DETECTING REGIME TRANSITIONS IN TIME SERIES USING DYNAMIC
MODE DECOMPOSITION

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ABSTRACT. We employ the framework of the Koopman operator and dynamic mode decomposition to devise a method to detect transient dynamics and regime changes in time series. We argue that typically transient dynamics experiences the full phase space dimension with subsequent fast relaxation towards the attractor. In equilibrium, on the other hand, the dynamics evolves on a lower dimensional attractor. The reconstruction error of a dynamic mode decomposition is used to monitor the effective dimension of the dynamics as well as the inability of the given observations to capture the fast relaxation towards the attractor. We illustrate our method by detecting transient dynamics in the Kuramoto-Sivashinsky equation. We further apply our method to atmospheric reanalysis data; our diagnostics detects the transition from a predominantly negative North Atlantic Oscillation (NAO) to a predominantly positive NAO around 1970, as well as the recently found regime change in the Southern Hemisphere atmospheric circulation around 1970.

1. INTRODUCTION

Being able to determine whether a dynamical system is evolving on an attractor exhibiting essentially equilibrium dynamics, or whether it exhibits transient dynamics is of utmost importance. Is a system exhibiting rare but natural equilibrium fluctuations or is the system transitioning, possibly to a new equilibrium state with possibly very different statistical behaviour? We develop here a method which aims at answering this question when only a time series is given. We consider dynamical systems which evolve, when in equilibrium, on an attractor the dimension of which is smaller than the full phase space dimension. We consider the case of an externally driven transition to a new attractor as well as transient non-equilibrium dynamics off the attractor.

We use the framework of Koopman operators and of dynamic mode decomposition (DMD) [13, 11, 10]. The Koopman operator is an abstract concept in dynamical systems theory which encodes the dynamics of a dynamical system and propagates observables from one instance of time to another instance of time [12]. A computationally cost-effective algorithm to compute a finite-dimensional approximation of the Koopman operator is given by DMD, which was proposed by Schmid [21, 20]. The connection between DMD and the Koopman operator has been made first in [19], and has lead
to further fruitful extensions [24, 26, 14]. DMD distills dynamically relevant structures, the so-called Koopman modes together with their temporal oscillation periods and/or their growth rates. DMD has been used in many areas of science to unravel dynamical features within dynamical systems such as instabilities and bifurcations (see, for example, [2, 11, 22, 10]). In particular, DMD allows for an approximate reconstruction of the dynamics, locally in time, by the eigenmodes of the Koopman operator. For chaotic dynamical systems evolving on a lower-dimensional attractor, it suffices to express the dynamics with a finite number of Koopman modes; the number of modes needed being proportional to the attractor dimension. The main idea of this work is the following: In equilibrium the dynamics evolves on a lower dimensional attractor, whereas transient dynamics feels the full phase-space dimension. Hence in transient dynamics the reconstruction by a finite number of Koopman modes, which has been sufficient to capture the equilibrium dynamics, may be poor. This poor representation of the observed dynamics by a finite number of numerically approximated Koopman modes is exacerbated by the typically fast attraction towards the attractor after perturbation in a non-equilibrium state off the attractor. To resolve this fast relaxation requires a sufficiently fine temporal resolution of the dynamics which may not be given in the time series under consideration. We propose here a simple and computationally cheap method to detect non-equilibrium dynamics such as transients or qualitative regime of the attractor by monitoring the reconstruction error of DMDs. We illustrate the effectiveness of our method using the Kuramoto-Sivashinsky equation for which the existence of a finite-dimensional attractor is proven [23]. Furthermore, we apply DMD to reanalysis data [9]. Our method is able to detect the transition from a predominantly negative North Atlantic Oscillation (NAO) phase to a predominantly positive phase in the late 1960ies which was shown to be related to a change in forecast skill [8, 27, 25]. The reconstruction error also detects the regime change of the Southern Hemisphere atmospheric dynamics around 1970 from a regime with more intense baroclinicity to a regime of more zonal barotropic dynamics [4, 3, 5], which has been attributed to an increased CO$_2$ concentration.

