The Numerical Approximation of Koopman Modes of a Nonlinear Operator Along a Trajectory

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Abstract The spectral theory of linear operators enables the analysis of their properties on stable subspaces. The Koopman operator allows to extend these approaches to a large class of nonlinear operators in a surprising way. This is even applicable for numerical analysis of time dependent data of simulations and measurements. We give here some remarks on the numerical approach, link it to spectral analysis by the Herglotz-Bochner theorem and are doing some steps for significance for partial differential equations.

1 Introduction

This paper is directly related to a first part [7] and a second part [8] from the author and is to be considered as an extension of the numerical approaches.

Linear operators are used and deeply analysed as well in mathematics and numerics as also in nearly any scientific discipline. Nevertheless most relevant models of nature are nonlinear, so that linear theory seems to be not applicable or in the best case only by local approximations. Here an even not new theory of functional analysis comes into play. The nonlinear operator induces in a natural way a linear one acting on the continuous functions defined on the space, where if nonlinear operator is defined. This linear Koopman operator has well known attributes as spectrum, eigenvalues, stable eigenspaces. What this means for a specific application is task for the different communities. The approach can be handled also in a numerical way, important for simulations, which has discussed already in in the Dynamic Mode Decomposition theory of Peter Schmid [12]. This is related to the Koopman operator theory, as pointed out by Igor Mesić and coworkers in [3] and Clarence Rowley and his coworkers in [4].

In that way the Ergodic Theory investigated by Ludwig Boltzmann, John von Neumann, George David Birkhoff, Bernard Osgood Koopman, Norbert Wiener,

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Aurel Friedrich Wintner and comprehensively described in the monograph [5] for new developments comes to modern numerical applications. We try here to make some steps further to general applicability and for understanding what that implies for the analysis of the solutions of nonlinear partial differential equations. in addition, we give also the link to spectral theory of Fourier analysis.

2 The Koopman Operator

This is a short description of the preliminaries given in [5] and recapitulating, what has been described in [8]. Let

$$\varphi : K \longrightarrow K \tag{1}$$

be a continuous nonlinear operator on the compact space K and assume $\mathscr{F} \subset C(K)$ being a linear subspace of "observables" in the continuous functions on K. $\mathscr{F}$ shall have the stability property

$$f \in \mathscr{F} \Rightarrow f \circ \varphi \in \mathscr{F} \tag{2}$$

that means, that an observable coupled with the operator is again in the observable space. This condition forces $\mathscr{F}$ typically to be large. Observables might be any useful functional on the space of interest as the mean pressure of a (restricted) fluid domain Ω or the evaluation operators δ_x at all points $x \in \Omega$. It might be also economic parameters describing the behaviour of models of national and global economies or of models of social science. The nonlinear operator φ has no further restrictions. It might describe non wellposed unsteady problems, the case where trajectories are not convergent (also strange attractors), chaotic or turbulent behaviour, mixing fluids, particle systems or ensembles of trajectories for weather forecast. The operator could also be defined by an agent based system for the simulation of traffic, epidemics, social dependencies, where the agents determine their next status by the current status of some other neighbouring agents. In this case K is the set product of the status of all agents with some topology and definitely not a subset of a vector space in contrast to $\mathscr{F}$. The operator φ might even not be known explicitly, but its effect on the observables measured at a number of time steps with constant difference is present. All models are described where an operator is changing the values of the observables to a new state, as long as the iterations are not leaving the limited region of interest.

An important numerical example is the discretization of the Navier-Stokes equations on a finite set of grid points in a domain and time steps. It is even possible to understand K here as the product of the status of all variables on the discretization grid together with varying boundary conditions and geometrical parameters.

By a simple mechanism the **nonlinear** operator φ acting on a set without linear structure induces a **linear** operator on the space of observables $\mathscr{F}$. The operator T_φ on the observables defined by

$$T_\varphi : \mathscr{F} \longrightarrow \mathscr{F} \tag{3}$$

$$f \mapsto T_\varphi f = f \circ \varphi \tag{4}$$

is named the Koopman operator of φ on $\mathscr{F}$ [6]. Hence T_φ is linear and continuous.

As an infinite dimensional operator T_φ may have a (complicated) spectrum with discrete and continuous parts. We are mainly interested in the point spectrum with eigenvalues providing eigenfunctions which are elements of $\mathscr{F}$ describing behaviour in K. The eigenvectors or eigenfunctions f are elements of the space of observables $\mathscr{F}$, not of the state space K as we know it form the linear case. They fulfill Schröders functional equation [13]

$$f(\varphi q) = \lambda f(q) \quad \forall\, q \in K \tag{5}$$

The compactness of the space K is forcing $|\lambda| \leq 1$ for any eigenvalue λ. For any application the meaning of these stable observables must be discussed. This might be a problem by itself.

It is a priori not clear, that eigenfunctions exist. The approach is addressing approximative eigenfunctions.

3 Trajectories and Observables

We study only single trajectories, even where ergodic theory [5] would allow for very general settings. But our target is to establish numerical procedures reflecting the implications of the theory at a level enabling computation. Even the trajectory might be large and dense in the space K. For numerical handling we assume that only the trajectory is given. We are not requesting the explicit knowledge of the operator. Also the space of observables is reduced as much as possible. We assume h to be an observable or a finite dimensional vector of observables. In the latter case we assume a dotproduct $< \cdot, \cdot >$. It might be also a function of a function space. We still avoid this setting because of the difficult questions involved. But h could be a function in a discrete finite space, as we have this in numerical approximations of function spaces.

Let $q_0 \in K$ be the starting point of the iteration or trajectory

$$\mathbb{N}_0 \ni k \mapsto q_k = \varphi^k q_0 \in K \tag{6}$$

Define g_k as the sequence

$$g_k = h(q_k) \quad \forall\, k \in \mathbb{N}_0 \tag{7}$$

These g_k are given by measurements or resulting iterations from a simulation. Because K is compact and h is continuous there norm has a common bound K_h with $\|g_k\| \leq K_h \quad \forall\, k \in \mathbb{N}_0$. They determine a matrix G by (n finite or infinite)

$$G = \left[g_0\ g_1 \cdots g_n\right] \tag{8}$$

The matrix $H = G^T G$ is symmetric positive semidefinite.

$$H_{j_1,j_2} = \left\langle g_{j_1}, g_{j_2} \right\rangle \quad \forall\, j_1, j_2 = 0, \cdots, n \tag{9}$$

Defining the sequence of vectors $\left(h_j\right)_j$ by overlapping the trajectory

$$h_j = \left(h\left(\varphi^j q_k\right)\right)_{k\in\mathbb{N}_0} = \left(h\left(\varphi^{j+k} q_0\right)\right)_{k\in\mathbb{N}_0} = \left(g_{j+k}\right)_{k\in\mathbb{N}_0} \tag{10}$$

we can define the space of observables $\mathscr{F}$ by

$$\mathscr{F} = \overline{LH}\left\{h_j | j \in \mathbb{N}_0\right\} \tag{11}$$

The space $\mathscr{F}$ has the stability property, necessary to define the Koopman operator on $\mathscr{F}$

$$g \in \mathscr{F} \Rightarrow g \circ \varphi \in \mathscr{F} \tag{12}$$

We define p arbitrary, but fixed. Let $a = \sum_{j_1=0}^{p} \alpha_{j_1} h_{j_1} \in \mathscr{F}$ and $b = \sum_{j_2=0}^{p} \beta_{j_2} h_{j_2} \in \mathscr{F}$. The Koopman operator T_φ acts on the space $\mathscr{F}$ via shifting on $h_j, j \in \mathbb{N}_0$.

$$T_\varphi\,(a) = \sum_{j=0}^{p} \alpha_j T_\varphi\left(h_j\right) = \sum_{j=0}^{p} \alpha_j h_{j+1} \tag{13}$$

or for the coefficient vector α

$$\left[\alpha_0\ \alpha_1\ \ldots\ \alpha_p\right] \mapsto \left[0\ \alpha_0\ \alpha_1\ \ldots\ \alpha_p\right] \tag{14}$$

