EDMD for expanding circle maps and their complex perturbations

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ABSTRACT. We show that spectral data of the Koopman operator arising from an analytic expanding circle map τ can be effectively calculated using an EDMD-type algorithm combining a collocation method of order m with a Galerkin method of order n. The main result is that if $m \geq \delta n$, where δ is an explicitly given positive number quantifying by how much τ expands concentric annuli containing the unit circle, then the method converges and approximates the spectrum of the Koopman operator, taken to be acting on a space of analytic hyperfunctions, exponentially fast in n. Additionally, these results extend to more general expansive maps on suitable annuli containing the unit circle.

1. Introduction

Identifying dynamically relevant signatures and effective degrees of freedom is among the most challenging and fruitful tasks in science in general. A specific method, termed dynamic mode decomposition (DMD), aims at combining the success of linear data analysis with dynamical systems theory. It exploits dynamical signatures which can be traced back to eigenmodes of an evolution operator defined on a suitable function space, thereby presenting a key example for data analysis inspired by abstract operator theory. While the term "dynamic mode decomposition" appears to have been coined in [30], it is hard to identify an exact single source for this approach. Related ideas have been used to reconstruct invariant measures of dynamical systems [12], and then considerably extended to estimate spectral properties of the Koopman operator from data [24]. In [35], the DMD algorithm was extended to cope with a broader range of observations. While there have been countless applications of DMD and its variants, here we restrict ourselves to a brief overview of a few of the major references, see [10, 36, 21, 16, 22, 9, 26] and references therein.

The main idea of dynamic mode decomposition follows concepts developed in the context of statistical data analysis and statistical physics. In particular, data-driven approaches to identify empirical modes with linear techniques can be traced back to [17], which has served as a seed for a wealth of linear decomposition techniques developed in the last decades. Beyond a plain data analysis aspect, the identification of relevant dynamical signatures adds to the theoretical understanding of motion. From a mathematical perspective, the role of phase space structures and, in particular, of the underlying function spaces have been pointed out in the context of theoretical physics, namely, as one of the main clues to understand the emergence of irreversibility in an otherwise time-invariant Hamiltonian setup [25], see also [28] for an illustration in an elementary setting. While these works provide some mathematical tools to rigorously underpin contemporary nonlinear data analysis techniques, identifying relevant dynamical signatures in general far-from-equilibrium processes remains a substantial challenge, and developing paradigms to identify effective degrees of freedom in general dynamical systems continues to be a very active area of research.

We will briefly outline the formal aspects of extended dynamic mode decomposition (EDMD) for a discrete dynamical system $z_{t+1} = \tau(z_t)$, see [35] for more explanations. Assuming that the dynamics is observed through a collection of N scalar functions $\{\psi_0, \dots, \psi_{N-1}\}$ and given a sequence of m points in phase space $z^{(0)}, \dots, z^{(m-1)}$, one constructs two $N \times N$ matrices

$$G_{k,l} = \frac{1}{m} \sum_{j=0}^{m-1} \psi_k \left(\tau \left(z^{(j)} \right) \right) \overline{\psi_l \left(z^{(j)} \right)}, \qquad (k, l = 0, \dots, N-1),$$

$$H_{k,l} = \frac{1}{m} \sum_{j=0}^{m-1} \psi_k \left(z^{(j)} \right) \overline{\psi_l \left(z^{(j)} \right)}, \qquad (k, l = 0, \dots, N-1),$$

and defines the matrix M as

$$M = GH^{-1} \tag{1}$$

(see also (21) in Section 2). This matrix provides an optimal finite-dimensional linear approximation to the original nonlinear system[1], and hence its eigendata are related to the time scales of the original dynamical system. It can be linked to the Koopman operator C_τ, the linear composition operator governing the underlying dynamics given by

$$C_\tau f = f \circ \tau \tag{2}$$

on some suitable function space. In particular, the EDMD method aims to establish convergence of the eigenvalues and eigenvectors of M to those of the Koopman operator in the limit of large number of observables, $N \to \infty$, and large number of nodes in phase space, $m \to \infty$.

Theoretical considerations of EDMD are often based on a Koopman operator defined on the space of square-integrable functions, which however raises fundamental technical issues. In the case of invertible measure-preserving dynamical systems, the Koopman operator defined on L^2 turns out to be unitary, which provides the necessary mathematical machinery for its rigorous study in terms of spectral measures, see for example [34, Chapter 1] and [13, Chapter 18] or [11, 23, 38] in the data-driven context. With the notable exception of the Hamiltonian setting, however, the assumption of invertibility appears to be very limiting, as in most applications a well-defined invertible global flow cannot be established. Even in cases where the Koopman operator is merely an isometry and can thus be decomposed into a unitary and a shift part by means of the Wold decomposition (see, for example, [27, Chapter 1.3]), a study focused solely on the unitary part may miss relevant dynamical features of the underlying dynamical system.

In the case of dissipative dynamics, one can still define the Koopman operator (2) on L^2, and the general spectral theory and properties of the trivial eigenvalue still provide essential information about ergodic and mixing properties of the system (see, for example, [34, Chapter 1]). However, in this setting the Koopman operator no longer enjoys nice spectral properties for this choice of function space. For a non-invertible discrete dynamical system preserving a mixing probability measure, the spectrum of the Koopman operator consists of the entire unit disk (see, for example, [19, Remark 4.4] or appeal to the Wold decomposition), and no non-trivial eigenvalues or eigenfunctions exist, precluding spectral convergence results or, in fact, any theoretical analysis which assumes the existence of eigenfunctions in L^2. Nevertheless, for various chaotic dynamical systems with enough regularity, EDMD as given above empirically still yields spectral data which correctly determines the correlation decay rates for sufficiently regular observables. This can indeed be rigorously understood by analysing the residual spectrum of the Koopman operator defined on L^2. For a value $\lambda \in \mathbb{C}$ in the residual spectrum, the range of $\lambda - C_\tau$ is not the entire Hilbert space, whereas its kernel is trivial as there are no eigenvalues in the residual spectrum. By enriching L^2 with "generalised functions" one can make $\lambda - C_\tau$ surjective, while for some selected values $\lambda \in \mathbb{C}$ the kernel of $\lambda - C_\tau$ becomes

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[1]To be precise, the matrix $M = GH^{-1}$ provides a least-squares solution $\arg\min_M \|MX - Y\|_2^2$ for $X = [\psi(z_0), \dots, \psi(z_{m-1})]$ and $Y = [\psi(\tau(z_0)), \dots, \psi(\tau(z_{m-1}))]$, with $\psi(z) = (\psi_0(z), \dots, \psi_{N-1}(z))^T$. This can be seen by noting that such solution is given by $M = YX^+ = (YX^H)(XX^H)^{-1} = GH^{-1}$ whenever XX^H is invertible, with X^+ and X^H denoting the Moore-Penrose pseudoinverse and conjugate transpose of X, respectively.

nontrivial. In the particularly nice setting of hyperbolic analytic systems one observes that the residual spectrum on this larger space vanishes in exchange for the occurrence of a point spectrum, while the Koopman operator becomes a compact operator, see the discussion in [32]. The corresponding eigenvalues are precisely the decay rates observed in the dynamical system, while the corresponding "physical" eigenfunctions are objects which are not in L^2 (see [14] for a striking visual demonstration), and EDMD detects this subtle structure. Again we want to stress that any analysis of the Koopman operator on L^2 which assumes the existence of nontrivial eigenfunctions misses this essential point and is problematic from a mathematical and physical perspective.

The results in non-equilibrium statistical mechanics alluded to earlier on suggest that the Koopman operator is best understood on physically relevant function spaces which guarantee compactness or, more generally, quasi-compactness of the operator and yield well-defined relaxation rates [33]. Using these ideas, we will clarify in Section 2 why EDMD is such a successful tool even in the case of chaotic dynamical systems, restricting our attention to the simplest such systems, one-dimensional expanding maps. As this method produces discrete spectra, it is well-suited to approximate compact Koopman operators. In fact, as our main result (Theorem 2.11) will show, EDMD implicitly treats compact Koopman operators on a suitably enriched function space which contains highly singular objects. Counterintuitively, it is precisely the presence of these highly singular objects that is responsible for the physical decay rates detected via EDMD. The main novelty of our results is a simple constraint on the two key parameters in EDMD, the number of observables and the number of nodes (that is, the size of the data set), which is sufficient to guarantee exponential convergence to the exact spectrum of a compact Koopman operator on the appropriate Hilbert space.

As the general statement of our main results requires some background explained in Section 2, we want to highlight its practical importance by presenting the following simple corollary of one of our results (Theorem 2.12), which applies to expanding maps on the circle. Writing $\tau'_{\min} = \min_{z \in \mathbb{T}} |\tau'(z)|$ (and $\tau'_{\max} = \max_{z \in \mathbb{T}} |\tau'(z)|$), we say $\tau \colon \mathbb{T} \to \mathbb{T}$ is an expanding circle map on $\mathbb{T} = \{z \in \mathbb{C} \colon |z| = 1\}$ if $\tau'_{\min} > 1$.