The paper is organized as follows. In Section 2 we briefly present the method of dynamic mode decomposition and propose our diagnostic for the detection of transients using the reconstruction error. In Section 3.1 we then apply our method to detect transitions and regime changes in the Kuramoto-Sivashinsky equation. In Section 3.2 we apply our method to analyze the regime change of the Northern Hemisphere atmospheric circulation dynamics and the NAO in reanalysis data. In Section 3.3 we apply our method to analyze the regime change of the Southern Hemisphere atmospheric circulation dynamics in reanalysis data. We conclude with a discussion in Section 4.

2. Dynamic mode decomposition and Koopman modes

In the following we introduce the Koopman operator and the computationally cheap algorithm to approximate the Koopman operator and its eigenfunctions, the dynamical mode decomposition. Let us consider a dynamical system

\[ \dot{x} = f(x) \]

with \( x(0) = x_0 \) for \( x \in \mathbb{R}^d \). Provided there is a unique solution of this initial value problem, we can introduce the flow map \( \varphi_t \) and write \( x(t) = \varphi_t(x_0) \). Consider observables \( \psi(x) \). Observables are
propagated in time according to $\psi(\varphi_t(x))$ which we express as
\begin{equation}
K_t\psi = \psi(\varphi_t(x)),
\end{equation}
where the propagator $K$ is termed the Koopman operator. Applying the chain rule one can verify that continuously differentiable observables satisfy the following linear partial differential equation
\begin{equation}
\partial_t v(x,t) = L v
\end{equation}
with the generator $L = f(x) \cdot \nabla$. We formally solve this Cauchy problem and write $v(x,t) = (e^{Lt}\psi)(x) = \psi(\varphi_t(x))$, and identify
\begin{equation}
K_t = e^{Lt}.
\end{equation}
The notion of the Koopman operator can be extended to bounded (not necessarily continuously differentiable) observables for which the limit defining the generator
\begin{equation}
L \psi = \lim_{t \to 0} \frac{e^{Lt}\psi - \psi}{t}
\end{equation}
exists. We remark that this can be readily extended for stochastic differential equations. For details the reader is referred to [12, 17].

Let us now describe DMD and how the Koopman operator and its eigenfunctions can be approximated given a set of observations. We follow here the exposition provided in [24, 11]. We are given snapshots $X$
\begin{equation}
X = \begin{pmatrix} x_1 & x_2 & \cdots & x_m \end{pmatrix}
\end{equation}
with $x_k = x(t_k) \in \mathbb{R}^n$. Successive vectors $x_k$ have evolved from $x_{k-1}$ under the dynamics for some, not necessarily small time interval $\Delta t$, i.e. $x_k = K_{\Delta t}x_{k-1}$. We are further given snapshots $X'$
\begin{equation}
X' = \begin{pmatrix} x'_1 & x'_2 & \cdots & x'_m \end{pmatrix}
\end{equation}
with $x'_k = x(t_k + \delta t) \in \mathbb{R}^n$. The variables $x$ may denote the state variables, or any observable of them\footnote{DMD was originally introduced in the case when $x$ denotes the state variables.}. Successive vectors $x'_k$ have evolved from $x_k$ under the dynamics for a time $\delta t$, i.e. $x'_k = K_{\delta t}x_k$. The size of $\delta t$ determines the accuracy of reconstructing the dynamics, as can be seen from (4). In DMD the Koopman operator $K_{\delta t}$ is approximated by a least square fit from $X' = K_{\delta t}X$ as
\begin{equation}
K = X'X^\dagger,
\end{equation}
where $X^\dagger$ denotes the pseudo-inverse of $X$. The finite dimensional approximation of the Koopman operator (5) may suggest that it is tacitly assumed that the dynamics is linear. This is not the case, only the infinite dimensional dynamics (3) determining the Koopman operator (or rather its generator) is linear. Recall that the Koopman operator acts on functions $\psi(x)$; in the case when the observables are the actual state variables we have $\psi(x) = \text{id}(x)$. If the observables span a
sufficiently large space the linear least square fit\cite{5} is indeed able to capture the full nonlinear dynamics\cite{11,24}. We express K as

\[ K = X'\Sigma^{-1}U*, \]

where we used a low rank \( r \leq m \) singular value decomposition of \( X = U\Sigma V^* \) with the proper orthogonal decomposition (POD) modes \( U \in \mathbb{C}^{n \times r} \), \( \Sigma \in \mathbb{C}^{r \times r} \) and \( V \in \mathbb{C}^{m \times r} \) and \( U^*U = Id \) and \( V^*V = Id \). For computational efficiency one projects K onto the POD modes and considers

\[ \tilde{K} = U^*KU = U^*X'\Sigma^{-1}. \]

