

Eigenmodes for nonlinear operators

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Micro Abstract

Even if spectral analysis seems to be restricted to linear operators, it turns out that it is also applicable to nonlinear operators by turning them linear by embedding these in a much larger space and analyzing the Koopman operator. Spectral analysis will be possible but in an infinite dimensional space. We show a numerical approach, which allows to separate different parts of instationary data in a time vanishing part and a remaining part. We discuss implications for calculation and IO.

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Introduction

Linear operators and different kind of matrices are used and deeply analysed as well in mathematics and numerics as also in nearly any application oriented research area. On the other hand most relevant models of nature are nonlinear, so that linear theory seems to be applicable only to local approximations. But a little trick extends the nonlinear to a linear operator, named Composition or Koopman operator, acting on a subspace of the continuous functions on the primary space. This extended linear operator has nice properties, it is bounded, say continuous, has a spectrum and typically eigenvalues and stable eigenspaces. This operator is subject to a discipline of functional analysis, the Ergodic Theory, going back to Ludwig Boltzmann, later investigated by John von Neumann, George David Birkhoff, Bernard Osgood Koopman [4], Norbert Wiener, Aurel Friedrich Wintner, and described in the monograph [3].

What the significance of the Koopman operator and its properties is for a specific scientific domain, has to be analysed. At least the Koopman operator reveals structures directly connected to the nonlinear operator in mind.

Another question is the numerical analysis of these relationships. Even for simple examples the relevant linear spaces are infinite dimensional and not directly accessible by finite dimensional matrix theory. But the approach of the Dynamic Mode Decomposition theory of Peter Schmid [5] turned out to be related to the Koopman operator as pointed out by Igor Mesić and coworkers in [1] and Clarence Rowley and his coworkers in [2].

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 a link to spectral theory of Fourier analysis.

1 The Koopman Operator

Assume a compact space K and a continuous transformation

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

K may be a subset of any topological space with or without any further structure as e.g. being a vector space. Assume a vector space of "observables" $\mathcal{F} \subset C(K)$ describing the nature of the elements of K which is stable in the sense

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

so that the observables can be applied to the composition with the operator. Because of this property, the observables might be infinite dimensional. This property enables the definition

$$f \in \mathcal{F} \Rightarrow T_\varphi f := f \circ \varphi \in \mathcal{F} \quad (3)$$

The operator T_φ is linear, continuous and bounded operator on the in general infinite dimensional space \mathcal{F} . If $f_1, f_2 \in \mathcal{F}$ with $f_1 f_2 \in \mathcal{F}$ then $T_\varphi (f_1 f_2) = (T_\varphi f_1) (T_\varphi f_2)$. T_φ has a spectrum and may have eigenvalues and eigenvectors, which are elements of \mathcal{F} and not of K . The Koopman operator of an linear operator acting on a compact subset of a finite dimensional space is not identical with this operator. With two eigenvalues also their product is an eigenvalue if the product of both eigenfunctions is not 0. All eigenvalues have to have a modulus not larger than 1 because K is compact. The eigenfunctions f fulfill Schröders equation [6]

$$f(\varphi q) = \lambda f(q) \quad \forall q \in K \quad (4)$$

The calculation of the spectrum in a numerical way is not clear because an operator on an infinite dimensional space has to be handled.

The operator φ on the space K has no restrictions in terms of potential applications. It might describe e.g. discretization of nonlinear time dependent partial differential equations (e.g. Navier-Stokes equations) including varying boundary conditions and geometrical boundaries. The iteration trajectories are not forced to converge. Ensembles as in weather forecast are allowed. Non well posed problems can be handled with chaotic or turbulent behaviour, or mixing fluids, particle systems. Also agent based systems as operators on changing graphs and any sequence of measurements can be handled as long as the defining operator is not changed. For the procedures given, it is not necessary to know the operator explicitly, only a sequence of observed values underlying the iterated operator.