4 The Relation to Time Series Analysis

For $m \in \mathbb{N}$ the semi-sesquilinear form can be defined by

$$\ll a, b \gg_m = \ll \sum_{j_1=0}^{p} \alpha_{j_1} h_{j_1}, \sum_{j_2=0}^{p} \beta_{j_2} h_{j_2} \gg_m = \sum_{j_1,j_2=0}^{p,p} \alpha_{j_1} \overline{\beta_{j_2}} \ll h_{j_1}, h_{j_2} \gg_m \tag{15}$$

using

$$\ll h_{j_1}, h_{j_2} \gg_m := \frac{1}{m} \sum_{k=0}^{m-1} \left\langle h\left(\varphi^{j_1+k} q_0\right), h\left(\varphi^{j_2+k} q_0\right)\right\rangle$$

$$= \frac{1}{m} \sum_{k=0}^{m-1} \left\langle g_{j_1+k}, g_{j_2+k}\right\rangle \quad \forall\ 0 \le j_1 \le p, 0 \le j_2 \le p \tag{16}$$

For all j_1, j_2 we have $| \ll h_{j_1}, h_{j_2} \gg_m | \le K_h^2$. The resulting matrix $\left(\ll h_{j_1}, h_{j_2} \gg_m\right)_{j_1,j_2}$ is the arithmetic mean H^{m-1} of the first m shifted submatrices $\frac{1}{m}\sum_{j=0}^{m-1} H_j$ of the matrix $H = G^T G$

$$H_j = H_{j:j+p,j:j+p} \tag{17}$$

with the size $[0:p] \times [0:p]$. We have

$$\ll a, b \gg_m = < H^{m-1}\alpha, \beta > \tag{18}$$

We assume, that the limit $\lim_{m\to\infty} \ll h_{j_1}, h_{j_2} \gg_m$ exist for all $j_1, j_2 \ge 0$.
This preassumption is not clear in case of applications.
Because for $j_1 \ge j_2$

$$H_{j_1,j_2}^{m-1} = \frac{1}{m} \sum_{k=0}^{m-1} \left\langle g_{j_1+k}, g_{j_2+k}\right\rangle = \frac{1}{m} \sum_{k=j_2}^{m-1+j_2} \left\langle g_{j_1-j_2+k}, g_k\right\rangle$$

$$= \frac{1}{m} \sum_{k=\max(0,-j_1+j_2)}^{m-1+\min(0,-j_1+j_2)} \left\langle g_{j_1-j_2+k}, g_k\right\rangle \text{ (Toeplitz matrix)} \tag{19}$$

$$- \frac{1}{m} \sum_{k=\max(0,-j_1+j_2)}^{j_2-1} \left\langle g_{j_1-j_2+k}, g_k\right\rangle$$

$$+ \frac{1}{m} \sum_{k=m+\min(0,-j_1+j_2)}^{m-1+j_2} \left\langle g_{j_1-j_2+k}, g_k\right\rangle \tag{20}$$

we get a decomposition in a Toeplitz matrix (the elements depend only on the difference $j_1 - j_2$) and initial and final matrices (https://en.wikipedia.org/wiki/Toeplitz_matrix), which are converging to zero as $m \to \infty$ for fixed j_1, j_2. For $m \gg j_1, j_2$ we end up with the relation

$$\gamma(j_1 - j_2) = \lim_{m\to\infty} \frac{1}{m} \sum_{k=0}^{m-1} \left\langle h\left(\varphi^{j_1-j_2+k} q_0\right), h\left(\varphi^k q_0\right)\right\rangle$$

$$= \lim_{m\to\infty} \frac{1}{m} \sum_{k=0}^{m-1} \left\langle h\left(\varphi^{j_1+k} q_0\right), h\left(\varphi^{j_2+k} q_0\right)\right\rangle \tag{21}$$

$$= \lim_{m\to\infty} \frac{1}{m} \sum_{k=0}^{m-1} \left\langle g_{j_1-j_2+k}, g_k\right\rangle = \lim_{m\to\infty} \frac{1}{m} \sum_{k=0}^{m-1} \left\langle g_{j_1+k}, g_{j_2+k}\right\rangle = H^\infty_{j_1,j_2} \tag{22}$$

for the symmetric positive semidefinite Toeplitz matrix H^∞ related to the autocorrelation coefficient $\gamma(j_1 - j_2)$, with a modulus bounded by K_h^2 (https://en.wikipedia.org/wiki/Autocorrelation). For such γ the theorem of Herglotz-Bochner (see [5] Theorem 18.6) assures the existence of a positive finite measure μ on the unit circle $\mathbb{T}$ depending on h and q_0 with the property (see also [1])

$$H^\infty_{j_1,j_2} = \gamma(j_1 - j_2) = \hat{\mu}(j_1 - j_2) = \int_{\mathbb{T}} \lambda^{-(j_1-j_2)}\, d\mu(\lambda) \tag{23}$$

so that the function γ on $\mathbb{Z}$ is the Fourier-transform of the measure μ identical to the entries of the Toeplitz matrix H^∞. All of this is well known in time series analysis.

In terms of the generating elements of the observables $\mathscr{F}$ we get

$$\ll T_\varphi^l \sum_{j_1=0}^{p} \alpha_{j_1} h_{j_1}, \sum_{j_2=0}^{p} \beta_{j_2} h_{j_2} \gg_\infty = \int_{\mathbb{T}} \overline{\lambda}^l \sum_{j_1=0}^{p} \alpha_{j_1} \lambda^{-j_1} \overline{\sum_{j_2=0}^{p} \beta_{j_2} \lambda^{-j_2}}\, d\mu(\lambda) \tag{24}$$

showing how T_φ is acting on $\mathscr{F}$ and with respect to μ for large m. The behaviour of small m, say the transition is not described.

Applied to coefficient vectors α, β, the related elements , $b \in \mathscr{F}$ and the related polynoms $\lambda \mapsto \alpha(\lambda), \beta(\lambda)$

$$\ll a, b \gg_\infty = \langle H^\infty \alpha, \beta\rangle = \int_{\mathbb{T}} \alpha\left(\overline{\lambda}\right) \overline{\beta\left(\overline{\lambda}\right)}\, d\mu(\lambda) \tag{25}$$

Following [1] Theorem 2.1 we see that the measure μ(23) is the weak limit of the sequence of measures μ_m given by the density for the Lebesgue measure $d\lambda$ on the unit circle

$$\int_{\mathbb{T}} r(\lambda)\, d\lambda = \int_0^{2\pi} r(\exp i\,\phi)\; d\phi \text{ for all integrable } r \tag{26}$$

so that

$$\mu_m(E) = \frac{1}{2\pi} \int_E d_m(\lambda)\, d\lambda \quad \forall \text{ measurable sets } E \subset \mathbb{T} \tag{27}$$

with the density function

$$\mathbb{T} \ni \lambda \mapsto d_m(\lambda) = \frac{1}{m} \left\| \sum_{k=0}^{m-1} g_k \, \overline{\lambda}^k \right\|^2 \tag{28}$$

which approximates the spectral density of the eigenvalues of modulus 1 and can be calculated on a computer. The function is not bounded with respect to m even for constant $g_k = g_0$.

Furthermore we have the relation (using, that $\int_{\mathbb{T}} \lambda^l \, d\lambda = 0$ for $l \neq 0$ and $\int_{\mathbb{T}} \lambda^l \, d\lambda = 2\pi$ for $l = 0$).

$$\frac{1}{2\pi} \int_{\mathbb{T}} \lambda^{-(j_1 - j_2)} \, d_m(\lambda) \, d\lambda = \frac{1}{2\pi} \frac{1}{m} \sum_{k_1, k_2 = 0}^{p} \langle g_{k_1}, g_{k_2} \rangle \int_{\mathbb{T}} \lambda^{-(j_1 - j_2) + k_1 - k_2} \, d\lambda \tag{29}$$

$$= \frac{1}{m} \sum_{k = \max(0, -j_1 + j_2)}^{m - 1 - \min(0, -j_1 + j_2)} \left\langle g_{j_1 - j_2 + k}, g_k \right\rangle \text{ for } j_1 \geq j_2 \tag{30}$$

$$= \frac{1}{m} \sum_{k = \max(0, j_1 - j_2)}^{m - 1 + \min(0, j_1 - j_2)} \left\langle g_k, g_{j_2 - j_1 + k} \right\rangle \text{ for } j_2 \geq j_1 \tag{31}$$

The last two identities reproduce the Toeplitz matrix appearing in Eq. (19). The elements are bounded by

$$\left| \frac{1}{2\pi} \int_{\mathbb{T}} \lambda^{-(j_1 - j_2)} \, d_m(\lambda) \, d\lambda \right| \leq K_h^2 \quad \forall \, 0 \leq j_1, \, j_2 \leq p \tag{32}$$

The density function (28) divided by m is the square of the norm of the discrete Fourier backtransform of the finite sequence $\left[g_0 \; g_1 \cdots g_{m-1} \right]$ which again is bounded by K_h^2. Additionally we recognize that

$$< H^{m-1} \alpha, \beta > - \frac{1}{2\pi} \int_{\mathbb{T}} \sum_{j_1 = 0}^{p} \alpha_{j_1} \overline{\lambda^{j_1}} \sum_{j_2 = 0}^{p} \overline{\beta_{j_2}} \lambda^{j_2} \, d_m(\lambda) \, d\lambda \overset{m \to \infty}{\longrightarrow} 0 \tag{33}$$

Definition 1 For a polynom c define the norm $\|c\|_{\infty, \mathbb{T}} = \max_{\lambda \in \mathbb{T}} |c(\lambda)|$. This is the H^∞ Hardy norm of the polynom $\|c\|_{H^\infty}$ on the unit circle (https://en.wikipedia.org/wiki/Hardy_space).