Performing an eigendecomposition of \( \tilde{K} \) with \( \tilde{K}W = W\Lambda \), eigenmodes of the approximation of the Koopman operator \( K_{\delta t} \) are expressed as

\[ \Phi = X'\Sigma^{-1}W\Lambda^{-1}, \]

satisfying \( K\Phi = \Phi\Lambda \). Note that eigenmodes of \( \tilde{K} \) are given by \( \tilde{\Phi} = UW \). Whereas the eigenmodes \( \tilde{\Phi} \) are orthonormal, this is not the case for \( \Phi \). Introducing \( \omega_j = \ln \lambda_j/\delta t \) the snapshots \( x_k = x(t_k) \) can now be approximated by the DMD-reconstructed field as

\[ x(t_{k+1}) \approx \sum_{j=1}^{r} \phi_j e^{\omega_j k\Delta t} b_j + c.c. = \Phi \exp(\Omega k\Delta t) b + c.c., \]

where \( b = \Phi^\dagger x(t_1) \) denotes the initial coefficients and \( \Omega \in \mathbb{R}^r \) has components \( \omega_j \), and c.c. denotes the complex conjugate.

In\cite{24} it was shown that DMD provides a good approximation of the Koopman operator and its spectral properties provided the data are sufficiently diverse – i.e. the sampling time \( \Delta t \) is sufficiently large to ensure sufficient diversity and a large range of \( X \) – and the observables are sufficiently rich in the sense that their span contains the eigenfunctions of the Koopman operator. It is pertinent to mention that it is a priori not possible to determine if given observables are sufficient to span the eigenfunctions of the Koopman operator.

We focus here only on reconstruction of the observations by the Koopman and not on forecasting. Hence the question whether the span of the observables is sufficiently large to contain all Koopman eigenmodes is not relevant here. A DMD reconstruction involves the reconstruction of the whole spatio-temporal evolution for a finite time window of \( m\Delta t \) with \( m \) snapshots (where the number of snapshots \( m \) is typically much smaller than the total number of observations which are available), and we do not employ the DMD approximation\cite{5} past the observations given in the time window \( m\Delta t \). We define the reconstruction error

\[ \mathcal{E}_{DMD}(t_k, r) = \sum_{l=0}^{m-1} \| x(t_k+l) - \Phi \exp(\Omega l\Delta t) b + c.c. \|, \]

with \( b = \Phi^\dagger x_k \). We are given data sets \( X \) and \( X' \) with \( M \gg m \) snapshots collected at intervals of length \( \Delta t \). We split these time series into windows of temporal length \( m\Delta t \) and reconstruct the field by means of DMD for each of the windows. Typically, the matrices \( X \) and \( X' \) are skinny and tall with the number of snapshot smaller than the dimension \( n \) of the snapshots \( x \). The reconstruction error is local in time and we reconstruct \( M/m \) time windows of temporal length \( m\Delta t \). If the
dynamics is in equilibrium at time $t_k$, evolving on an attractor with dimension $d_a \ll d$ we expect that the reconstruction error $E_{\text{DMD}}(t_k, r)$ is large for $r \leq r_a$ with $r_a \sim O(d_a)$, and then rapidly decreases for larger values of $r$. If the dynamics is, on the other hand, not in equilibrium at time $t_k$ and experiences the full phase space dimension $d$, the value of $r$ needed for good reconstruction may be larger than the the chosen $m$, based on previous knowledge of the equilibrium dynamics. More importantly, the fast attraction towards the attractor with rate $\lambda_{\text{relax}}$ may not be resolved by $\delta t$ if $\delta t \gg 1/\lambda_{\text{relax}}$, implying a bad reconstruction with large values of $E_{\text{DMD}}(t_k, r)$. The latter point we will see is crucial in identifying transitions.