1.1. THEOREM. *Let τ be an analytic expanding circle map, C_τ the associated Koopman operator given in (2), and $\tau'_{\min}, \tau'_{\max}$ the minimal and maximal derivatives of τ on $\mathbb{T}$. Then the following holds.*

(1) *There exists a Hilbert space $\mathcal{H}$ such that C_τ is a well-defined compact operator from $\mathcal{H}$ to $\mathcal{H}$. In particular, its spectrum $\mathrm{spec}(C_\tau)$ is either a finite set or a sequence converging to zero together with zero itself and each non-zero spectral point is an eigenvalue of finite algebraic multiplicity.*

(2) *For $m, n \in \mathbb{N}$ and $\alpha \in \mathbb{R}$ let $\{\psi_l\}_{-(n-1) \leq l \leq (n-1)}$ with $\psi_l(z) = z^l$ be the set of observables, $\{z^{(j)}\}_{0 \leq j \leq m-1}$ with $z^{(j)} = e^{2\pi i j/m + i\alpha}$ be the set of phase space points and $M = M_n$ the $(2n-1) \times (2n-1)$ matrix given in (1). If for every $n \in \mathbb{N}$, the number of phase space points $m = m(n) \in \mathbb{N}$ is chosen such that*

$$m \geq (\tau'_{\min} + \tau'_{\max})n, \tag{3}$$

then the following hold:

(a) *Any convergent sequence $(\lambda_n)_{n \in \mathbb{N}}$ with $\lambda_n \in \mathrm{spec}(M_n)$ converges to a spectral point of C_τ.*

(b) *Conversely, for any $\lambda \in \mathrm{spec}(C_\tau)$ there is a sequence $(\lambda_n)_{n \in \mathbb{N}}$ with $\lambda_n \in \mathrm{spec}(M_n)$ such that $\lambda_n \to \lambda$ as $n \to \infty$. Moreover,*

$$|\lambda - \lambda_n| = O(e^{-an}) \quad \text{as } n \to \infty,$$

for some $a > 0$.

(c) *Suppose $\lambda \in \mathrm{spec}(C_\tau)$ is non-zero and $(\lambda_n)_{n \in \mathbb{N}}$ denotes the approximating sequence of eigenvalues of M_n given in (b). If $\xi_n = (\xi_{n,-n+1}, \ldots, \xi_{n,0}, \ldots, \xi_{n,n-1})^T \in \mathbb{C}^{2n-1}$ is a generalised eigenvector of the transpose M_n^T of M_n, then setting*

$$h_n(z) = C \sum_{|k| < n} \xi_{n,k} z^k \quad (z \in \mathbb{C}),$$

where C is a constant chosen so that $\|h_n\|_{\mathcal{H}} = 1$, yields a sequence of Laurent polynomials $(h_n)_{n \in \mathbb{N}}$ with

$$\|\mathcal{P}h_n - h_n\|_{\mathcal{H}} = O(e^{-bn}) \quad \text{as } n \to \infty,$$

where $\mathcal{P}$ is the spectral projection associated to the eigenvalue λ of C_τ and some $b > 0$.

In short, for analytic expanding maps on the circle, this theorem guarantees exponential convergence of eigenvalues and eigenvectors of the EDMD matrix in (1) constructed using $2n-1$ Laurent polynomials as observables and m equidistant points in the phase space, to those of the associated Koopman operator, if m is a linear function of n satisfying (3). In the setting of non-invertible maps, it is more common (in the dynamical systems community) to approximate the adjoint of the Koopman operator, known as the Perron-Frobenius or transfer operator, as it can be considered on ordinary function spaces such as spaces of functions of bounded variation, Sobolev spaces, or spaces of analytic functions, see [18, 12, 20, 2] for a small snapshot of a large body of works or [15, 8, 37] for some more recent contributions. Whilst working with the transfer operator requires knowledge of the local inverse branches of τ and their derivatives, EDMD only requires knowledge of the map itself, and can be leveraged as an alternative way to approximate the spectrum of either of the operators.

In order to benchmark our results and the sharpness of our bound in (3) we will resort in Section 3 to a class of analytic maps where full spectral information is accessible [31, 7], and which has been used recently to clarify some convergence properties of EDMD [32]. Within this class of chaotic systems we demonstrate that the rigorous convergence estimates are surprisingly sharp (see Figure 2 in Section 3), and that EDMD correctly identifies the spectrum of the compact Koopman operator considered on a space of generalised functions.

2. Koopman operator for holomorphically expansive maps on spaces of generalised functions

For $r \in (0, 1)$ let $A_r = \{z \in \mathbb{C} : r < |z| < r^{-1}\}$ denote an annulus containing the unit circle $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$. Let τ be an *analytic expanding circle map*, that is, $\tau : \mathbb{T} \to \mathbb{T}$ has an analytic extension to some annulus A_r with $r \in (0, 1)$ and $\min_{z \in \mathbb{T}} |\tau'(z)| > 1$. We start by showing that the expansivity assumption on the unit circle entails a type of expansivity in the complex plane in the following sense.

2.1. LEMMA. *Let τ be an analytic expanding circle map. Then there is $\tilde{r} \in (0, 1)$, such that the following holds:*

(1) *τ is holomorphic on $A_{\tilde{r}}$.*
(2) *For every $r_1 \in (\tilde{r}, 1)$ there are radii r_2 and r_3 with $0 < r_3 < r_2 < r_1 < 1$ with the following property:*
   if τ is orientation-preserving then

$$\begin{aligned} r_3 &< |\tau(z)| < r_2 \quad \text{for any } z \in \mathbb{C} \text{ with } |z| = r_1, \\ r_2^{-1} &< |\tau(z)| < r_3^{-1} \quad \text{for any } z \in \mathbb{C} \text{ with } |z| = r_1^{-1}; \end{aligned} \tag{4}$$

   while if τ is orientation-reversing then

$$\begin{aligned} r_2^{-1} &< |\tau(z)| < r_3^{-1} \quad \text{for any } z \in \mathbb{C} \text{ with } |z| = r_1, \\ r_3 &< |\tau(z)| < r_2 \quad \text{for any } z \in \mathbb{C} \text{ with } |z| = r_1^{-1}. \end{aligned} \tag{5}$$

Moreover, the above radii r_1, r_2 and r_3 can be chosen so that

$$\lim_{r_1 \uparrow 1} \frac{\log(r_2)}{\log(r_1)} = \tau'_{\min} \quad \text{and} \quad \lim_{r_1 \uparrow 1} \frac{\log(r_3)}{\log(r_1)} = \tau'_{\max},$$

where $\tau'_{\min} = \min_{z \in \mathbb{T}} |\tau'(z)|$ and $\tau'_{\max} = \max_{z \in \mathbb{T}} |\tau'(z)|$.

PROOF. Note that the unit circle $\mathbb{T}$ is an invariant set for the map τ. Then setting $\tau(\exp(it)) = \exp(if(t))$ for $t \in \mathbb{R}$ defines an analytic map $f : \mathbb{R} \to \mathbb{R}$ with

$$f'(t) = \frac{\tau'(e^{it})}{\tau(e^{it})}e^{it},$$

see, for example, [4, Lemma 5.1]. We shall only consider the case of orientation-preserving τ here, which implies $f'(t) > 0$ for $t \in \mathbb{R}$. The orientation-reversing case is similar.

For later use, we note that setting $f'_{\min} = \min_{t \in \mathbb{R}} f'(t)$ and $f'_{\max} = \max_{t \in \mathbb{R}} f'(t)$ we have $f'_{\min} = \tau'_{\min}$ and $f'_{\max} = \tau'_{\max}$.

For $z = \exp(it)$ and $w = r \exp(it)$ with τ analytic and non-zero on the line-segment $[z, w]$, we have

$$\log \tau(z) - \log \tau(w) = \int_w^z \frac{\tau'(\zeta)}{\tau(\zeta)}d\zeta$$

so that

$$\log |\tau(e^{it})| - \log |\tau(re^{it})| = \operatorname{Re} \int_r^1 \frac{\tau'(\rho e^{it})}{\tau(\rho e^{it})}e^{it}d\rho.$$

Since $|\tau(\exp(it))| = 1$ we have

$$-\log |\tau(re^{it})| = \int_r^1 f'(t)d\rho + \operatorname{Re} \int_r^1 \left(\frac{\tau'(\rho e^{it})}{\tau(\rho e^{it})}e^{it} - f'(t) \right) d\rho \tag{6}$$
$$= (1 - r)f'(t) + R(r, t).$$

Since the integrand of the second integral is analytic and vanishes at the upper limit, there is a constant $C > 0$, such that for all real r sufficiently close to 1 we have

$$\sup_{t \in \mathbb{R}} |R(r, t)| \le C(1 - r)^2. \tag{7}$$

Now fix a function $\epsilon : (0, \infty) \to (0, \infty)$ with

$$0 < \epsilon(r) < f'_{\min} - 1 \quad (\forall r \in (0, 1)) \tag{8}$$

such that

$$\lim_{r \to 1} \epsilon(r) = 0 \quad \text{and} \quad \lim_{r \to 1} \frac{\epsilon(r)}{|1 - r|} = \infty. \tag{9}$$

To be definite, we could choose

$$\epsilon(r) = \frac{1}{2}(f'_{\min} - 1)\sqrt{|1 - r|}.$$

Using (7), the fact that $\lim_{r \to 1} \log(r)/(r - 1) = 1$ and the properties (8) and (9) of ϵ we see that there is $\tilde{r} \in (0, 1)$ with τ analytic on $A_{\tilde{r}}$ such that

$$\left| \frac{R(r, t)}{1 - r} \right| < \epsilon(r) \quad (\forall r \in (\tilde{r}, 1) \cup (1, \tilde{r}^{-1})) \tag{10}$$

and

$$f'_{\min} - \epsilon(r) > \frac{-\log(r)}{1 - r} \quad (\forall r \in (\tilde{r}, 1)). \tag{11}$$