Proposition 1 *Assume, the finite measure μ (23) is discrete and that $\epsilon > 0$ is given.*

1. *μ must be the sum of at most countable number of point measures*

$$\mu = \sum_{l=1}^{\infty} \rho_l \, \delta_{\{\lambda_l\}} \text{ with } |\lambda_l| = 1 \quad \forall \, l \tag{34}$$

with decreasing weights $\rho_l > 0$.

It exists l_ϵ, so that the last part of the sum is small $\sum_{l=l_\epsilon+1}^{\infty} \rho_l < \epsilon$.

2. *Let $c = c_\epsilon$ be a polynom coefficient vector c, so that $c\left(\overline{\lambda_l}\right) = 0$ for $l = 1, \cdots, l_\epsilon$. Then*

$$\begin{aligned} \frac{\langle H^\infty c, c\rangle}{\|c\|^2_{\infty,\mathbb{T}}} &= \frac{1}{\|c\|^2_{\infty,\mathbb{T}}} \int_{\mathbb{T}} \left| \sum_{j=0}^{p} c_j \lambda^{-j} \right|^2 d\mu\,(\lambda) = \frac{1}{\|c\|^2_{\infty,\mathbb{T}}} \sum_{l=1}^{\infty} \rho_l \, |c\left(\overline{\lambda_l}\right)|^2 \\ &= \frac{1}{\|c\|^2_{\infty,\mathbb{T}}} \sum_{l=l_\epsilon+1}^{\infty} \rho_l \, |c\left(\overline{\lambda_l}\right)|^2 \leq \epsilon \end{aligned} \tag{35}$$

3. *By definition of H^∞ there exists an m_0 so that*

$$\frac{\frac{1}{m}\left\langle \sum_{j=0}^{m-1} H_j c, c\right\rangle}{\|c\|^2_{\infty,\mathbb{T}}} \leq 2\epsilon \quad \forall \, m \geq m_0 \tag{36}$$

4. *Multiplying c by any other non zero polynom b would maintain the roots of c and therefore also this estimate for $c * b$.*
5. *Because the l_2-norm of the polynom coefficient vector c is identical to the H^2 Hardy space norm of the polynom c which itself is lower or equal to the H_∞ Hardy space norm of the polynom*

$$\|c\|_2^2 = \|c\|^2_{H_2} = \frac{1}{2\pi} \int_{\mathbb{T}} \left| \sum_k c_k \lambda^k \right|^2 d\lambda \leq \frac{1}{2\pi} \int_{\mathbb{T}} \max_{\lambda' \in \mathbb{T}} |c\left(\lambda'\right)|^2 \, d\lambda = \|c\|^2_{\infty,\mathbb{T}} \leq \|c\|_1^2 \tag{37}$$

the Rayleigh quotient of c is an upper estimate of (35)

$$\frac{\langle H^\infty c, c\rangle}{\|c\|^2_{\infty,\mathbb{T}}} \leq \frac{\langle H^\infty c, c\rangle}{\|c\|_2^2} \tag{38}$$

meaning, that for a polynom coefficient vector c with $\frac{\langle H^\infty c, c\rangle}{\|c\|_2^2} \leq \epsilon$, we have also an estimate for (35).

It is not clear , that $\|c_\epsilon\|_{\infty,\mathbb{T}}$ remains limited for $\epsilon \to 0$. In numerical tests we got the impression, that this is the case if the roots are nearly uniformly distributed near the unit circle.

For a measure μ (23) with continuous parts, the existence of a polynomial approximation of nullfunctions of H^∞ is not yet clear.

The analysis as far shows the relation to a Fourier analysis by the Herglotz-Bochner theorem. That means it shows the behaviour of a long running sequence neglecting the damped parts of the sequence. Only the spectral part on the unit circle $\mathbb{T}$ is relevant in this context and not the inner part of the unit circle describing the part, which will vanish during the iteration. Nevertheless a numerical scheme must show the correct results in the terms described in the previous section.

The following examples will give insight into typical situations for given sequences $(g_k)_{k=0,1,2,\ldots}$. All these can be part of a single sequence.

Example 1 (Converging Sequences) If the iteration $h\left(\varphi^k\right) \overset{k\to\infty}{\to} h\left(q_*\right)$ converges, the measure μ in (23) is the single point measure at 1.

To see this

$$\begin{aligned}
&\left|\frac{1}{m}\sum_{k=k_0}^{m-1+k_0}\left\langle h\left(\varphi^{j_1+k}q_0\right), h\left(\varphi^{j_2+k}q_0\right)\right\rangle - \left\langle h\left(q_*\right), h\left(q_*\right)\right\rangle\right| \\
&\quad\le \left|\frac{1}{m}\sum_{k=k_0}^{m-1+k_0}\left\langle h\left(\varphi^{j_1+k}q_0\right) - h\left(q_*\right), h\left(\varphi^{j_2+k}q_0\right) - h\left(q_*\right)\right\rangle\right| \\
&\quad+ \left|\frac{1}{m}\sum_{k=k_0}^{m-1+k_0}\left\langle h\left(\varphi^{j_1+k}q_0\right) - h\left(q_*\right), h\left(q_*\right)\right\rangle\right| \\
&\quad+ \left|\frac{1}{m}\sum_{k=k_0}^{m-1+k_0}\left\langle h\left(q_*\right), h\left(\varphi^{j_2+k}q_0\right) - h\left(q_*\right)\right\rangle\right|
\end{aligned} \tag{39}$$

so that for given $\epsilon > 0$ and appropriate k_0 , that $\|h\left(\varphi^{j+k}q_0\right) - h\left(q_*\right)\| < \epsilon$ for all $k, j \ge 0$ with $k \ge k_0$ we find

$$\left|\lim_{m\to\infty}\frac{1}{m}\sum_{k=k_0}^{m-1+k_0}\left\langle h\left(\varphi^{j_1+k}q_0\right), h\left(\varphi^{j_2+k}q_0\right)\right\rangle - \left\langle h\left(q_*\right), h\left(q_*\right)\right\rangle\right| \le \epsilon^2 + \epsilon\|h\left(q_*\right)\| \tag{40}$$

and therefore $\lim_{m\to\infty}\frac{1}{m}\sum_{k=0}^{m-1}\left\langle h\left(\varphi^{j_1+k}q_0\right), h\left(\varphi^{j_2+k}q_0\right)\right\rangle = \lim_{m\to\infty}\frac{1}{m}\sum_{k=k_0}^{m-1+k_0}\left\langle h\left(\varphi^{j_1+k}q_0\right), h\left(\varphi^{j_2+k}q_0\right)\right\rangle = \|h\left(q_*\right)\|^2$. That means

$$\|h\left(q_*\right)\|^2 = \int_{\mathbb{T}} \lambda^{-(j_1-j_2)}\, d\mu\left(\lambda\right) \quad \forall\, j_1, j_2 \ge 0 \tag{41}$$

which is possible only for the point measure $\mu = \|h\left(q_*\right)\|^2\, \delta_{\{1\}}$.

This example shows the measure μ (23) for a practically relevant case, but which is of less interest in our context.