3. Applications

We now explore how DMD reconstruction error can be used to detect transitions and regime changes. We start with artificially generated data from numerical simulations of a partial differential equation, before applying our method to confirm recent findings in regime changes and transitions in the atmospheric circulation of the northern and the southern hemisphere.

3.1. Detecting regime changes in the Kuramoto-Sivashinsky equation. We first consider artificially generated time series obtained from a numerical simulation of the Kuramoto-Sivashinsky equation

$$u_t + uu_x + \alpha u_{xx} + u_{xxxx} = 0.$$  

(8)

For fixed system length $L$ the Kuramoto-Sivashinsky equation becomes chaotic upon increasing the driving $\alpha$. The most unstable wave number is given through linearization around $u = 0$ as $k_{\text{max}} = \sqrt{\alpha/2}$ suggesting that the observed spatio-temporal patterns have around $(L/2\pi)\sqrt{\alpha/2}$ peaks. We choose a fixed domain length $L = 53.35$, and integrate the equation using a pseudo-spectral Crank-Nicolson scheme where the nonlinearity is treated with a second-order Adams-Bashforth scheme. We employ a discretization step of $dt = 0.01$ and use 128 spatial grid points.

Our first experiment involves transient dynamics from an initial condition of $u(x, 0) = u_0 \exp\left(-w(x - \frac{L}{2})^2\right)$ for 250,000 time units with $u_0 = 0.67$ and $w = 0.62$ for $\alpha = 2.53$ for which the dynamics is non-chaotic. The dynamics settles on a limit cycle with regular behaviour around 125,000 time units. We choose $m = 100$ snapshots to reconstruct the dynamics separated by $\Delta t = 2.5$ and a time interval of $\delta t = 2.5$. In Figure 1 we show the reconstruction error $E_{\text{DMD}}(t_k, r)$. It is clearly seen that during the transient dynamics the reconstruction error is large but drops off significantly when the dynamics has settled down on the limit cycle near $t = 125,000$. Note that the number of POD modes required for an accurate reconstruction is roughly 10 and is larger than the number of linearly unstable modes $\sqrt{\alpha L/2\pi} = 4$. The reason for this bad reconstruction is the fast relaxation towards the attractor from the initial condition which was chosen far form the attractor. We have checked that for finely sampled observations with $\delta t = \Delta t = 0.1$ one obtains very good reconstruction for reconstruction windows of 10 time units corresponding to $m = 100$; for the sampling times $\delta t = \Delta t = 2.5$ time units, which were used in the simulations depicted in Figure 1, one is not able to accurately reconstruct the observations past the 4 observed snapshots using $m = 6$, after which the reconstruction is dominated by the Koopman modes associated with the largest real part of the eigenvalues, leading to large reconstruction errors $E_{\text{DMD}}$. It is important to realize that the
transition needs to involve a sufficiently strong non-equilibrium character with fast attraction to be detectable with the DMD reconstruction error.

We further show the reconstruction error $E_{\text{DMD}}(t_k, r)$ for dynamics exhibiting a regime change from one chaotic attractor to another chaotic attractor, induced by a change of the driver $\alpha$. It is important to notice that the regime change needs to be sufficiently strong in the sense that the two attractors need to be sufficiently different to allow for a significant fast transition between the two attractors. We consider changes from $\alpha = 3.16$ to $\alpha = 3.79$ at $t = 250$ time units. We have assured that at time $t = 0$ the dynamics is on the attractor, by having employed a preceding integration for the long integration time of $10^6$ time units. We choose again $m = 100$ snapshots to reconstruct the dynamics separated by $\Delta t = 0.01$ and a time interval of $\delta t = 0.01$. It is seen that the number of POD modes required for accurate reconstruction is higher for the larger value of $\alpha$, consistent with the analytical results that the attractor dimension increases with $\alpha$ \cite{23}. However, the change in the attractor is not sufficient to allow for sufficiently fast transitory dynamics towards equilibrium in this case.