For $r \in (\tilde{r}, 1)$ we now define radii

$$r_2(r) = \exp(-(1 - r)(f'_{\min} - \epsilon(r))),$$

$$r_3(r) = \exp(-(r^{-1} - 1)(f'_{\max} + \epsilon(r))).$$

We shall now show that these radii have the desired properties, that is, for every $r \in (\tilde{r}, 1)$ and every $t \in \mathbb{R}$ we have

$$r_3(r) < r_2(r) < r, \tag{12}$$

$$r_3(r) < |\tau(re^{it})| < r_2(r), \tag{13}$$

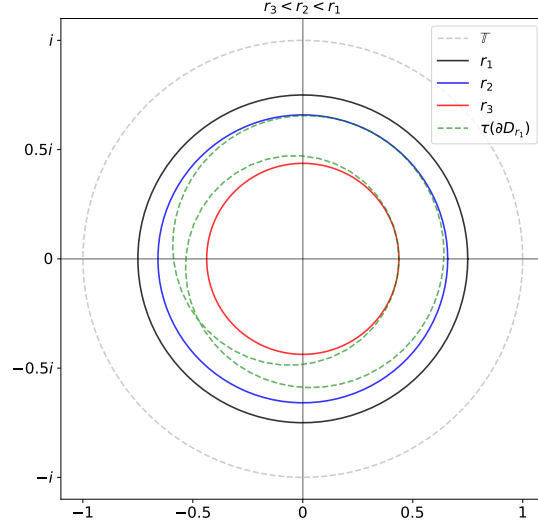$$(r_2(r))^{-1} < |\tau(r^{-1}e^{it})| < (r_3(r))^{-1}. \tag{14}$$

FIGURE 1. Illustration of radii $r_3 < r_2 < r_1$ for a holomorphically expansive τ satisfying (15).

We start by observing that (12) follows from (11) and the fact that $1 - r < r^{-1} - 1$ for $r \in (0, 1)$. Next note that (10) implies that for $r \in (\tilde{r}, 1)$ we have

$$(f'_{\min} - \epsilon(r)) < f'(t) + \frac{R(r, t)}{1 - r} < \frac{r^{-1} - 1}{1 - r}(f'_{\max} + \epsilon(r))$$

and

$$\frac{1 - r}{r^{-1} - 1}(f'_{\min} - \epsilon(r)) < f'(t) - \frac{R(r^{-1}, t)}{r^{-1} - 1} < (f'_{\max} + \epsilon(r))$$

which together with (6) imply (13) and (14).

Finally, using the definition of the radii r_2 and r_3 it is not difficult to see that

$$\lim_{r \uparrow 1} \frac{\log(r_2(r))}{\log(r)} = f'_{\min} \text{ and } \lim_{r \uparrow 1} \frac{\log(r_3(r))}{\log(r)} = f'_{\max},$$

which finishes the proof. □

It turns out that our convergence results hold for a larger class of maps defined below, which do not need to preserve the unit circle.

2.2. DEFINITION. Given radii $0 < r_3 < r_2 < r_1 < 1$ we say that $\tau : A_{r_1} \to \mathbb{C}$ is *holomorphically (r_2, r_3)-expansive on A_{r_1}* (or *holomorphically expansive on A_{r_1}, for short*) if τ is holomorphic on the closure of A_{r_1} and either

$$\begin{aligned} r_3 \ &< |\tau(z)| < r_2 \quad \text{for any } z \in \mathbb{C} \text{ with } |z| = r_1, \\ r_2^{-1} \ &< |\tau(z)| < r_3^{-1} \quad \text{for any } z \in \mathbb{C} \text{ with } |z| = r_1^{-1}; \end{aligned} \tag{15}$$

or

$$\begin{aligned} r_2^{-1} \ &< |\tau(z)| < r_3^{-1} \quad \text{for any } z \in \mathbb{C} \text{ with } |z| = r_1, \\ r_3 \ &< |\tau(z)| < r_2 \quad \text{for any } z \in \mathbb{C} \text{ with } |z| = r_1^{-1}. \end{aligned} \tag{16}$$

hold.

For an illustration of the role played by the radii r_1, r_2 and r_3 see Figure 1.

2.3. REMARK.

(1) Note that in order for a τ which is holomorphic on the closure of an annulus A_{r_1} to be holomorphically expansive on A_{r_1} it suffices that

either
$$\sup_{t\in\mathbb{R}}|\tau(r_1 e^{it})| < r_1 \text{ and } r_1^{-1} < \inf_{t\in\mathbb{R}}|\tau(r_1^{-1}e^{it})|$$

or
$$\sup_{t\in\mathbb{R}}|\tau(r_1^{-1}e^{it})| < r_1 \text{ and } r_1^{-1} < \inf_{t\in\mathbb{R}}|\tau(r_1 e^{it})|\,.$$

(2) By Lemma 2.1 every analytic expanding circle map is holomorphically expansive on any A_r with r sufficiently close to 1.

Our next task will be to define a class of Hilbert spaces on which the Koopman operator of a holomorphically expansive map has good spectral properties. We start by recalling the definition of the Hardy-Hilbert space $H^2(A_r)$ with $r \in (0,1)$ which consists of those functions f holomorphic on the annulus A_r for which

$$\sup_{\rho\in(r,1]}\left(\frac{1}{2\pi}\int_0^{2\pi}|f(\rho e^{it})|^2\,dt + \frac{1}{2\pi}\int_0^{2\pi}|f(\rho^{-1}e^{it})|^2\,dt\right) < \infty\,.$$

It turns out that $H^2(A_r)$ is a Hilbert space with scalar product

$$(f,g)_{H^2(A_r)} = \frac{1}{2\pi}\int_0^{2\pi} f^*(re^{it})\overline{g^*(re^{it})}\,dt + \frac{1}{2\pi}\int_0^{2\pi} f^*(r^{-1}e^{it})\overline{g^*(r^{-1}e^{it})}\,dt\,,$$

where f^* and g^* denote the respective non-tangential boundary values of f and g. More details on this construction can be found in [7] or [29]. For later use we note that $(e_n)_{n\in\mathbb{Z}}$ with

$$e_n(z) = \frac{z^n}{\sqrt{r^{2n}+r^{-2n}}} \quad (n\in\mathbb{Z}) \tag{17}$$

is an orthonormal basis for $H^2(A_r)$. We shall use this space later on to control the quadrature error inherent in EDMD.

The space on which we shall study the Koopman operator is denoted by $H^2(A_r^c)$ and is constructed as follows. Let $L^2(\mathbb{T})$ denote the Hilbert space of square-integrable functions on the unit circle. Given $f \in L^2(\mathbb{T})$ we write

$$c_n(f) = \frac{1}{2\pi}\int_0^{2\pi} f(e^{it})e^{-int}\,dt \quad (n\in\mathbb{Z})$$

for the Fourier coefficients of f.

Let $r \in (0,1)$ and let L denote the set of all finite linear combinations of positive and negative powers of z, that is, L is the set of Laurent polynomials in z. We construct a norm $\|\cdot\|_{H^2(A_r^c)}$ on L as follows

$$\|f\|_{H^2(A_r^c)} = \sqrt{\sum_{n\in\mathbb{Z}}|c_n(f)|^2 r^{2|n|}}\,,$$

and define $H^2(A_r^c)$ to be the completion of L with respect to this norm. It turns out that $H^2(A_r^c)$ is a Hilbert space with scalar product

$$(f,g)_{H^2(A_r^c)} = \sum_{n\in\mathbb{Z}} c_n(f)\overline{c_n(g)}r^{2|n|}\,,$$

and orthonormal basis $(e_n^c)_{n\in\mathbb{Z}}$ where

$$e_n^c(z) = r^{-|n|}z^n \quad (n\in\mathbb{Z})\,. \tag{18}$$

The space $H^2(A_r^c)$ is quite large. It contains $L^2(\mathbb{T})$, but also all distributions, and other highly singular objects, such as hyperfunctions. The reason for the notation, which looks peculiar at first sight, stems from the fact that $H^2(A_r^c)$ can be identified with the Hardy-Hilbert space of functions holomorphic on the complement A_r^c of A_r in the Riemann sphere $\hat{\mathbb{C}}$, see, for example, [7].

We shall now show that the Koopman or composition operator $C_\tau\colon f \mapsto f\circ\tau$ is a well-defined compact operator on $H^2(A_r^c)$. We start with the following crucial lemma.

2.4. LEMMA. *Let τ be holomorphically (r_2, r_3)-expansive on A_{r_1} and let $r \in (r_2, r_1)$. Then the following holds:*

$$C_\tau e_k^c \in H^2(A_r^c) \quad (k \in \mathbb{Z}),$$

$$\left| (C_\tau e_k^c, e_l^c)_{H^2(A_r^c)} \right| \le \left(\frac{r_2}{r} \right)^{|k|} \left(\frac{r}{r_1} \right)^{|l|} \quad (k, l \in \mathbb{Z}),$$

where $(e_n^c)_{n \in \mathbb{Z}}$ is the orthonormal basis for $H^2(A_r^c)$ given in (18).

PROOF. We start with a simple observation. For $\rho > 0$ let ∂D_ρ denote the positively oriented boundary of the disk $D_\rho = \{ z \in \mathbb{C} : |z| < \rho \}$. For any $\rho \in [r_1, r_1^{-1}]$ we have

$$c_l(C_\tau e_k^c) = \frac{r^{-|k|}}{2\pi i} \int_{\partial D_\rho} \tau(z)^k z^{-(l+1)} \, dz \quad (k, l \in \mathbb{Z}). \tag{19}$$

This follows by rewriting the definition of the l-th Fourier coefficient c_l as a contour integral and then using the fact that τ is holomorphic on the closure of A_{r_1} to shift the contour. We claim that the above equation implies

$$r^{|l|} c_l(C_\tau e_k^c) \le \left(\frac{r_2}{r} \right)^{|k|} \left(\frac{r}{r_1} \right)^{|l|} \quad (k, l \in \mathbb{Z}). \tag{20}$$

The proof of the inequality above splits into two cases depending on whether τ satisfies (15) or (16). We shall only consider τ satisfying (16) here, the other case can be treated similarly.