Example 2 (Besicovitch Sequences) Assume, that the values $g_k = \sum_{l=1}^{p} v_l \ \lambda_l{}^k$ $\forall \ k \in \mathbb{N}_0$ are given by decomposition in modes with all λ_l pairwise different and $|\lambda_l| \leq 1$. If for all $|\lambda_l| = 1$, the decomposition is a so called Besicovitch sequence [2]. Then

$$H_{j_1,j_2}^{m-1} = \frac{1}{m} \sum_{k=0}^{m-1} \left\langle g_{j_1+k}, g_{j_2+k} \right\rangle = \frac{1}{m} \sum_{k=0}^{m-1} \sum_{l_1,l_2} \langle v_{l_1}, v_{l_2} \rangle \ \lambda_{l_1}^{j_1+k} \overline{\lambda_{l_2}}^{j_2+k}$$

$$= \sum_{l_1,l_2} \langle v_{l_1}, v_{l_2} \rangle \, \lambda_{l_1}^{j_1} \overline{\lambda_{l_2}}^{j_2} \, \frac{1}{m} \sum_{k=0}^{m-1} \lambda_{l_1}^{k} \overline{\lambda_{l_2}}^{k} \tag{42}$$

$$= \sum_{l_1,l_2} \langle v_{l_1}, v_{l_2} \rangle \ \lambda_{l_1}^{j_1} \overline{\lambda_{l_2}}^{j_2} \, \frac{1}{m} \, \frac{1 - \left(\lambda_{l_1} \overline{\lambda_{l_2}}\right)^m}{1 - \lambda_{l_1} \overline{\lambda_{l_2}}} \tag{43}$$

The last term converges to zero for $m \to \infty$ if $\lambda_{l_1} \overline{\lambda_{l_2}} \neq 1$ because $|\lambda_{l_1} \overline{\lambda_{l_2}}| \leq 1$. The convergence is relatively slow. For $\lambda_{l_1} \overline{\lambda_{l_2}} = 1$ we simply have $\frac{1}{m} \sum_{k=0}^{m-1} \lambda_{l_1}^{k} \overline{\lambda_{l_2}}^{k} = 1$. Therefore

$$H_{j_1,j_2}^{\infty} = \lim_{m \to \infty} \frac{1}{m} \sum_{k=0}^{m-1} \left\langle g_{j_1+k}, g_{j_2+k} \right\rangle = \sum_{l} \langle v_l, v_l \rangle \ \lambda_l^{j_1-j_2} \tag{44}$$

Thus the measure μ (23) is discrete and given by

$$\mu = \sum_{l} \|v_l\|^2 \, \delta_{\{\overline{\lambda_l}\}} \tag{45}$$

meaning, that the values $\overline{\lambda_l}$ of the Besicovitch sequence determine the measure μ. Because the measure μ is finite, the sum $\sum_l \|v_l\|^2$ must be bounded. The assumption $|\lambda_l| \leq 1$ is essential for the construction. Modes with $|\lambda_l| < 1$ are disappearing for $k \to \infty$. The measure μ (23) cannot represent these.

Let c be an polynom coefficient vector and define the linear combination $\sum_{k=0}^{p} c_k g_{k+j} = \sum_l v_l \lambda_l^j c\,(\lambda_l)$. We assume, that a finite number of λ_l are roots of the polynom $\lambda \mapsto c\,(\lambda)$. Estimating the linear combination by

$$\| \sum_{k=0}^{p} c_k g_{k+j} \| \leq \sum_{l} \|v_l\| |\lambda_l^j| |c\,(\lambda_l)\,| \tag{46}$$

$$\leq \sum_{l, c(\lambda_l) \neq 0} \|v_l\| |c\,(\lambda_l)\,| \tag{47}$$

$$\leq \sum_{l, c(\lambda_l) \neq 0} \|v_l\| \max_{|\lambda|=1} |c\,(\lambda)\,| \tag{48}$$

so that for finite $\sum_l \|v_l\| < \infty$ it is possible to define the roots of c in way, that the remaining part is arbitrary small independent on the index j as long as $\max_{|\lambda|=1} |c(\lambda)|$ remains bounded.

Example 3 (Impact of Continuous Segments) Assume, that the values g_k for $k \in \mathbb{N}_0$ have a linear decomposition containing also continuous parts of the following kind as summands.

$$g_k = \sum_m \int_{[\rho_m, \sigma_m]} \lambda^k f_m(\lambda)\, d\lambda \quad \forall\, k \in \mathbb{N}_0 \tag{49}$$

For simplicity we consider one element of the sum.

The function $\lambda \mapsto f(\lambda)$ should be continuously differentiable. $[\rho, \sigma]$ is a segment on the unit circle. Because of the definition of (26) (remark the difference to the usual product rule)

$$\int_{[\rho,\sigma]} \lambda^k f(\lambda)\, d\lambda = \left[\frac{1}{i\,k}\, \lambda^k f(\lambda)\right]_\rho^\sigma - \int_{[\rho,\sigma]} \frac{1}{k}\, \lambda^{k+1}\, \partial_\lambda f(\lambda)\, d\lambda \tag{50}$$

these terms converge to 0 for $k \to \infty$ with $\frac{1}{k}$ and not exponentially as in the case of a discrete atomic measure for a point λ with $|\lambda| < 1$. Even a constant f will be interesting.

By these contiguous segments continuous parts of the spectrum can be formulated for numerical purposes. Used as density for the Lebesgue measure on the unit circle they are special examples for so called Rajchman measures, which nth Fourier Transform vanish for $n \to \infty$ (https://en.wikipedia.org/wiki/Rajchman_measure).

5 Approximation of an λ-Eigenmode Along a Trajectory

As before we assume here φ as an operator and a sequence $f = (f_j)_{j=0,1,\cdots}$ with $f_j = f(\varphi^j q_0)$ of scalars or vectors as in (10) or even functions as elements of a function space $C(\Omega, \mathbb{R}^s)$, f_j are the elements of an iteration observed by a vector of observables f. s might be any natural number given by a number of components in the analysed process defined by the operator φ. $s = 4$ in case of the incompressible Navier-Stokes equations with three velocity components and the pressure. To simplify the problem we handle only discretized versions with a finite set of discretization points Ω which makes the function space finite dimensional. j is the time step number of the time discretization given by the operator φ in this case. We define finite complex linear combinations of values along the trajectory starting at each step j. The coefficients are given by the vector $\alpha = (\alpha_k)_{k=0,\cdots,p-1}$ and do not dependent on j. The coefficients are understood also as coefficients of a

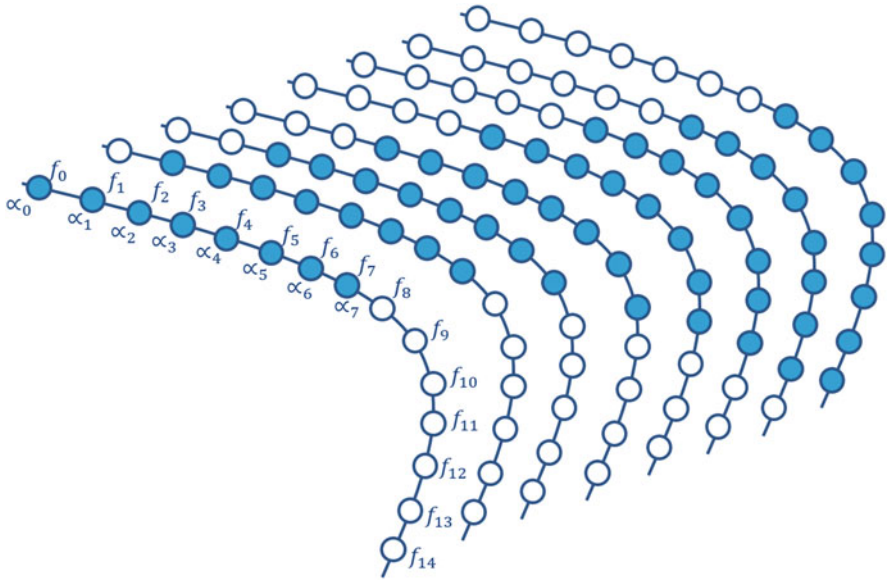

Fig. 1 Moving linear combination of values along a trajectory

polynom $\lambda \mapsto \alpha(\mu) = \sum_{k=0}^{p-1} \alpha_k \mu^k$. We fix here a value λ which must not be a root of this polynom and define the sequence

$$\widehat{f}_j^{\alpha,\lambda} = \frac{\sum_{k=0}^{p-1} \alpha_k f_{j+k}}{\sum_{k=0}^{p-1} \alpha_k \lambda^k} \quad \forall\, j = 0, 1, 2, \cdots \tag{51}$$

Figure 1 shows the linear combinations on the trajectory for $p - 1 = 8$ elements moving along 7 starting points j. This approach is motivated by the fact, that for a sequence $\left(f_j\right)_j$, already fulfilling the rule $f_j = \lambda^j f_0$, we conserve this property $\widehat{f}_j^{\alpha,\lambda} = \lambda^j f_0$. That means we conserve Schröders equation $f(\varphi q) = \lambda f(q)\ \forall q$, or in other words have a Koopman eigenvector.