![Figure 1. Reconstruction error $E_{\text{DMD}}(t_k, r)$ for the Kuramoto-Sivashinsky equation with $\alpha = 2.53$ during transient dynamics from an initial condition off the attractor.](image)

3.2. Detecting the inter-decadal changes in the North Atlantic Oscillation. The North Atlantic Oscillation is a major source of low frequency variability in the Northern Hemisphere (defined as variability on time scales larger than 10 days) \cite{22}. The NAO involves changes of the locations of the storm tracks, separating air masses between the Arctic and the subtropical Atlantic, with major impact on heat and moisture transport. The oscillations are reflected in the NAO index which quantifies the difference of atmospheric pressure at sea level between the Icelandic Low and the Azores High. NAOs are coarsely distinguished in a positive and a negative phase where the former is associated with more zonal flow patterns over Europe and the latter is associated with a
higher frequency of atmospheric blocking events over the North Atlantic. The NAO has experienced significant changes in the past decades. In particular, the NAO has changed from a predominantly negative phase during the 1950-1970 to a predominantly positive phase \cite{8}. The regime transition has been linked to a change in forecast skill, with improved forecast skill in the positive phase after 1970 \cite{25}.

We shall use the DMD reconstruction error diagnostics to identify this change in NCEP/NCAR (National Centers for Environmental Prediction/National Center for Atmospheric Research) reanalysis data \cite{9}. We use their 6 hourly reanalysis data of the 500hPa geopotential height covering the temporal period 1948-2017 for the spatial region of the Northern Hemisphere in the region [30N–90N, 80W–40E] with a spatial resolution of 2.5° × 2.5°. We consider only anomalies with respect to the climatological mean without detrending. Figure 3 shows a snapshot of the geopotential height anomalies at July 5 1960 at noon.

The time intervals for the Koopman analysis are ∆t = 6t = 6hours. We choose as the time window over which DMD reconstruction is sought a synoptic time scale of 4 days, which corresponds to m = 16. We have also performed an analysis using m = 40, which corresponds to a characteristic time scale of atmospheric blocking events, with qualitatively similar results. The observations have dimension n = 1225. In Figure 3 an instance of a good reconstruction error with E_DMD is shown with E_DMD ≈ 88. The DMD reconstruction relies on the singular value decomposition. It is well known that for observations which are noise contaminated to some degree, only the first singular values and their associated left and right eigenvectors are reliable, and one should truncated the singular value decomposition. For additive measurement noise, \cite{6} provide a criterion for an optimal truncation. The criterion amounts to an optimal truncation at r = 6. Figure 4 shows the reconstruction error E_DMD for the whole period 1949-2017 for r ≤ 16. We observe an increased error for values of r
around the optimal truncation value $r = 6$ for the years around 1970. To quantify this we plot $N_{\text{DMD}}$, the moving average of the number of $r$-values with acceptable reconstruction accuracy with $\mathcal{E}_{\text{DMD}} \leq 400$ between $7 \leq r \leq 16$ (the average is performed over ten years). Note that large values of $N_{\text{DMD}}$ imply good reconstruction and that by construction $N_{\text{DMD}} \leq 16 - 7 + 1 = 10$. There is a clear dip in $N_{\text{DMD}}$ around 1970, suggesting transitory dynamics, consistent with the observed regime change associated with a decrease of blocking instances [16, 15]. Noticeable, the reconstruction error increases (i.e. $N_{\text{DMD}}$ decreases) continuously after 1990. This may be due to further hitherto unidentified transitory dynamics which occurs on a slow time scale.

3.3. Detecting the inter-decadal changes in the large-scale circulation of the Southern Hemisphere. As the Northern Hemisphere atmospheric dynamics the Southern Hemisphere atmospheric dynamics and its climate has experienced significant changes in the past decades. In particular, the frequency of blocking events has decreased significantly around the mid 1970ies and has given way to a more zonal flow regime [16, 15]. The regime change has been shown to be likely caused by anthropogenic CO$_2$ emissions [3, 5].

We use again reconstruction error diagnostics to detect this change in the NCEP/NCAR reanalysis data [9]. We use again the 6 hourly reanalysis data of the 500hPa geopotential height covering the temporal period 1948–2017 but consider now the spatial region of the full Southern Hemisphere. The observations have dimension $n = 5328$. As before, we consider only anomalies with respect to the climatological mean (no detrending has been performed). We provide in Figure 5 a snapshot of the geopotential height anomalies at July 5 1960 at noon.