To start with suppose that $k \ge 0$. Since (16) holds, we know that for all z with $|z| = r_1^{-1}$ we have $|\tau(z)| \le r_2$, and so, since $k \ge 0$ we have $|\tau(z)|^k \le r_2^k$ for any z with $|z| = r_1^{-1}$. Using (19) we have

$$r^{|l|} c_l(C_\tau e_k^c) \le \frac{r^{|l|-k}}{2\pi} \int_{\partial D_{r_1^{-1}}} |\tau(z)|^k \, |z|^{-(l+1)} \, |dz| \le r^{|l|-k} r_2^k r_1^l \le \left(\frac{r_2}{r} \right)^k \left(\frac{r}{r_1} \right)^{|l|},$$

since $r_1^l \le r_1^{-|l|}$ for all $l \in \mathbb{Z}$.

Suppose now that $k < 0$. By (16) we know that for all z with $|z| = r_1$ we have $|\tau(z)| \ge r_2^{-1}$, and so, since $k < 0$ we have $|\tau(z)|^k \le r_2^{-k}$ for any z with $|z| = r_1$. Using (19) we have

$$r^{|l|} c_l(C_\tau e_k^c) \le \frac{r^{|l|+k}}{2\pi} \int_{\partial D_{r_1}} |\tau(z)|^k \, |z|^{-(l+1)} \, |dz| \le r^{|l|+k} r_2^{-k} r_1^{-l} \le \left(\frac{r_2}{r} \right)^{-k} \left(\frac{r}{r_1} \right)^{|l|},$$

since $r_1^{-l} \le r_1^{-|l|}$ for all $l \in \mathbb{Z}$. This finishes the proof of (20). The first assertion of the lemma now follows since, using (20) we have

$$\| C_\tau e_k^c \|_{H^2(A_r^c)}^2 = \sum_{l \in \mathbb{Z}} r^{2|l|} |c_l(C_\tau e_k^c)|^2 < \infty.$$

The remaining assertion also follows from (20), since $(C_\tau e_k^c, e_l^c)_{H^2(A_r^c)} = r^{|l|} c_l(C_\tau e_k^c)$.   □

An immediate consequence of the previous lemma is that the Koopman operator C_τ is Hilbert-Schmidt on $H^2(A_r^c)$.

2.5. COROLLARY. *Let τ be holomorphically (r_2, r_3)-expansive on A_{r_1} and let $r \in (r_2, r_1)$. Then C_τ is a Hilbert-Schmidt operator from $H^2(A_r^c)$ into itself with Hilbert-Schmidt norm bounded by*

$$\| C_\tau \|_{S^2(H^2(A_r^c))} = \sqrt{ \sum_{k, l \in \mathbb{Z}} \left| (C_\tau e_k^c, e_l^c) \right|^2 } \le \sqrt{ \frac{(r^2 + r_2^2)(r_1^2 + r^2)}{(r^2 - r_2^2)(r_1^2 - r^2)} }.$$

Since C_τ is compact, its spectrum is a finite set or a sequence converging to zero together with zero itself, and every non-zero spectral point is an eigenvalue of finite algebraic multiplicity. Next we shall show that spectral data of C_τ on $H^2(A_r^c)$ is effectively approximated by spectral data of matrices $M_{\tau;m,n}$ constructed as follows. Let a family of complex-valued functions be defined by

$$f_{\tau;k,l}(z) = \tau(z)^k z^{-l} \quad (k, l \in \mathbb{Z})$$

and, for $m \in \mathbb{N}$, let L_m denote the following continuous functional on $H^2(A_r)$

$$L_m(f) = \frac{1}{m} \sum_{l=0}^{m-1} f(\exp(\frac{2\pi i l}{m} + i\alpha)) \quad (f \in H^2(A_r)),$$

where $m \in \mathbb{N}$ and $\alpha \in \mathbb{R}$. As we shall see later L_m provides a quadrature rule for functions in $H^2(A_r)$ converging to the functional

$$L(f) = \frac{1}{2\pi} \int_0^{2\pi} f(\exp(it)) \, dt \quad (f \in H^2(A_r))$$

at exponential speed in the strong dual topology of $H^2(A_r)$. For $m, n \in \mathbb{N}$ define the $(2n-1) \times (2n-1)$ matrix $M_{\tau;m,n}$ by

$$M_{\tau;m,n} = (L_m(f_{\tau;k,l})_{k,l}) \quad (k, l \in \{-n+1, \ldots, n-1\}). \tag{21}$$

As we shall see the above two-parameter family of matrices yield effective spectral approximants for C_τ, where the parameter n describes the order of truncation of a Galerkin-type approximation, while the parameter m describes the order of truncation in a collocation-type method. Numerical experiments suggest that in order to achieve convergence m has to be chosen at least twice as large as n in order to achieve convergence. In the following we shall state and prove a more precise version of this observation.

First recall that by Corollary 2.5 we know that C_τ is Hilbert-Schmidt on $H^2(A_r^c)$. It turns out that C_τ can be approximated at exponential speed in Hilbert-Schmidt norm by the finite-rank Galerkin approximants $P_n C_\tau P_n$, where for $n \in \mathbb{N}$ the operator $P_n \colon H^2(A_r^c) \to H^2(A_r^c)$ is the orthogonal projection given by

$$P_n f = \sum_{|k|<n} (f, e_k^c)_{H^2(A_r^c)} e_k^c,$$

as we shall see now.

2.6. LEMMA. *Let τ be holomorphically (r_2, r_3)-expansive on A_{r_1} and let $r \in (r_2, r_1)$. Then there is a constant K_1 depending on r, r_1 and r_2 only, such that*

$$\|C_\tau - P_n C_\tau P_n\|_{S^2(H^2(A_r^c))} \le K_1 \rho^n \quad (n \in \mathbb{N}),$$

where $\rho = \max\left\{\frac{r_2}{r}, \frac{r}{r_1}\right\}$.

PROOF. Writing $c_{k,l} = (C_\tau e_k^c, e_l^c)_{H^2(A_r^c)}$ for $k, l \in \mathbb{Z}$ we have

$$\|C_\tau - P_n C_\tau P_n\|_{S^2(H^2(A_r^c))}^2 = \sum_{\substack{|k|\ge n \\ |l|<n}} |c_{k,l}|^2 + \sum_{\substack{|k|<n \\ |l|\ge n}} |c_{k,l}|^2 + \sum_{\substack{|k|\ge n \\ |l|\ge n}} |c_{k,l}|^2 \, .$$

Using Lemma 2.4 the first sum can be bounded by

$$\sum_{\substack{|k|\ge n \\ |l|<n}} |c_{k,l}|^2 \le \sum_{\substack{|k|\ge n \\ |l|<n}} \left(\frac{r_2}{r}\right)^{2|k|} \left(\frac{r}{r_1}\right)^{2|l|} \le 2\frac{r^2(r_1^2 + r^2)}{(r^2 - r_2^2)(r_1^2 - r^2)} \left(\frac{r_2}{r}\right)^{2n},$$

while the second sum can be bounded by

$$\sum_{\substack{|k|<n \\ |l|\ge n}} |c_{k,l}|^2 \le \sum_{\substack{|k|<n \\ |l|\ge n}} \left(\frac{r_2}{r}\right)^{2|k|} \left(\frac{r}{r_1}\right)^{2|l|} \le 2\frac{r_1^2(r^2 + r_2^2)}{(r_1^2 - r^2)(r^2 - r_2^2)} \left(\frac{r}{r_1}\right)^{2n},$$

and the third sum by

$$\sum_{\substack{|k|\ge n \\ |l|\ge n}} |c_{k,l}|^2 \le \sum_{\substack{|k|\ge n \\ |l|\ge n}} \left(\frac{r_2}{r}\right)^{2|k|} \left(\frac{r}{r_1}\right)^{2|l|} \le 4\frac{(r^2 + r_2^2)(r_1^2 + r^2)}{(r^2 - r_2^2)(r_1^2 - r^2)} \left(\frac{r_2}{r}\right)^{2n} \left(\frac{r}{r_1}\right)^{2n},$$

from which the assertion follows. □

2.7. REMARK. From Corollary 2.5 we know that C_τ is Hilbert-Schmidt. The lemma above implies that C_τ enjoys an even stronger property, namely, it is of exponential class (see [3]), that is, its sequence of singular values (and hence its sequence of eigenvalues) is bounded from above by a decreasing exponential, in common with other naturally occurring evolution operators associated with holomorphic data considered on spaces of holomorphic functions (see, for example, [4, 5, 6]).

Using the definition of $H^2(A_r^c)$ the matrix elements of C_τ on $H^2(A_r^c)$ can be written as integrals over the unit circle as follows

$$(C_\tau e_k^c, e_l^c)_{H^2(A_r^c)} = \frac{r^{|l|-|k|}}{2\pi} \int_0^{2\pi} \tau(\exp(it))^k \exp(-ilt)\, dt = r^{|l|-|k|} L(f_{\tau;k.l}) \quad (k, l \in \mathbb{Z})\,.$$

For computational purposes the integration over the unit circle given by the functional L on $H^2(A_r)$ is replaced by the numerical quadrature functionals L_m on $H^2(A_r)$ introduced earlier

$$L_m(f) = \frac{1}{m} \sum_{l=0}^{m-1} f(\exp(\frac{2\pi i l}{m} + i\alpha)) \quad (f \in H^2(A_r))\,,$$

where $m \in \mathbb{N}$ and $\alpha \in \mathbb{R}$. We shall now show that L_m converges to L at exponential speed in the strong dual topology of $H^2(A_r)$.