The error $\epsilon^{\alpha,\lambda}$ of the pair $\left(\lambda, \widehat{f}^{\alpha,\lambda}\right)$ of being a Koopman eigenvalue-eigenvector pair is given by

$$\epsilon_j^{\alpha,\lambda} = -\lambda \widehat{f}_j^{\alpha,\lambda} + \widehat{f}_{j+1}^{\alpha,\lambda} = \frac{1}{\alpha(\lambda)} \left(-\sum_{k=0}^{p-1} f_{j+k}\, \lambda \alpha_k + \sum_{k=0}^{p-1} f_{j+1+k}\, \alpha_k \right) \tag{52}$$

$$= \frac{1}{\alpha(\lambda)} \left(-f_j\, \lambda \alpha_0 + \sum_{k=1}^{p-1} f_{j+k}\, \left(-\lambda \alpha_k + \alpha_{k-1}\right) + f_{j+p}\, \alpha_{p-1} \right) \tag{53}$$

$$= \frac{1}{\alpha(\lambda)} \sum_{k=0}^{p} f_{j+k}\, c_k \quad \forall\, j = 0, 1, \cdots \tag{54}$$

with the polynom coefficient vector

$$\begin{aligned} c_0 &= -\lambda\alpha_0 \\ c_k &= -\lambda\alpha_k + \alpha_{k-1} \quad \forall\, k = 1, \cdots, p-1 \\ c_p &= \qquad\quad \alpha_{p-1} \end{aligned} \tag{55}$$

Example 4 (Wiener-Wintner) An example are the sums in the Wiener-Wintner theorem [5]

$$\tilde{f_\omega}\left(q_j\right) \approx \frac{1}{p}\sum_{k=0}^{p-1} f\left(\varphi^k q_j\right) e^{i\,2\pi\,\omega k} \quad \forall\, j \in \mathbb{N}_0 \tag{56}$$

where $\alpha_k = e^{i\,2\pi\,\omega k}$ for all k, the eigenvalue $\lambda = e^{-i\,2\pi\,\omega}$ and $\alpha\left(\lambda\right) = p$. For $p \to \infty$ they approximate the eigenmode $\tilde{f_\omega}$ for λ.

c is given by $c = \left[-e^{-i\,2\pi\,\omega}\ 0 \cdots 0\ e^{i\,2\pi\,\omega(p-1)}\right]$ and the approximation error by $\epsilon_j^{\alpha,\lambda} = \frac{1}{p}\left(-f_j e^{-i\,2\pi\,\omega} + f_{j+p} e^{i\,2\pi\,\omega(p-1)}\right)$ which is small for bounded f, if p is large.

As a polynom, c is the product of polynom α and the linear divisor given by $\mu \mapsto \mu - \lambda$. Understood as polynom coefficient vector c is the convolution $c = \alpha * \begin{bmatrix} -\lambda \\ 1 \end{bmatrix}$. By definition, λ is a root of the polynom $\mu \mapsto c\left(\mu\right)$.

For a matrix $\mathfrak{A}_p(c)$ build by the repeatedly shifted vector c we request equivalently

$$\epsilon^{\alpha,\lambda} = \frac{1}{\alpha\left(\lambda\right)}\left[f_0, f_1, f_2, \cdots\right] \begin{bmatrix} c_0 & & & \\ c_1 & c_0 & & \\ c_2 & c_1 & c_0 & \\ \cdot & c_2 & c_1 & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ c_p & c_{p-1} & c_{p-2} & \cdot \\ & c_p & c_{p-1} & \cdot \\ & & c_p & \cdot \\ & & & \cdot \end{bmatrix} = \frac{1}{\alpha\left(\lambda\right)} f\, \mathfrak{A}_p(c) \overset{!}{\approx} 0 \tag{57}$$

The existence of a polynom coefficient vector c with this property is a necessary condition for the existence of approximative eigenvectors. Using the same notation we have $\widehat{f^{\alpha,\lambda}} = \frac{1}{\alpha(\lambda)} f\, \mathfrak{A}_{p-1}(\alpha)$ for the approximative eigenmode (51) .

The sequence $\widehat{f^{\alpha,\lambda}}$ will be an approximative eigenmode of the underlying iteration operator if and only if $\|\widehat{f^{\alpha,\lambda}}\| \gg \|\epsilon^{\alpha,\lambda}\|$ and $\|\epsilon^{\alpha,\lambda}\| \approx 0$. In the following we assume that $\epsilon^{\alpha,\lambda}$ is small.

If a vector c with the property (57) has been found, it provides λ as root of the polynom c. Furthermore, all roots λ_l of c together with the related polynom coefficient vectors α_l for $l = 1, \cdots, p$ are candidates for approximating Koopman

modes, as long they are not multiple roots and as long $|\lambda_l| \leq 1$. These pairs all share the same approximation quality $\frac{1}{\alpha(\lambda_l)} f\ \mathfrak{A}_p(c)$ depending solely on the fraction $\frac{1}{\alpha(\lambda_l)}$. By providing a single coefficient vector α, we get many other coefficient vectors α_l by dividing the polynom c by the linear divisors of the different roots. If $|\alpha_l\,(\lambda_l)\,|$ is large, we expect a good approximation quality. The degree p has to be as small as possible.

5.1 Determining the Polynom Coefficient Vector c

Given are a finite sequence of vectors $G = \left[g_0\ g_1\ \ldots\ g_n\right]$. To find a polynom coefficient vector c with small approximation error

$$\epsilon^{\alpha,\lambda} = G\,\mathfrak{A}_p(c) \approx 0,$$

we apply the following procedure. For any given c determine the minimal number $\rho_c \geq 0$ so that

$$\mathfrak{A}(c)^* H\ \mathfrak{A}(c) \leq \rho_c\ \ \mathfrak{A}(c)^* \mathfrak{A}(c) \tag{58}$$

ρ_c is the largest eigenvalue of the generalized eigenvalue problem. Determine c with fixed degree p so that $\rho = \rho_c$ is minimal and that the roots of the polynom defined by c have modulus not more than 1. This can be reached by an iterative process following the theorem of Rellich [10], that for a real symmetric parametrized matrix eigenvalues and eigenvectors depend analytically on the parameter. During the iteration the roots of c are tested and changed, if there modulus exceeds 1.

The value of ρ determines the error of the approximation.

Projecting to the jth row and column of both sides of the matrix inequality we find

$$\left\langle H_j\ c, c\right\rangle \leq \rho\ \|c\|^2 \tag{59}$$

for the jth submatrix H_j (17).

Taking the mean over the $m = n - p + 1$ first submatrices H_j we find for H^{m-1} as in (18)

$$\left\langle H^{m-1} c, c\right\rangle \leq \rho \|c\|^2 \tag{60}$$

So we get by (38) and (35) the estimate for m which is sufficiently large

$$\frac{\langle H^{\infty} c, c\rangle}{\|c\|^2_{\infty,\mathbb{T}}} \approx \frac{\left\langle H^{m-1} c, c\right\rangle}{\|c\|^2_{\infty,\mathbb{T}}} \leq \frac{\left\langle H^{m-1} c, c\right\rangle}{\|c\|^2_2} \leq \rho \tag{61}$$

Minimizing $\frac{\left\langle H^{m-1} c, c\right\rangle}{\|c\|^2_{\infty,\mathbb{T}}}$ directly with respect to c might result in a better c.

There are other alternatives to calculate the vector c. The whole procedure is related to DMD of Peter Schmid [12].

5.2 Roots and Pseudo-Eigenvectors

The roots λ_l for all $l = 1, \cdots, p$ of the polynom c are determined by the solution of the eigenvalues of the c-companion matrix.

For each λ_l with $|\lambda_l| \leq 1$ a "pseudo-eigenvector" α_l is determined by factorizing the linear divisor of root λ_l out of c

$$\alpha_l(\lambda)\ (\lambda - \lambda_l) = c(\lambda) \quad \forall\ \lambda \in \mathbb{C} \tag{62}$$

We assume, that there are no multiple roots of c, so that $\alpha_l(\lambda) \neq 0$. The vectors α_l with degree $p-1$ define the linear combinations (51) along the trajectory delivering approximate Koopman eigenvectors for the eigenvalues λ_l.

The matrix consisting on the vectors $\frac{\alpha_l}{\alpha(\lambda_l)}$ is the inverse of the Vandermonde matrix (https://en.wikipedia.org/wiki/Vandermonde_matrix) defined by the eigenvalues λ_l.

