initial jolt and do not offer much insight at the first glance. We can use the sum of membrane heights as an observable that reduces the system’s behaviour into a single scalar value to visualise the oscillation and the effect of different damping rates as shown in the left graph of Figure 2.

We use DMD on 1000 uniformly sampled snapshots from the interval $t \in [0, 10]$ that are composed into the data matrix $\mathbf{V}$ with stacking $m = 10$. Each snapshot is composed of 3985 height values in computational nodes for the mesh-free partial differential equation solving, which are uniformly positioned within $\Omega$. 

![Figure 1. Analytic eigenvectors for the oscillation of a square membrane, ordered by increasing frequency.](image)
The resulting frequencies, calculated from DMD eigenvalues as described in Eq. (2), are shown in the top graph of Figure 3. The results provide a good estimation for the analytic results with sub percent relative error for the first ∼30 modes as shown in the central graph. Estimated frequencies remain good even for the relatively strongly damped γ = 1 case showing promise for eigenfrequency estimation on experimental data obtained from complex objects.

There is a slight inconsistency in the results with a sharp increase in the relative error for the γ = 0 frequencies. We would expect that the least damped case would give the best results but there seems to be an additional non-physical mode at index 11 that has caused a shift in the following frequencies. Fortunately we can use the mode power described in Sec. II-C and shown in the bottom graph of Figure 3 to detect and remove the highlighted spurious mode with a significantly lower strength. It is surprising how little nonsensical modes we identified even though we initially disturbed the membrane in a non-symmetric location and how chaotic the actual system shown in the heat maps of Figure 2 looks to a human observer.

We can also compare the analytic eigenvectors shown in Figure 1 and DMD eigenvectors in Figure 4. The DMD vector positions in the grid are shifted by one compared to the analytic due to the non-oscillatory background mode that is always present in the decomposition of data with non-zero average. Some eigenvectors match almost perfectly while others wildly differ. This might seem inconsistent at the first glance but can be explained with degeneracy in the analytical spectrum. Linear combinations of degenerate eigenvectors still constitute a valid eigenvector. The non-symmetric eigenvector ϕ_{11} can quickly be identified as the one corresponding to the previously mentioned spurious mode.

D. Oddly shaped membrane

Now that we have shown that DMD can be used to identify inherent oscillatory modes we apply it to an irregularly shaped membrane. The duck-shaped membrane is again disturbed with a Gaussian initial state, resulting in the oscillation shown in Figure 5. This combination of meshless computational nodes, the time evolution of the system, the DMD spectrum, and the DMD eigenvectors ordered by frequency provides a condensed overview of the dynamics and shows how DMD could be used in engineering analysis. The DMD spectrum is a convenient and commonly used display of DMD mode frequency and power in the same graph, which can, when sorted by frequency, be used similarly to the Fourier transform.

IV. NON-NEWTONIAN FLUID

The last example is a practical use case for DMD applied to hydrodynamics. We solve, with details available in [15], the
system of partial differential equations
\[
\nabla \cdot \mathbf{v} = 0, \\
\rho \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \nabla \cdot (\eta \nabla \mathbf{v}) - \mathbf{g} \rho \beta T, \\
\rho c_p \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \nabla \cdot (\lambda \nabla T),
\]
with \(\mathbf{v}, T, p, \rho, \mathbf{g}, \beta, T_\Delta, c_p, \eta_0, n\) representing the flow velocity field, temperature field, pressure field, density, gravity, thermal expansion coefficient, temperature offset, heat capacity, viscosity constant and non-Newtonian index respectively.

The system is used to describe the natural convection in an incompressible non-Newtonian fluid. Non-Newtonian fluids have a variable viscosity meaning that the relationship between the shear-strain and the shear-stress is non-linear. We use a simple power-law model to describe the relationship with non-Newtonian power index \(n\) as the main parameter of behaviour. Smaller values of \(n\) indicate stronger shear-thinning non-Newtonian effects while \(n = 1\) equals to a normal, Newtonian fluid.

We will be using the dimensionless Rayleigh number (Ra) that has a similar meaning for natural convection as Reynolds number, meaning stronger dynamics for higher values, as a case parameter, with details unimportant for the demonstration.

The model is solved in a square cavity with differentially heated walls schematically shown in the upper left graph of Figure 6. The left and right walls are kept at a temperature differential causing the fluid to form a vortex as it heats and rises at the right boundary and cools and descends on the left. This circulation is stationary for low Ra with a transition into an oscillatory and later chaotic regime as Ra increases. The upper right graphs in Figure 6 show a selection of system temperature and velocity field snapshots for the oscillatory and later chaotic regime as Ra increases. The case parameter, with details unimportant for the demonstration. The system is stationary for low Ra with a transition into the oscillatory behaviour occurring at Ra = 10^6. A set of parameters where the transition into the oscillatory behaviour occurs has been identified by Kosec et al. [16] and we use DMD to analyse the differences in dynamics as we push past that point with increasing Ra and decreasing \(n\).

As mentioned in the introduction we can use the Nusselt number, shown in the bottom graph of Figure 6 as an observable into the systems behaviour. The system is stationary for Ra = 5 \cdot 10^3 and \(n = 1\) but oscillations occur both when we increase Ra and when we decrease \(n\).

We use DMD to decompose the 5 cases utilising 500 snapshots of the system between \(t = 10\) and \(t = 11\) with stacking \(m = 5\). The results are shown in Figure 7a for increasing Ra and Figure 7b for decreasing \(n\). The mode power defined in Eq. (12) is used to identify the strongest modes and display the corresponding eigenvectors. The first observation that is common to both modes of spurring the dynamics pertains to the DMD spectrum. The initial stationary case has the vast majority of its power in the first constant mode with others most likely only containing noise. As the intensity of the dynamics increases we get more distinct modes but the power of the background modes also increases as expected with ever wilder dynamics heading towards chaos, where all modes would be present and indistinguishable by power.

We can be reasonably certain that the oscillatory dynamics are in fact different for the Ra and \(n\) spurred dynamics by using the eigenvectors of DMD modes sorted by power to identify the important parts. The strongest areas are clearly
different with eigenvectors for the Ra induced dynamics in Figure 7a present mainly as perturbations to the main central vortex while the modes for the n induced dynamics in Figure 7b point to activity in corners where counter vortices occur. This is consistent with the typical shear-thinning non-Newtonian behaviour where the larger velocity gradients are penalised less providing better conditions for smaller vortices.

V. CONCLUSION

We have presented the algorithm for dynamic mode decomposition and applied it to various test and example cases. The examples progressed from the most basic, where we were able to verify the results against known closed-form values, towards a concrete hydrodynamics example where DMD provided valuable insight into the system that would be difficult to obtain otherwise. The DMD has proved to be a very practical tool for dynamical system analysis and it is recommended that anyone dealing with hydrodynamics or similarly complex systems should be at least familiar with its fundamentals. The algorithm is only a decade old and has an active community working on extensions for the concept of Koopman operator decomposition and applications for the existing versions of DMD.

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