2.8. LEMMA. Let $\rho \in (0,1)$. Then for any $m \in \mathbb{N}$ the m-th order quadrature error for functions $f \in H^2(A_\rho)$ is bounded by

$$|L(f) - L_m(f)| \le \frac{\|f\|_{H^2(A_\rho)}}{\sqrt{1-\rho^2}} \rho^m\,.$$

PROOF. Recall that

$$e_k(z) = \frac{z^k}{\sqrt{\rho^{2k} + \rho^{-2k}}} \quad (k \in \mathbb{Z}, z \in A_\rho)$$

is an orthonormal basis in $H^2(A_\rho)$, so

$$f(z) = \sum_{k \in \mathbb{Z}} \frac{(f, e_k)_{H^2(A_\rho)}}{\sqrt{\rho^{2k} + \rho^{-2k}}} z^k \quad (f \in H^2(A_\rho), z \in A_\rho)\,.$$

Thus for any $f \in H^2(A_\rho)$ we have

$$L(f) = \sum_{k \in \mathbb{Z}} \frac{(f, e_k)_{H^2(A_\rho)}}{\sqrt{\rho^{2k} + \rho^{-2k}}} \frac{1}{2\pi} \int_0^{2\pi} \exp(ikt)\, dt = \frac{1}{\sqrt{2}} (f, e_0)_{H^2(A_\rho)}\,.$$

and

$$L_m(f) = \sum_{k \in \mathbb{Z}} \frac{(f, e_k)_{H^2(A_\rho)}}{\sqrt{\rho^{2k} + \rho^{-2k}}} \frac{1}{m} \sum_{l=0}^{m-1} \exp(\frac{2\pi i l k}{m} + ik\alpha) = \sum_{k \in \mathbb{Z}} \frac{(f, e_{km})_{H^2(A_\rho)}}{\sqrt{\rho^{2km} + \rho^{-2km}}} \exp(ikm\alpha)$$

since

$$\frac{1}{m} \sum_{l=0}^{m-1} \exp(\frac{2\pi i l k}{m} + ik\alpha) = \begin{cases} \exp(ik\alpha) & \text{if } k \in m\mathbb{Z}, \\ 0 & \text{if } k \notin m\mathbb{Z}. \end{cases}$$

Thus for any $m \in \mathbb{N}$ the m-th order quadrature error is given by

$$|L(f) - L_m(f)| = \left| \sum_{k \in \mathbb{Z} \setminus \{0\}} \frac{(f, e_{km})_{H^2(A_\rho)}}{\sqrt{\rho^{2km} + \rho^{-2km}}} \right|$$

$$\le \sqrt{\sum_{k \in \mathbb{Z} \setminus \{0\}} \frac{1}{\rho^{2km} + \rho^{-2km}}} \|f\|_{H^2(A_\rho)} \le \frac{\|f\|_{H^2(A_\rho)}}{\sqrt{1-\rho^2}} \rho^m$$

as required.   □

For $m, n \in \mathbb{N}$ let $C_{\tau;m.n}$ denote the finite-rank operator on $H^2(A_r^c)$ given by

$$(C_{\tau;m,n} e_k^c, e_l^c)_{H^2(A_r^c)} = r^{|l|-|k|} L_m(f_{\tau;k,l}) \quad (k, l \in \{-n+1, \ldots, n-1\}). \qquad (22)$$

The operator above has the same non-zero eigenvalues counting algebraic multiplicities as the matrix $M_{\tau;m,n}$ introduced earlier. Moreover, by Lemma 2.8, for fixed n, the sequence $(C_{\tau;m,n})_{m \in \mathbb{N}}$ converges to $P_n C_\tau P_n$ in Hilbert-Schmidt norm.

2.9. LEMMA. *Let τ be holomorphically (r_2, r_3)-expansive on A_{r_1} and let $r \in (r_2, r_1)$. Then there is a constant K_2 depending on r, r_1 and r_3 only such that*

$$\|P_n C_\tau P_n - C_{\tau;m,n}\|_{S^2(H^2(A_r^c))} \le K_2 \frac{r_1^m}{(rr_3)^n} \quad (m, n \in \mathbb{N}).$$

PROOF. Using Lemma 2.8 it follows that for any $m, n \in \mathbb{N}$

$$\|P_n C_\tau P_n - C_{\tau;m,n}\|_{S^2(H^2(A_r^c))}^2 = \sum_{\substack{|k|<n \\ |l|<n}} r^{2|l|-2|k|} \left| L(f_{\tau;k,l}) - L_m(f_{\tau;k,l}) \right|^2$$

$$\le \sum_{\substack{|k|<n \\ |l|<n}} r^{2|l|-2|k|} \frac{\|f_{\tau;k,l}\|_{H^2(A_{r_1})}^2}{1-r_1^2} r_1^{2m}.$$

Since τ is holomorphically (r_2, r_3)-expansive on A_{r_1} we have

$$\|f_{\tau;k,l}\|_{H^2(A_{r_1})} \le \sqrt{2} r_3^{-|k|} r_1^{-|l|} \quad (k, l \in \mathbb{Z}).$$

In order to see this suppose for the moment that τ satisfies (15). Then for $k \ge 0$ we have the bound

$$\|f_{\tau;k,l}\|_{H^2(A_{r_1})}^2 \le r_2^{2k} r_1^{-2l} + r_3^{-2k} r_1^{2l} \le 2 r_3^{-2k} r_1^{-2|l|},$$

and for $k < 0$ the bound

$$\|f_{\tau;k,l}\|_{H^2(A_{r_1})}^2 \le r_3^{2k} r_1^{-2l} + r_2^{-2k} r_1^{2l} \le 2 r_3^{2k} r_1^{-2|l|}.$$

The proof for τ satisfying (16) is similar. Thus

$$\|P_n C_\tau P_n - C_{\tau;m,n}\|_{S^2(H^2(A_r^c))}^2 \le \frac{4(r_1^2 + r^2)}{(1-r_1^2)(r_1^2 - r^2)(1-(rr_3)^2)} \frac{r_1^{2m}}{(rr_3)^{2n}},$$

where we have used the bound

$$\sum_{|k|<n} \alpha^{-|k|} = 1 + \frac{2}{\alpha} \frac{\alpha^{-(n-1)} - 1}{\alpha^{-1} - 1} \le \frac{2}{1-\alpha} \alpha^{-n},$$

with $\alpha \in (0, 1)$. $\qquad \square$

Looking back at what we have achieved so far, we see that for τ holomorphically (r_2, r_3)-expansive on A_{r_1} and $r \in (r_2, r_1)$ the Koopman operator C_τ acting on $H^2(A_r^c)$ can be approximated in Hilbert-Schmidt norm by the operators $C_{\tau;m,n}$. By Lemma 2.6 and Lemma 2.9, we have the following upper bound for the error in approximation

$$\|C_\tau - C_{\tau;m,n}\|_{S^2(H^2(A_r^c))} \le \|C_\tau - P_n C_\tau P_n\|_{S^2(H^2(A_r^c))} + \|P_n C_\tau P_n - C_{\tau;m,n}\|_{S^2(H^2(A_r^c))}$$

$$\le K_1 \max\left\{ \frac{r_2}{r}, \frac{r}{r_1} \right\}^n + K_2 \frac{r_1^m}{(rr_3)^n}.$$

The first term, depending on n only, arises from the error of the Galerkin approximation, while the second term, depending on both m and n, is due to the quadrature error of the collocation method. We shall now seek to minimise the two sources of error, given the available bounds. The Galerkin truncation error is minimised if we choose $r = \sqrt{r_1 r_2}$. For the quadrature error, we need to choose m so that the quadrature error is asymptotically not larger than the error

arising from the Galerkin truncation. For each $n \in \mathbb{N}$, we want to choose $m = m(n) \in \mathbb{N}$ such that $m \geq \delta n$. Having fixed $r = \sqrt{r_1 r_2}$, we thus seek $\delta > 0$, so that

$$\limsup_{n \to \infty} \frac{\|P_n C_\tau P_n - C_{\tau; \lceil \delta n \rceil, n}\|_{S^2(H^2(A_r^c))}}{\|C_\tau - P_n C_\tau P_n\|_{S^2(H^2(A_r^c))}} < \infty$$

Using the bounds obtained in Lemma 2.6 and Lemma 2.9 the above yields

$$\limsup_{n \to \infty} \frac{K_2 r_1^{\lceil \delta n \rceil}}{K_1 r_2^n r_3^n} < \infty\,,$$

which is equivalent to

$$\delta \geq \frac{\log(r_2 r_3)}{\log(r_1)}\,.$$

Summarising, we have proven the following theorem, which yields an optimised method to approximate C_τ in Hilbert-Schmidt norm by the finite rank operators $C_{\tau;m,n}$.

2.10. THEOREM. *Let τ be holomorphically (r_2, r_3)-expansive on A_{r_1} and $r \in (r_2, r_1)$. Then the Koopman operator C_τ is Hilbert-Schmidt on $H^2(A_r^c)$ and*

$$\|C_\tau - C_{\tau;m,n}\|_{S^2(H^2(A_r^c))} \leq K_1 \max\left\{\frac{r_2}{r}, \frac{r}{r_1}\right\}^n + K_2 \frac{r_1^m}{(rr_3)^n} \quad (m, n \in \mathbb{N}) \tag{23}$$

for some constants $K_1, K_2 > 0$. Moreover, choosing $r = \sqrt{r_1 r_2}$ and $m \geq \delta n$ with $\delta = \frac{\log(r_2 r_3)}{\log(r_1)}$ yields

$$\|C_\tau - C_{\tau;m,n}\|_{S^2(H^2(A_r^c))} \leq K \left(\sqrt{\frac{r_2}{r_1}}\right)^n \quad (n \in \mathbb{N})$$

for some $K > 0$.