The approximative eigenvectors are given by

$$v_l = G\,\frac{\alpha_l}{\alpha(\lambda_l)} \tag{63}$$

The vectors with complex elements are also named Koopman modes [3].

For small ρ (61) we get the following approximation

$$g_k \approx \sum_{l=1}^{p} v_l\,\lambda_l^{\,k} \quad \forall\ k \tag{64}$$

which is Besicovitch like sequence including potentially some λ_l with $|\lambda_l| < 1$.

5.3 Handling Intermediate Data Steps

If the number of data steps is large, or if the data from step to step are very slowly changing, or if the data size per step is large (e.g. 100,000 steps of a weather simulation), it is reasonable to analyse only intermediate steps, e.g. every mth out of n steps. There is basically no difference to the given approach. How to analyse the

influence of the intermediate data on the eigenvalues? This can be done by enlarging the matrix G in the following way:

$$\widehat{G} = \begin{bmatrix} G_{0+0} & G_{m+0} & G_{2\,m+0} & \cdots & G_{q\,m+0} \\ G_{0+1} & G_{m+1} & G_{2\,m+1} & \cdots & G_{q\,m+1} \\ G_{0+2} & G_{m+2} & G_{2\,m+2} & \cdots & G_{q\,m+2} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ G_{0+m-1} & G_{m+m-1} & G_{2\,m+m-1} & \cdots & G_{q\,m+m-1} \end{bmatrix} \tag{65}$$

q is defined so that $qm + m - 1 \leq n$. Every line out of m consists on intermediate steps with distance m. The next line is shifted by 1. Be aware, that the matrix size is essentially the same as before. The degree $q\,m$ vector $c = \left[c_0\ 0_{m-1}\ c_m\ 0_{m-1}\ c_{2\,m}\ 0_{m-1} \cdots 0_{m-1}\ c_{q\,m}\right]$ where 0_{m-1} represents a vector of $m-1$ zeros. After suppressing these zeros $\widehat{G}\ c \approx 0$ is handled as before. c leads to a polynom

$$\lambda \mapsto \sum_{k=0}^{q} c_{k\,m}\,(\lambda^m)^k \tag{66}$$

The $q\,m$ roots of this polynom are $\lambda_l^m = \lambda_{l,j}^m$ where

$$\lambda_{l,j} = \lambda_{l,0}\ \exp\left(i\,2\pi\ \frac{j}{m}\right) \quad \forall\, j = 0, 1, \cdots, m-1, \text{ and } l = 1, \cdots, q \tag{67}$$

If $\lambda_{l_1,j}^m \neq \lambda_{l_2,j}^m$ for $l_1 \neq l_2$ than all the m roots belonging to both values are different. These roots are related to pseudoeigenvectors $w_{l,j}$ which are calculated in the following way. Similar to c let w_l be the polynom coefficient vector of degree $(q-1)\,m$ $w_l = \left[w_{l,0}\ 0_{m-1}\ w_{l,m}\ 0_{m-1}\ w_{l,2\,m}\ 0_{m-1} \cdots w_{l,q\,m}\right]$ defined by the factorization $w_l = c/\left[-\lambda_l^m\ 0_{m-1}\ 1\right]$. The complete pseudoeigenvectors are then given by the convolution

$$w_{l,j} = \frac{1}{m}\left(\frac{1}{\lambda_{l,0}^k}\ \exp\left(-i\,2\pi\ \frac{j\,k}{m}\right)\right)_{k=0,\cdots,m-1} * w_l \quad \forall\, j = 0, \cdots, m-1 \tag{68}$$

The eigenmodes $v_{l,j}$ are calculated by

$$u_{l,j} = \frac{1}{m}\left(\exp\left(-i\,2\pi\ \frac{j\,k}{m}\right)\right)_{k=0,\cdots,m-1} diag\left(\frac{1}{\lambda_{l,0}^k}\right)_k\ \widehat{G}\ w_l / w_l\left(\lambda_l^m\right) \tag{69}$$

The first part is a discrete Fouriertransform and is identical for all different $l = 1, \cdots, q$. The second part $\widehat{G}\ w_l / w_l\left(\lambda_l^m\right)$ is constant with respect to j and represents the whole space belonging to the eigenvalues given by λ_l^m. The modes $u_{l,j}$ for

fixed l are not related to each other. Some of them might be nearly vanishing. The calculation requires the special definition of $\widehat{G}$ with replicated shifted lines.

6 The λ-Eigenmode Mapping Operator

For a given pair (λ, α) we denominate the map $\widehat{\bullet}^{\lambda}$ defined by approximative eigenmode (51)

$$\widehat{\bullet}^{\lambda} : f \mapsto \widehat{f}^{\lambda} = \widehat{f}^{\alpha,\lambda} \tag{70}$$

the λ-eigenmode mapping operator. This linear operator can be applied to a sequence of scalars or vectors or functions or vector fields in the appropriate spaces.

Under reasonable conditions we found in our simulations (no proof) empirically for the pairs (α, λ), that

$$\frac{1}{|\alpha(\lambda)|} \sum_{k=0}^{p-1} |\alpha_k| = \frac{\|\alpha\|_1}{|\alpha(\lambda)|} = O(1) \tag{71}$$

This helps in analysing the behaviour in combination with diverse operators. This property together with an uniformly bounded approximation-error $\epsilon^{\alpha,\lambda}$ (57) shows the following properties.

In the case of continuous or differentiable or integrable functions f the operator $\widehat{\bullet}^{\lambda}$ is linear and commutes with limits and (discrete) differentiable and integration operators, substantial for the definition of partial differential equations, e.g.

$$\widehat{af + bg}^{\lambda} = a\widehat{f}^{\lambda} + b\widehat{g}^{\lambda}$$

$$\widehat{\lim_{n\to\infty} f_n}^{\lambda} = \lim_{n\to\infty} \widehat{f_n}^{\lambda}$$

$$\widehat{\text{grad}\, f}^{\lambda} = \text{grad}\, \widehat{f}^{\lambda}$$

$$\widehat{\Delta f}^{\lambda} = \Delta \widehat{f}^{\lambda}$$

$$\widehat{\mathrm{D}\, v}^{\lambda} = \mathrm{D}\, \widehat{v}^{\lambda}$$

$$\widehat{\text{div}\, v}^{\lambda} = \text{div}\, \widehat{v}^{\lambda}$$

$$\widehat{\text{rot}\, v}^{\lambda} = \text{rot}\, \widehat{v}^{\lambda}$$

$$\widehat{\int_V f(x)dx}^{\lambda} = \int_V \widehat{f}^{\lambda}(x)\, dx$$

$$\widehat{\oint_{\partial V} < v(x), df(x) >}^{\lambda} = \oint_{\partial V} < \widehat{v}^{\lambda}(x)\, df(x) >$$

all these elements are approximative eigenmodes for the eigenvalue λ as long as approximation-error $\epsilon^{\alpha,\lambda}$ (57) is small. The approximation error will surely changed by these operations. If the finite sums by coefficients would be changed to infinite sums, additional restrictions have to be expected.

Assume a time dependent solution of a partial differential equation with boundary conditions given. The λ-eigenmode mapping operator $\widehat{\bullet}^{\lambda}$ can be applied to the trajectory of boundary conditions as well. A timewise constant boundary condition b is an eigenvector for $\lambda = 1$.

6.1 Incompressible Navier-Stokes Equations as Example

The Navier-Stokes equations can be defined in integral or differential form. The difference is not important here. In differentiable form

$$\operatorname{div} v = 0 \tag{72}$$

$$\partial_t v = -\operatorname{div} v \otimes v - \frac{1}{\rho} \operatorname{grad} p + \nu \Delta v \tag{73}$$

$\operatorname{div} v \otimes v$ is the sole nonlinear term using the local tensor product of the velocity field. The density is here simply 1. ν is the kinematic viscosity.

We discretize the time derivative in a simple way, which is here not relevant, and get for $k = 0, \cdots, p-1$ and $j = 0, 1, 2, \cdots$

$$\operatorname{div} v_{j+k} = 0 \tag{74}$$

$$v_{j+k+1} = v_{j+k} + \Delta t \left(-\operatorname{div} (v \otimes v)_{j+k} - \frac{1}{\rho} \operatorname{grad} p_{j+k} + \nu \Delta v_{j+k} \right) \tag{75}$$

The operators in 3D-space are to be understood as differentiable operators or their discretization.