The time intervals for the Koopman analysis are $\Delta t = \delta t = 6$hours. We choose again a reconstruction window of $m = 16$, corresponding to a characteristic time synoptic scale of 4 days. We found qualitatively similar results when extending the time window to 10 days, resolving the typical time scale for atmospheric blocking events. The optimal truncation criterion [8] yields again $r = 6$. 

Figure 3. Anomaly of the 500hPa geopotential height on July 5 1960 at noon in the Northern Hemisphere. Left: Reanalysis data. Right: DMD reconstruction for $r = 6$ initiated at July 1 1960 at noon. Figures were made using [18].
Figure 4. Diagnostics of the reconstruction error for the reanalysis data of the 500hPa geopotential height anomalies in the Northern Hemisphere. Left: Reconstruction error $\mathcal{E}_{\text{DMD}}(t_k, r)$. Right: Average number of instances of good reconstruction with reconstruction errors $\mathcal{E}_{\text{DMD}} \leq 400$ for $7 \leq r \leq 16$.

Figure 5. Anomaly of the 500hPa geopotential height on July 5 1960 at noon in the Southern Hemisphere. Left: Reanalysis data. Right: DMD reconstruction for $r = 6$ initiated at July 1 1960 at noon. Figures were made using [18].

Figure 5 shows an instance of a good reconstruction error $\mathcal{E}_{\text{DMD}} \approx 322$ for $r = 6$. The reconstruction error $\mathcal{E}_{\text{DMD}}$ for the whole period 1948–2017 is shown for $r \leq 16$ in Figure 6. We observe an increased error around the optimal reconstruction error $r = 6$ for the years around 1970. To quantify this we evaluate again the moving average $\mathcal{N}_{\text{DMD}}$ of the number of $r$-values with acceptable reconstruction accuracy with $\mathcal{E}_{\text{DMD}} \leq 400$ between $7 \leq r \leq 16$ (the average is performed over ten years). By construction $\mathcal{N}_{\text{DMD}} \leq 16 - 7 + 1 = 10$. There is a clear dip in $\mathcal{N}_{\text{DMD}}$ around
1970, suggesting transitory dynamics, consistent with the observed regime change associated with a decrease of blocking instances [16, 15]. Noticeably, the reconstruction error increases continuously after 1990. This may be due to further hitherto unidentified slow transitory dynamics.

Figure 6. Diagnostics of the reconstruction error for the reanalysis data of the 500hPa geopotential height anomalies in the Southern Hemisphere. Left: Reconstruction error $\varepsilon_{\text{DMD}}(t_k, r)$. Right: Average number of instances of good reconstruction with reconstruction errors $\varepsilon_{\text{DMD}} \leq 400$ for $7 \leq r \leq 16$.

4. Discussion

We proposed a data-driven method to detect eventual regime changes and transient dynamics in time series. Our method is based on the Koopman operator and determining its eigenmodes using dynamic mode decomposition. Our approach exploits the fact that transient non-equilibrium dynamics explores the full-dimensional phase space as opposed to equilibrium dynamics which is typically supported on a lower dimensional attractor. It further exploits the fact that for a given temporal sampling interval DMD may fail to reconstruct the dynamics during periods of fast relaxation towards an attractor. We use the reconstruction error between the observations and their DMD approximations as a diagnostic tool to analyze the dynamics and probe transient behaviour and regime changes. We have illustrated the effectiveness of our method in artificially prepared data from a chaotic partial differential equation as well as in reanalysis data of the Southern and Northern Hemisphere atmospheric climate data. Our method is cost-effective and is able to detect regime changes and transitory dynamics in both cases. The diagnostics we propose crucially depends on the transition evolving on a time scale faster than the resolution time scale $\delta t$ used to estimate the Koopman operator. If the transition time scale is of the same order as the equilibrium dynamics then the transition dynamics is not detectable, even using subsampling of the time series to increase the time step $\delta t$. 
We were concerned here with identifying periods of transient dynamics and regime changes. In future work it may be interesting to see whether DMD is able to identify precursors of transitions, and thereby is able to predict transitions. The choice of observables will then be of importance.

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