PROOF. The first estimate (23) follows by combining Lemma 2.6 and Lemma 2.9. The remaining assertion is a simple calculation. $\qquad\square$

The theorem above immediately implies our main theorem.

2.11. THEOREM. *Let τ be holomorphically (r_2, r_3)-expansive on A_{r_1} and let $r = \sqrt{r_1 r_2}$. Then C_τ is a well-defined Hilbert-Schmidt operator on $H^2(A_r^c)$. In particular, its spectrum $\mathrm{spec}(C_\tau)$ is either a finite set or a sequence converging to zero together with zero itself and each non-zero spectral point is an eigenvalue of finite algebraic multiplicity.*

Furthermore, for $m, n \in \mathbb{N}$ and $\alpha \in \mathbb{R}$, let $\{\psi_l\}_{-(n-1) \leq l \leq (n-1)}$ with $\psi_l(z) = z^l$ be the set of observables, $\{z^{(j)}\}_{0 \leq j \leq m-1}$ with $z^{(j)} = e^{2\pi i j/m + i\alpha}$ be the set of phase space points and $M = M_n$ the $(2n-1) \times (2n-1)$ matrix given in (1). If for every $n \in \mathbb{N}$, the number of phase space points $m = m(n) \in \mathbb{N}$ is chosen such that

$$m \geq \frac{\log(r_2 r_3)}{\log(r_1)} n,$$

then the following hold:

  (1) *Any convergent sequence $(\lambda_n)_{n \in \mathbb{N}}$ with $\lambda_n \in \mathrm{spec}(M_n)$ converges to a spectral point of C_τ.*
  (2) *Conversely, for any $\lambda \in \mathrm{spec}(C_\tau)$ there exists a sequence $(\lambda_n)_{n \in \mathbb{N}}$ with $\lambda_n \in \mathrm{spec}(M_n)$ such that $\lambda_n \to \lambda$ as $n \to \infty$. More precisely, if λ is an eigenvalue with ascent[2] p, we have*

$$|\lambda - \lambda_n| = O\left(\left(\frac{r_1}{r_2}\right)^{n/(2p)}\right) \quad \text{as } n \to \infty.$$

---

[2]An eigenvalue λ of an operator T is said to have *ascent* p, if p is the smallest integer such that the kernel of $(\lambda I - T)^p$ equals that of $(\lambda I - T)^{p+1}$. In particular, if λ is algebraically simple, then $p = 1$.

(3) *Suppose $\lambda \in \operatorname{spec}(C_\tau)$ is non-zero and $(\lambda_n)_{n \in \mathbb{N}}$ denotes the approximating sequence of eigenvalues of M_n given in (2) above. If $\xi_n = (\xi_{n,-n+1}, \ldots, \xi_{n,0}, \ldots, \xi_{n,n-1})^T \in \mathbb{C}^{2n-1}$ is a generalised eigenvector of the transpose M_n^T of M_n normalised so that*

$$\sum_{|k|<n} |\xi_{n,k}|^2 r^{2|k|} = 1,$$

then setting

$$h_n(z) = \sum_{|k|<n} \xi_{n,k} z^k \quad (z \in \mathbb{C})$$

yields a sequence of Laurent polynomials $(h_n)_{n \in \mathbb{N}}$ with

$$\|\mathcal{P} h_n - h_n\|_{H^2(A_r^c)} = O\left(\left(\frac{r_1}{r_2}\right)^{n/2}\right) \quad \text{as } n \to \infty,$$

where $\mathcal{P}$ is the spectral projection associated to the eigenvalue λ of C_τ.

PROOF. We start with a few observations. First we note that the EDMD matrix M_n defined above coincides with the matrix $M_{\tau;m,n}$ given in (21), since the matrix H occurring in the definition of M is the identity in our case. Next we observe that by (22)

$$\operatorname{spec}(M_{\tau;m,n}) = \operatorname{spec}(C_{\tau;m,n}).$$

Finally, defining the operator $J_n : \mathbb{C}^{2n-1} \to H^2(A_r^c)$ by

$$J_n : (\xi_{-n+1}, \ldots, \xi_0, \ldots, \xi_{n-1})^T \mapsto \left(z \mapsto \sum_{|k|<n} \xi_k z^k\right)$$

we see, after a short calculation, that

$$J_n M_{\tau;m,n}^T = C_{\tau;m,n} J_n,$$

which in turn implies that for any non-zero $\lambda \in \mathbb{C}$ and any $\nu \in \mathbb{N}$

$$J_n(\ker((\lambda I - M_{\tau;m,n}^T)^\nu)) = \ker((\lambda I - C_{\tau;m,n})^\nu).$$

Thus, J_n maps generalised eigenvectors of $M_{\tau;m,n}^T$ corresponding to a non-zero eigenvalue λ to generalised eigenvectors of $C_{\tau;m,n}$ corresponding to the eigenvalue λ.

The assertions now follow from Theorem 2.10 and standard perturbation theory. To be precise, assertions (1) and (2) follow from [1, Corollaries 2.7, 2.13]; for the bound on the convergence, see Theorems 2.17, 2.18, and ensuing remarks in [1]. Finally, [1, Proposition 2.9] yields statement (3). □

If the map τ is additionally assumed to preserve the unit circle, we obtain the following result, which yields a practical numerical approximation scheme of the Koopman operator without having to compute the quantities r_1, r_2 and r_3.

2.12. THEOREM. *Let τ be an analytic expanding circle map with $\tau'_{\max}$ the maximal derivative of τ on $\mathbb{T}$. Furthermore, for $n \in \mathbb{N}$ let $M = M_n$ be the $(2n-1) \times (2n-1)$ EDMD matrix constructed from the $2n-1$ observables and $m \in \mathbb{N}$ phase space points specified in Theorem 2.11.*

Suppose now that δ is any positive real number with

$$\delta > 1 + \tau'_{\max}.$$

Then there is $r \in (0,1)$ such that C_τ is Hilbert-Schmidt on $H^2(A_r^c)$. Moreover, if for every $n \in \mathbb{N}$, the number of phase space points $m = m(n) \in \mathbb{N}$ is chosen such that

$$m \geq \delta n, \tag{24}$$

then the following holds.

(1) *Any convergent sequence $(\lambda_n)_{n \in \mathbb{N}}$ with $\lambda_n \in \operatorname{spec}(M_n)$ converges to a spectral point of C_τ.*

(2) *Conversely, for any $\lambda \in \operatorname{spec}(C_\tau)$ there exist a sequence $(\lambda_n)_{n \in \mathbb{N}}$ with $\lambda_n \in \operatorname{spec}(M_n)$ such that $\lambda_n \to \lambda$ as $n \to \infty$. Moreover,*

$$|\lambda - \lambda_n| = O(e^{-an}) \quad as \ n \to \infty,$$

for some $a > 0$.

(3) *Suppose $\lambda \in \operatorname{spec}(C_\tau)$ is non-zero and $(\lambda_n)_{n \in \mathbb{N}}$ denotes the approximating sequence of eigenvalues of M_n given in (2) above. If $\xi_n = (\xi_{n,-n+1}, \ldots, \xi_{n,0}, \ldots, \xi_{n,n-1})^T \in \mathbb{C}^{2n-1}$ is a generalised eigenvector of the transpose M_n^T of M_n normalised so that*

$$\sum_{|k|<n} |\xi_{n,k}|^2 r^{2|k|} = 1,$$

then setting

$$h_n(z) = \sum_{|k|<n} \xi_{n,k} z^k \quad (z \in \mathbb{C})$$

yields a sequence of Laurent polynomials $(h_n)_{n \in \mathbb{N}}$ with

$$\|\mathcal{P}h_n - h_n\|_{H^2(A_r^c)} = O(e^{-bn}) \quad as \ n \to \infty,$$

where $\mathcal{P}$ is the spectral projection associated to the eigenvalue λ of C_τ and some $b > 0$.

PROOF. Fix $\delta > 1 + \tau'_{\max}$. By Lemma 2.1 there are r_1, r_2 and r_3 with $0 < r_3 < r_2 < r_1 < 1$ such that τ is holomorphically (r_2, r_3)-expansive on A_{r_1} and such that

$$\delta > 1 + \frac{\log(r_3)}{\log(r_1)}.$$

Next choose $r \in (r_2, r_1)$ such that

$$\delta > \frac{\log(r)}{\log(r_1)} + \frac{\log(r_3)}{\log(r_1)},$$

and finally $\gamma > 0$ with

$$\delta > \gamma + \frac{\log(r)}{\log(r_1)} + \frac{\log(r_3)}{\log(r_1)}.$$

Thus, if $m \geq \delta n$ we have $r_1^m \leq r_1^{\gamma n}(rr_3)^n$ and so, by Theorem 2.10,

$$\|C_\tau - C_{\tau;m,n}\|_{S^2(H^2(A_r^c))} \leq K_1 \max\left\{\frac{r_2}{r}, \frac{r}{r_1}\right\}^n + K_2 r_1^{\gamma n} \leq K e^{-cn} \quad (n \in \mathbb{N}).$$

for some positive constants K_1, K_2 and K and $c > 0$.