Applying the λ-eigenmode mapping operator $\widehat{\bullet}^{\lambda}$ with respect to eigenvalue λ to this equation system

$$\operatorname{div} \widehat{v_j}^{\lambda} = 0$$

$$\frac{1}{\Delta t} \left(\lambda \widehat{v_j}^{\lambda} - \widehat{v_j}^{\lambda} \right) = -\operatorname{div} \overbrace{\left(v_j \otimes v_j \right)^{\lambda}} - \frac{1}{\rho} \operatorname{grad} \widehat{p_j}^{\lambda} + \nu \Delta \widehat{v_j}^{\lambda} \quad \forall\, j = 0, 1, 2, \cdots \tag{76}$$

After dividing by λ^j this gives an approximate decomposition into time independent complex components.

Remark, that the equation reflects the actual spacial discretizations of grad, div, Δ as long as these are linear. E.g. the approximate eigenvector of the velocity field is divergence free.

Remark further, that

$$\widehat{(v_j \otimes v_j)}^{\lambda} \neq \left(\widehat{v}_j^{\lambda} \otimes \widehat{v}_j^{\lambda}\right) \quad \forall\, j = 0, 1, 2, \cdots \tag{77}$$

This is the nonlinear term and couples eigenmodes of different eigenvalues (but not all).

To get all of this with a small approximation-error $\epsilon^{\alpha,\lambda}$ (57) we assume that the relevant entities are small after multiplication by $\mathfrak{A}_p(c)$ from the right

$$\begin{bmatrix} v \\ v \otimes v \\ p \end{bmatrix} \mathfrak{A}_p(c) = G\, \mathfrak{A}_p(c) \overset{!}{\approx} 0 \tag{78}$$

The operator G consists on the sequences of all iterations $v = \left[v_j\right]_j$, $v \otimes v = \left[v_j \otimes v_j\right]_j$ and $p = \left[p_j\right]_j$. Remark that we are using (discrete) functions. Practically it turns out, that the term $v \otimes v$ involving many variables, is not necessary. We still don't know, why and under what circumstances.

In the case of a small approximation-error $\epsilon^{\alpha,\lambda}$ (57) we then have for $\forall j = 0, 1, 2, \cdots$

$$\begin{aligned} \widehat{v_{j+1}}^{\lambda} &\approx \lambda\, \widehat{v}_j^{\lambda} \\ \widehat{(v_{j+1} \otimes v_{j+1})}^{\lambda} &\approx \lambda\, \widehat{(v_j \otimes v_j)}^{\lambda} \\ \widehat{p_{j+1}}^{\lambda} &\approx \lambda\, \widehat{p}_j^{\lambda} \end{aligned} \tag{79}$$

7 Remarks

Having a decomposition of the real iterated values g_k as

$$\mathbb{N}_0 \ni k \mapsto g_k = \sum_{l=1}^{p} v_l\, {\lambda_l}^k \tag{80}$$

with $|\lambda_l| \leq 1$ then with (λ_l, v_l) appear also the conjugated elements $\left(\overline{\lambda_l}, \overline{v_l}\right)$. So the decomposition can be written as sum of terms $2\,\mathrm{Re}\, v_l\, {\lambda_l}^k$. These terms could be understood as vectors in a two dimensional subspace moving with the time step k. They can be animated in this form.

Eigenvalues with modulus lower than 1 belong to eigenmodes, which disappear during ongoing iterations. Even for eigenvalues with modulus near to 1, e.g. $|\lambda_l| = 0.999$ the term $v_l \, {\lambda_l}^k$ is reduced by a factor of 0.37 for $k = 1000$.

Changing the degree p of the polynom coefficient vector c has influence on some eigenvalues but not on all. The latter might be candidates for determining the continuous part of the spectrum. On the one hand the degree p of c should be small to limit the number of modes; on the other hand a small degree enlarges the approximation error μ. There must be a balance between the degree p of c, this is the number of eigenvalues, and m as number to take the mean of submatrices. The sum $m + p$ is the number of given measurements. The continuous part of the spectrum is not addressed by this approach. It might be that it numerically shows up by the eigenvalues with eigenvectors with a small norm which are locally uniformly distributed. Our example gives an impression.

For the largest possible $p = n$, we have $\mathfrak{A}(c) = c$ and (c, ρ) can be an eigenpair for smallest eigenvalue of H. This is the setting for the Dynamic Mode Decomposition (DMD) of [12].

8 Computational Costs and Performance Aspects

An essential part of the computational effort is the calculation of the product $G^T G$ in (8) resp. $\widehat{G}^T \widehat{G}$ in (65).

The number of columns of the matrix G is the number of used time steps. The number of rows of G is typically very large. In case of a discretized PDE this number is #(variables per node)∗#(discretization nodes) ∗# (repetitions of the sequence). The effort for reading might be large. Assume a discretization grid with 10^9 nodes with 4 variables per node with 8 B and $n = 1000$ time steps. The stored data are $10^9 * 4 * 1000 * 8$ B = 29.1 TB. A system with a effective read bandwidth of 100 GB/sec would need 298 s to read the data.

The number of operations for the calculation of $G^T G$ is $2 * 4 * 10^9 * 1000^2$ Flop= $8 * 10^{15}$ Flop= $8 * 10^3$ TFlop. On a system running with an effective performance of 10 TFlops we need 800 s computing time which is comparable with the read time. The computing time increases with second order of the number of time steps whereas the reading the input data with the first order. That means, that the process is computationally limited. The second compute intensive part is the multiplication of the matrix G with the matrix consisting on the pseudoeigenvectors $(w_l)_{l=1,\cdots,p}$. The needed effort is comparable to the effort for the calculation of $G^T G$.

Opposite to the size of G the matrix $G^T G$ typically has a relatively small size given by the number of intermediate time steps.

A generalized eigenproblem of size $n - p$ has to be solved iteratively for determining c with degree p. This takes relevant time, if p is relatively small and many iterations have to be made.

9 Application Example

As example we show the simulation of the flow in an artery near the heart aortic-valve with OpenFOAM. The geometry was taken from MRI-data of Fraunhofer Mevis [9] (https://www.mevis.fraunhofer.de/) as well as the estimations of inflow and outflow conditions. The simulation has been done by [11]. Figures 2 and 3 show the square root of the norm of the eigenmodes over the phase of their eigenvalues for time step 0 and time step 2457. The second figure shows disappearing modes with modulus smaller 1 . The distribution also shows prominent eigenvalues which are nearly multiples of a smallest. This property is expected, because λ being a Koopman eigenvalue, also λ^m for $m \in \mathbb{N}$ is an Koopman eigenvalue.

Figures 4, 5, 6, and 7 show the the vector field $2\,\mathrm{Re}\, v_l\ \lambda_l^k$ of the eigenmode l with the second largest norm in the upper part of the aorta for the time steps