The assertions of the theorem now follow as in the proof of Theorem 2.11 from standard perturbation theory. $\square$

3. Numerical illustration of convergence properties

The purpose of this section is to demonstrate the practical usefulness of the bound $m \geq \delta n$, which establishes the connection between the number of phase space points m and the number of observables n. For any holomorphically expansive map τ on the annulus, there is an open interval $I_{r_1} = (r_1^-, r_1^+)$ with $r_1 \in I_{r_1}$ so that τ satisfies either (15) or (16), and hence our main Theorem 2.11 holds with δ being a function of r_1. Whilst this theorem holds for all $r_1 \in I_{r_1}$ and the corresponding δ, for practical purposes it is of interest to know the smallest such δ, which we denote by $\delta_{\min}$, as it determines the minimal number m of equidistant phase space points required for a given set of n observables.

We shall next look at a particular class of nontrivial maps τ, perform a numerical search of $r_1 \in I_{r_1}$ to find a suitable δ, and empirically observe convergence or non-convergence of the respective eigenvalue approximations obtained using the EDMD algorithm to the true eigenvalues of C_τ, depending on the chosen δ. We consider the family of maps

$$\tau(z) = b_a(z)b_b(z) + c, \tag{25}$$

where $b_\mu(z) = \frac{z-\mu}{1-\bar{\mu}z}$ is a Möbius map for $\mu \in \mathbb{C}$ with $|\mu| < 1$, and $c \in \mathbb{C}$.

3.1. Convergence for circle maps. We shall first focus on the case $c = 0$. In this case these maps belong to the class of finite Blaschke products, which can be viewed as maps on $\mathbb{C} \cup \{\infty\}$, giving rise to expanding maps when restricted to the circle. If additionally $a = b = 0$ then τ reduces to the map $z \mapsto z^2$, which is the usual doubling map when considered on the unit circle. For non-zero a, b one can think of τ as a (strong) analytic perturbation of the doubling map. The main reason for considering this class of maps for numerical experiments is that the entire spectrum of the Koopman operator C_τ considered on a suitable space $H^2(A_r^c)$ is known, being determined by the fixed point properties of τ inside the unit disk [32]. In particular, the spectrum of C_τ is given by

$$\operatorname{spec}(C_\tau) = \{0, 1\} \cup \{\lambda(z_0)^n \colon n \in \mathbb{N}\} \cup \{\lambda(z_\infty)^n \colon n \in \mathbb{N}\}, \tag{26}$$

where $\lambda(z_0)$ and $\lambda(z_\infty)$ are the multipliers of the unique attracting fixed points $z_0 \in D_r$ and $z_\infty \in D_{1/r}^\infty$. Moreover, the non-zero subleading eigenvalues come as complex-conjugate pairs, as in this case we have $\lambda(z_\infty) = \overline{\lambda(z_0)}$.

Having access to the eigenvalues of C_τ allows us to compare the distance between exact and approximated eigenvalues. For this, we measure the distance between the first subleading eigenvalue $\lambda_2 = \lambda(z_0)$ and the corresponding eigenvalue λ_2^{nm} of $C_{\tau;m,n}$ represented by the $(2n-1) \times (2n-1)$ matrix M_n computed in the EDMD algorithm. We choose $a = b = 0.33 \exp(i\pi/25)$ for the map (25), the same setting as considered in [32]. The results are presented in Figure 2, where for each $m \in [2, 400]$ and $n \in [2, 100]$ we plot the error $|\lambda_2^{nm} - \lambda_2|$ in log scale, with the darkness of the colour corresponding to the size of the error.

Using Theorem 1.1, we have computed an admissible value for δ as $\tau'_{\min} + \tau'_{\max} \approx 4.98$, which also coincides with $\delta_{\min}$ obtained using a numerical search of $r_1 \in I_{r_1}$ as described above. The line $m = 5n$ depicted in Figure 2 aligns well with the (numerically observed) boundary between convergence and non-convergence. Here the value $\delta = 5$ was chosen merely for convenience, as this appears to be a sharp bound for integer-valued δ.

In Figure 3 we plot the error $|\lambda_2^{nm} - \lambda_2|$ as a function of n for different regimes of $m = m(n)$. Choosing a fixed large value of m, for example $m = 300$, initially results in exponentially fast convergence in n, up to numerical precision. The error however deteriorates significantly as we increase n, here $n > 55$, while holding m constant, as there are too few phase space points to resolve highly oscillatory modes. Choosing m as a linear function of n, that is $m = \delta n$, we observe for $\delta = 5 \approx \delta_{\min}$ exponential convergence of the error, albeit slower than the initial convergence for a fixed regime of $m = 300$. Choosing $m = 6n > \delta_{\min} n$, we observe fast exponential convergence with the same (initial) rate as for a fixed regime $m = 300$, which does not deteriorate. Choosing δ too small, here $m = 4n < \delta_{\min} n$ we observe no convergence of the error. To summarize, the threshold value provided by Theorem 1.1 is not only sufficient for guaranteeing convergence, but appears to be close to $\delta_{\min}$, that is the boundary between convergence and non-convergence for this example.

3.2. Convergence for maps not preserving the unit circle. Theorem 2.11 also applies to holomorphically expansive maps on the annulus which do not necessarily preserve the unit circle $\mathbb{T}$. To demonstrate our bounds in this setting we consider maps τ in (25) with $c \neq 0$, in which case τ no longer preserves the unit circle. We shall choose a, b and c in such a way that τ is holomorphically expansive on an annulus containing the unit circle, and whose Julia set is a quasicircle[3]. Using the same arguments as in the proof of [7, Theorem 5.4(b)], one can show that the spectrum of C_τ considered on a suitable space $H^2(A_r^c)$ is again given by (26), that is, given by the powers of the multipliers of the two fixed points in the two respective Fatou components of τ (however the two multipliers are no longer complex conjugates of each other).

In the same vein as before, in Figure 4(right) we show the approximation error $|\lambda_2^{nm} - \lambda_2|$ for $n \in [2, 100]$ and different choices of $m = m(n)$. We note that since τ does not preserve the unit circle, the chosen phase space points are typically in its Fatou set, which tends to make the computations numerically less stable, as the size of the matrix entries grows with n. To

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[3]If $a = b = 0$ then $\tau(z) = z^2 + c$ is the well-known quadratic family. If $c \in \{z \in \mathbb{C} \colon |1 - \sqrt{1 - 4z}| < 1\}$ then τ is hyperbolic and its Julia set is a quasicircle, that is, the image of a circle under a quasi-conformal map of $\hat{\mathbb{C}}$.
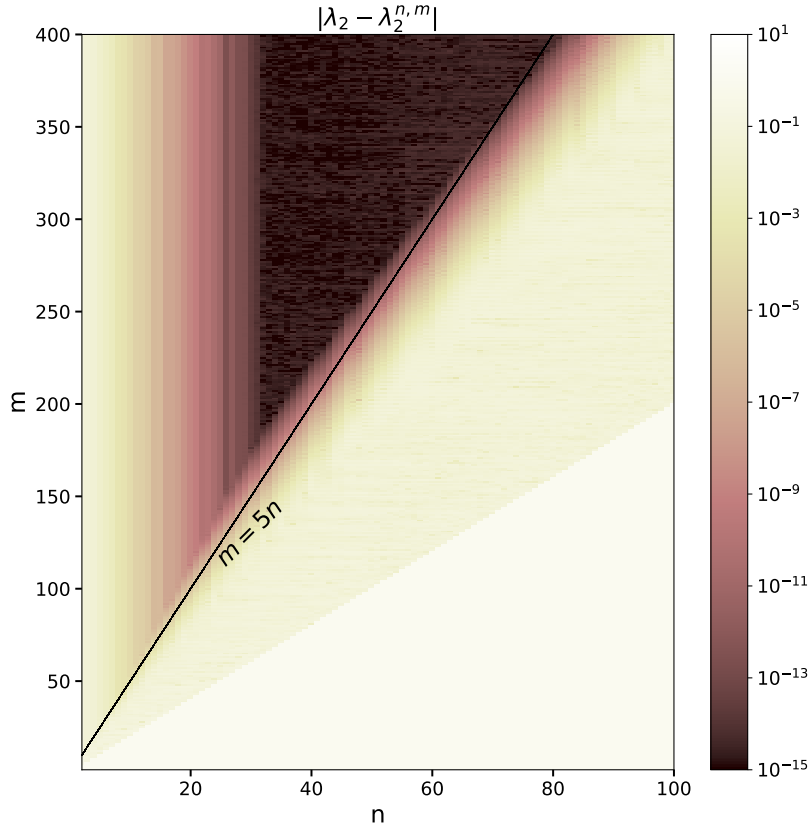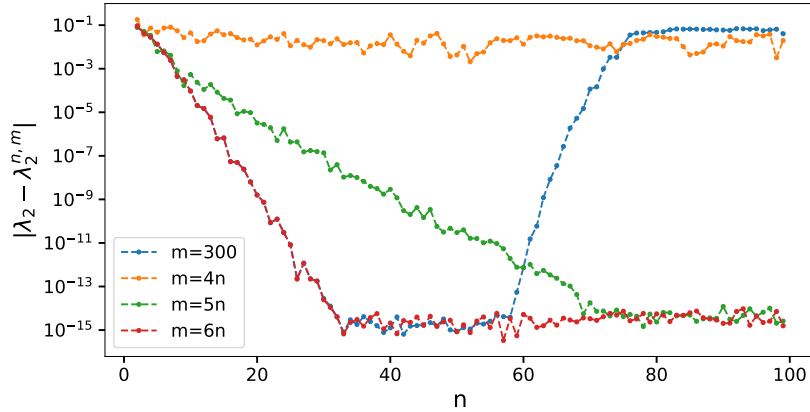
FIGURE 2. Absolute error of the first subleading eigenvalue (plotted in log scale) for the circle map in (25) with $a = b = 0.33 \exp(i\pi/25)$ and $c = 0$ obtained from the EDMD matrix for different values of m and n. The black line in the middle is $m = \delta n$ for $\delta = 5$ nicely indicates our theoretical bound, that is choosing $m \geq 5n$, we are seeing exponential convergence in n of the first subleading eigenvalue.

FIGURE 3. Absolute error of the first subleading eigenvalue (plotted in log scale) for the circle map in (25) with $a = b = 0.33 \exp(i\pi/25)$ and $c = 0$ obtained from the EDMD matrix, plotted as a function of n for different regimes of choosing m.
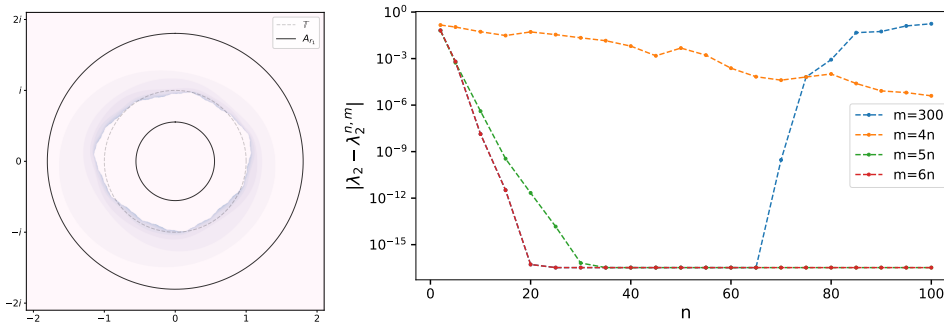
FIGURE 4. (Left) The Julia set $\mathcal{J}_\tau$ for τ in (25) for $a = 0.25i + 0.11, b = 0.078$ and $c = 0.164$. The annulus A_{r_1} containing $\mathcal{J}_\tau$ for $r_1 \approx 0.554$ satisfies condition (15) with corresponding $\delta \approx 4.18$. (Right) EDMD approximation error of the first subleading eigenvalue, as a function of n for different regimes of $m = m(n)$.

obtain good approximations, the use of high-precision computation is therefore required in this case. As this involves substantially higher computational cost, we limit ourselves to a sparse grid of n values in the plots provided. Qualitatively, we obtain a very similar picture to the previous case, with a value of $\delta \approx 4.18$ (obtained as before, using a numerical search of $r_1 \in I_{r_1}$) again appearing to be close to $\delta_{\min}$. We note that the approximation error in Figure 4 can not improve below $\approx 10^{-16}$, as our reference value λ_2 is only computed to this regular floating point precision.

4. Acknowledgments

5. Declaration

The authors have no relevant financial or non-financial interests to disclose.

References

[1] M. Ahues, A. Largillier and B.V. Limaye. *Spectral Computations for Bounded Operators*, Boca Raton, Chapman and Hall/CRC (2001).

[2] V. Baladi and M. Holschneider, *Approximation of nonessential spectrum of transfer operators*, Nonlinearity **12(3)**, 525–538 (1999).

[3] O.F. Bandtlow, *Resolvent estimates for operators belonging to exponential classes*, Integral Equations Operator Theory **61(1)**, 21–43 (2008).

[4] O.F. Bandtlow and F. Naud, *Lower bounds for the Ruelle spectrum of analytic expanding circle maps*, Ergodic Theory Dynam. Systems **39(2)**, 289–310 (2019).

[5] O.F. Bandtlow and O. Jenkinson, *Explicit eigenvalue estimates for transfer operators acting on spaces of holomorphic functions* Adv. Math. **218(3)**, 902–925 (2008).

[6] O. F. Bandtlow and O. Jenkinson, *On the Ruelle eigenvalue sequence*, Ergodic Theory Dynam. Systems **28(6)**, 1701–1711 (2008).

[7] O.F. Bandtlow, W. Just, and J. Slipantschuk, *Spectral structure of transfer operators for expanding circle maps*, Ann. Inst. H. Poinc. C **34**, 31–43 (2017).

[8] O.F. Bandtlow and J. Slipantschuk, *Lagrange approximation of transfer operators associated with holomorphic data*, arXiv preprint, arXiv:2004.03534 (2020).

[9] S. L. Brunton, M. Budišić, E. Kaiser and J. N. Kutz, *Modern Koopman theory for dynamical systems*, SIAM Rev. **64(2)**, 229–340 (2022).

[10] M. Budišić, R. Mohr, and I. Mezić, *Applied Koopmanism*, Chaos **22(4)**, 7510, 33 pp (2012).

[11] M. J. Colbrook and A. Townsend, *Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*, to appear in Comm. Pure Appl. Math.

[12] M. Dellnitz and O. Junge, *On the approximation of complicated dynamical behavior*, SIAM J. Num. Anal. **36(2)**, 491–515 (1999).

[13] T. Eisner, B. Farkas, M. Haase, R. Nagel, *Operator Theoretic Aspects of Ergodic Theory*, Springer, Cham (2015).

[14] G. Froyland, C. Gonzalez-Tokman and A. Quas, *Detecting isoloated spectrum of Transfer and Koopman operators with Fourier analytic tools*, J. Comput. Dyn **1(2)**, 249–278 (2014).

[15] S. Galatolo, M. Monge, I. Nisoli, F. Poloni, *A general framework for the rigorous computation of invariant densities and the coarse-fine strategy*, Chaos, Solitons & Fractals **170**, 113329, 21 pp (2023).

[16] D. Giannakis, *Data-driven spectral decomposition and forecasting of ergodic dynamical systems*, Appl. Comput. Harmon. Anal. **47(2)**, 338–396 (2019).

[17] K. Karhunen, *Über lineare Methoden in der Wahrscheinlichkeitsrechnung*, Ann. Acad. Sci. Fennicae Ser. A. I. Math.-Phys. **37** (1947).

[18] G. Keller, *Stochastic stability in some chaotic dynamical systems*, Monatsh. Math. **94**, 313–333 (1982).

[19] G. Keller, *Markov extensions, zeta functions, and Fredholm theory for piecewise invertible dynamical systems*, Trans. Amer. Math. Soc. **314(2)**, 433–497 (1989).

[20] G. Keller and C. Liverani, *Stability of the spectrum for transfer operators*, Ann. Scuola Norm. Sup. Pisa Cl. Sci. **28(1)**, 141–152 (1999).

[21] S. Klus, P. Koltai, and C. Schütte, *On the numerical approximation of the Perron-Frobenius and Koopman operator*, J. Comput. Dyn. **3(1)**, 51–79 (2016).

[22] S. Klus, F. Nüske, S. Peitz, J.-H. Niemann, C. Clementi, and C. Schütte, *Data-driven approximation of the Koopman generator: Model reduction, system identification, and control*, Phys. D **406**, 132416, 15 pp (2020).

[23] M. Korda, M. Putinar, and I. Mezić, *Data-driven spectral analysis of the Koopman operator*, Appl. Comput. Harm. Anal. **48(2)**, 599–629 (2020).

[24] I. Mezić, *Spectral properties of dynamical systems, model reduction and decompositions*, Nonl. Dyn. **41**, 309–325 (2005).

[25] I. Prigogine, F. Mayné, C. George, and M. De Haan, *Microscopic theory of irreversible processes*, Proc. Nat. Acad. Sci. **74(10)**, 4152–4156 (1977).

[26] Q. Li, F. Dietrich, E.M. Bollt, and I.G. Kevrekidis, *Extended dynamic mode decomposition with dictionary learning: a data-driven adaptive spectral decomposition of the Koopman operator*, Chaos **27(10)**, 103111, 10 pp (2017).

[27] M. Rosenblum and J. Rovnyak, *Hardy Classes and Operator Theory*, Oxford, Oxford University Press (1985).

[28] W.C. Saphir and H.H. Hasegawa, *Spectral representation of the Bernoulli map*, Phys. Lett. A **171**, 317–322 (1992).

[29] D.Sarason. *The H^p spaces of an annulus*, Mem. Amer. Math. Soc., **56** (1965).

[30] P. J. Schmid, *Dynamic mode decomposition of numerical and experimental data*, J. Fluid Mech. **656** 5–28 (2010).

[31] J. Slipantschuk, O.F. Bandtlow, and W. Just, *Analytic expanding circle maps with explicit spectra*, Nonlinearity **26(12)**, 3231–3245 (2013).

[32] J. Slipantschuk, O.F. Bandtlow, and W. Just, *Dynamic mode decomposition for analytic maps*, Comm. Nonl. Sci. Num. Sim. **84**, 105179, 9pp (2020).

[33] Z. Suchanecki, I. Antoniou, S. Tasaki, and O. Bandtlow, *Rigged Hilbert spaces for chaotic dynamical systems*, J. Math. Phys. **37**, 5837–5847 (1996).

[34] P. Walters, *An Introduction to Ergodic Theory*, Springer, New York (1982).

[35] M. Williams, I. G. Kevrekidis, and C. Rowley, *A data–driven approximation of the Koopman operator: Extending dynamic mode decomposition*, J. Nonl. Sci. **25**, 1307–1346 (2015).

[36] M. Williams, C. Rowley, I. Mezić, and I. Kevrekidis, *Data fusion via intrinsic dynamic variables: An application of data-driven Koopman spectral analysis*, Europhys. Lett. **109(4)**, 40007, 6pp (2015).

[37] C. Wormell, *Spectral Galerkin methods for transfer operators in uniformly expanding dynamics*, Numer. Math. **142** 421–463 (2019).

[38] C. Zhang and E. Zuazua, *A quantitative analysis of Koopman operator methods for system identification and predictions*, to appear in C. R. Mécanique.

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