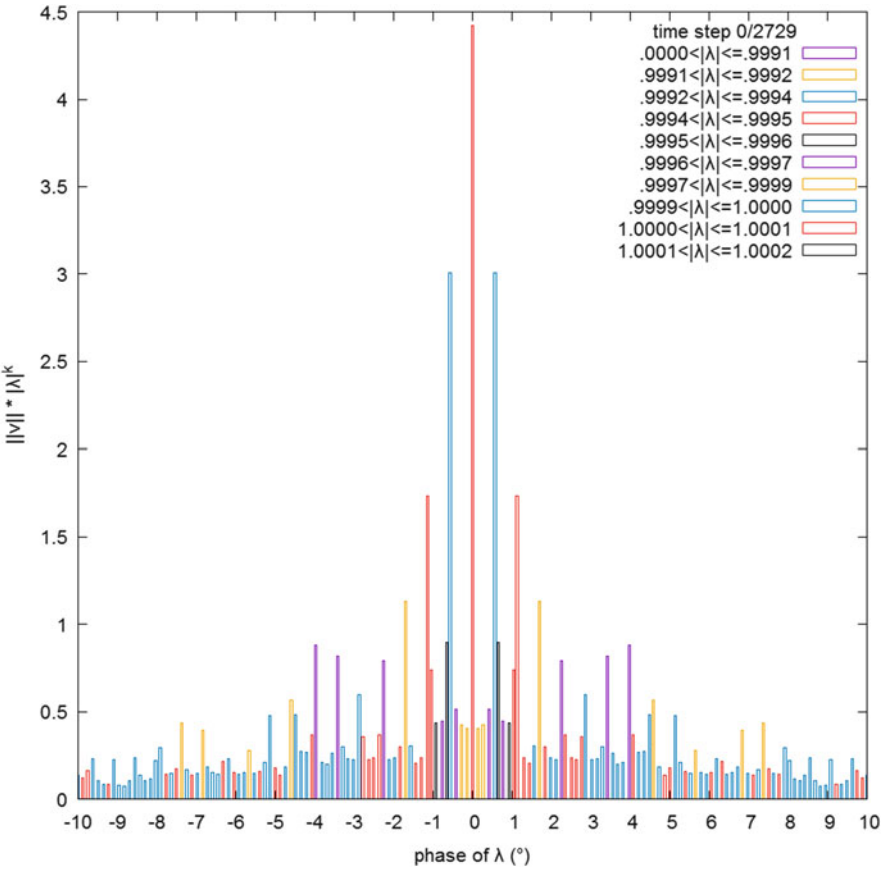

Fig. 2 $\|v_l \lambda_l^k\|$ over phase for time step $k = 0$ in $[-10° : +10°]$

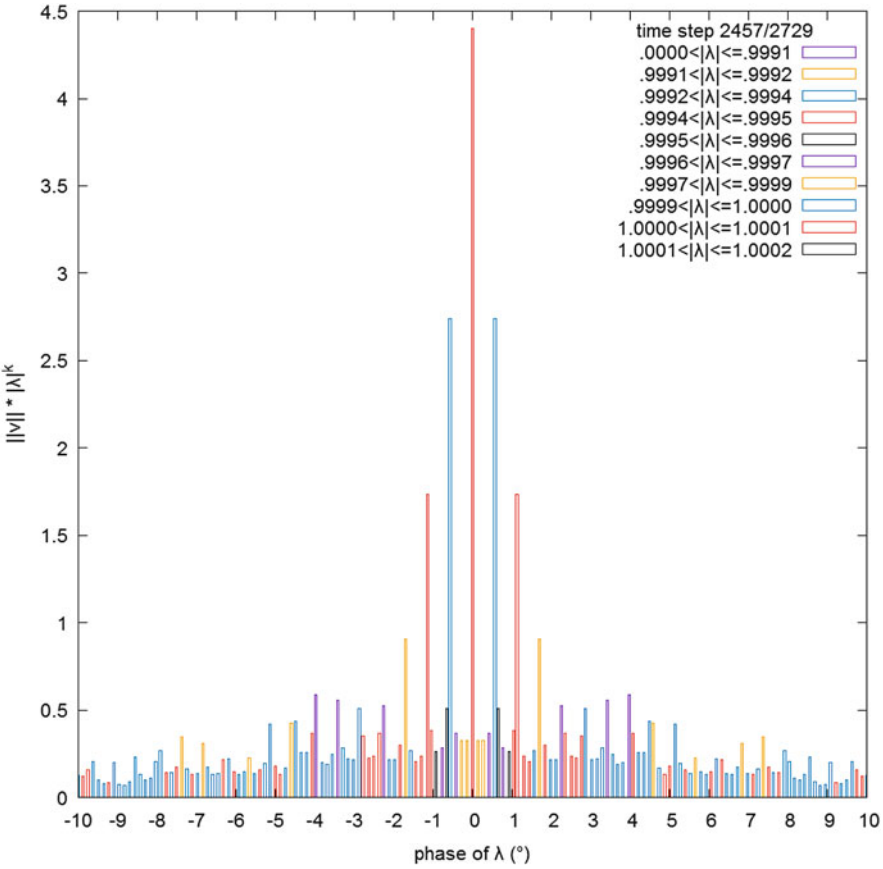

Fig. 3 $\|v_l \lambda_l^k\|$ over phase for time step $k = 2457$ in $[-10° : +10°]$

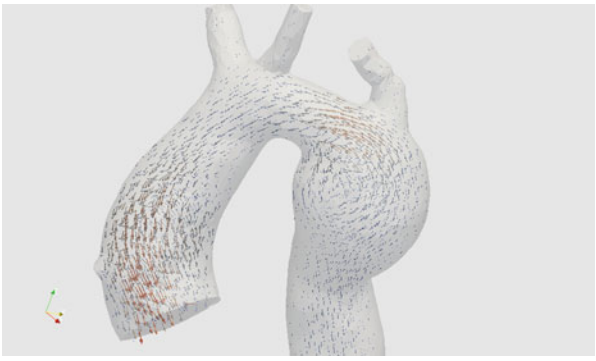

Fig. 4 Time step 661

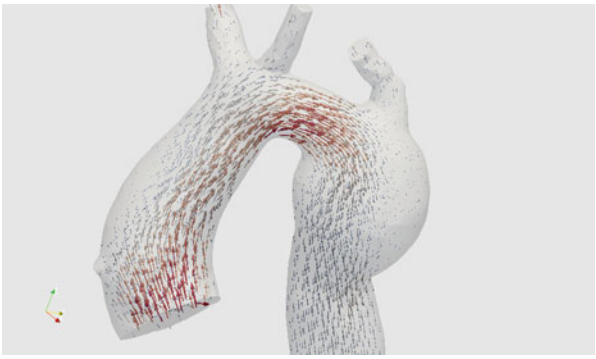

Fig. 5 Time step 841

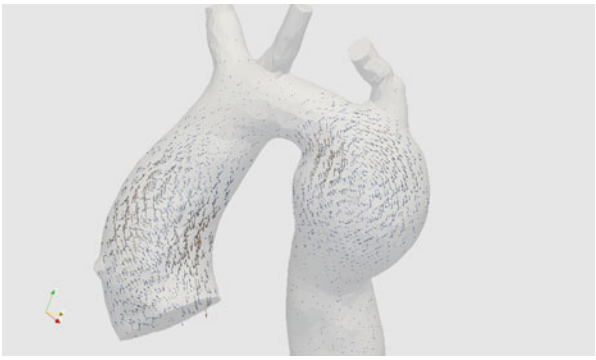

Fig. 6 Time step 1021

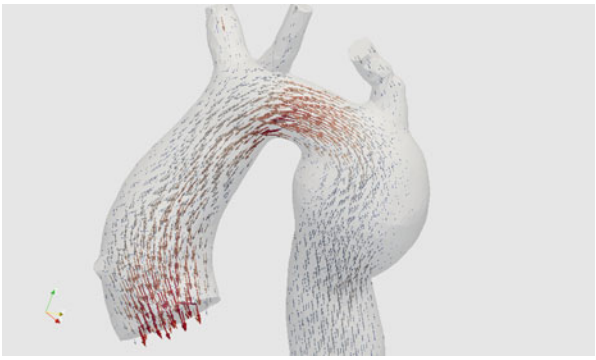

Fig. 7 Time step 1201

$k = 661, 841, 1021, 1201$. It can be seen, that the direction of the vector field is reversed going from time step 841 (5) to time step 1201 (7) and that the vector field disappears in some regions at time step 1021 (6).

The simulated nearly periodic flow is nearly stagnating at a certain time. Interesting is, that the eigenvalues λ_l of the dominant eigenmodes all nearly satisfy $\lambda_l^q = 1$ where $\Delta T = q\ \Delta t$ is the time difference of two flow stagnation events. This is expected because if

$$\sum_{l=1}^{p} v_l\ {\lambda_l}^k = \sum_{l=1}^{p} v_l\ {\lambda_l}^{k+q} \tag{81}$$

it is clear that $\sum_{l=1}^{p} v_l\ \left({\lambda_l}^{k+q} - {\lambda_l}^k\right) = 0$ and for linearly independent v_l that also ${\lambda_l}^{k+q} - {\lambda_l}^k = 0$ implying for $\lambda_l \neq 0$ that $\lambda_l^q = 1$ for all l. This remains true even for linearly dependent v_l if the identity is given for several steps k. We see here the peculiarity of periodic sequences $k \mapsto g_k$.

10 Conclusions

It is possible to determine numerically approximative Koopman eigenvectors for nonlinear operators by linear combinations of iterated values on a trajectory. This is in line with the Wiener-Wintners theorem. These approximative eigenvectors have a direct relation to the partial differential equation defining the operator. The physical meaning is not clear.

We have shown the relationship of variants of the Dynamic Mode Decomposition to Fourier analysis using the theorem of Herglotz-Bochner for the eigenvalues with modulus 1. Whereas this theory handles on spectral parts on the unit circle for an infinite sequence, the proposed methods deliver also eigenvalues with modulus less than 1. We found empirically, that with an eigenvalue λ with a large eigenvector also $\lambda^2, \lambda^3, \cdots$ are appearing. It remains open, how continuous parts of the spectrum can be handled, if they are not yet visible by the proposed procedures.

The approach allows for handling ensembles by integrating all members in the matrix G. The algorithms deliver common eigenvalues and by the described procedures eigenvectors, which are related to each other.

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