1.0.1 Minimum Sets

For handling a PDE (e.g. the incompressible Navier-Stokes equations) discretized by operator ϕ we restrict the compact space K to a single trajectory $(q_k)_{k=0:\infty[}$ defined by $q_{k+1} = \varphi q_k = \varphi^k q_0$ including the accumulation points. $K = \overline{\{\varphi^k q_0 \mid k \in \mathbb{N}_0\}}$ is part of the product space over \mathbb{N}_0 of all state variables at all different discretization nodes. For the analysis it is sufficient to have a vector of observables f and the sequence $f_k = f(q_k) = T_\varphi f(q_{k-1})$. Trajectory and observables are stable with respect to φ . The Koopman operator acts on the sequence by shifting.

If the vector of observables f consists on the evaluation functionals δ_x for all discretization nodes x , then f could be understood as embedding and $f_k = q_k$. This assumes, that K has a linear structure.

1.0.2 Approximation of an λ -eigenmode along a trajectory

Assume a polynom coefficient vector $\alpha = (\alpha_k)_{k=0:p-1}$ defining the polynom $\mathbb{C} \ni \mu \mapsto \alpha(\mu) = \sum_{k=0}^{p-1} \alpha_k \mu^k$. Assume further a complex number λ not being root of this polynom, $\alpha(\lambda) \neq 0$.

Define an induced sequence

$$\widehat{f}_j^{\alpha, \lambda} = \frac{1}{\alpha(\lambda)} \sum_{k=0}^{p-1} f_{j+k} \alpha_k \quad \forall j = 0, 1, 2, \dots \quad (5)$$

summing up p sequential weighted values along the trajectory. The approximate eigenvector condition for shifted elements is

$$0 \approx -\lambda \widehat{f}_j^{\alpha, \lambda} + \widehat{f}_{j+1}^{\alpha, \lambda} = \frac{1}{\alpha(\lambda)} \sum_{k=0}^p f_{j+k} c_k \quad \forall j = 0, 1, \dots \quad (6)$$

where the polynom coefficient vector c is given by the product of polynom α and the polynom $\mu \mapsto \mu - \lambda$. Finding eigenvectors is equivalent in finding nullvectors along the trajectory. An important eigenvalue is 1, which is related to the arithmetic mean along the trajectory. The constant boundary conditions are special eigenvectors of the eigenvalue 1.

The in this way defined λ -eigenmode mapping operator

$$\hat{\bullet}^\lambda : f \mapsto \hat{f}^\lambda = \hat{f}^{\alpha, \lambda} \quad (7)$$

can be applied to a sequence of scalars or vectors or functions or vector fields in the appropriate spaces. By some some reasonable conditions for α and c this operator can be interchanged with spatial (discrete) differential or integration operators making partial differential equations accessible.

2 Numerical techniques

All the numerical techniques define a large matrix consisting on all measured or calculated values

$$G = G_{[0:n]} = [f_0 \ f_1 \ \cdots f_n] \quad (8)$$

1. The Dynamic Mode Decomposition (DMD) method of Peter Schmid [5] can be formulated in a way of determining a vector $c_{[0:n]}$, so that $G_{[0:n-1]}^T G_{[0:n]} c_{[0:n]} = 0$. The roots of the associated polynom of $c_{[0:n]}$ are the approximative eigenvalues λ_l , the vectors $G_{[0:n-1]} w_l / w_l(\lambda_l)$ the approximative eigenvectors.
2. Define the matrix $H = G^T G$ and the convolution matrix (a Toeplitz matrix) for $p \leq n$

$$\mathfrak{A}(c) = \begin{matrix} & 0 & & n-p \\ & \begin{pmatrix} c_0 & & & \\ c_1 & \ddots & & \\ \cdot & \cdot & & c_0 \\ \cdot & \cdot & & c_1 \\ p & c_p & & \vdots \\ \cdot & & \ddots & \\ n & & & c_p \end{pmatrix} \end{matrix} \quad (9)$$

and search c with the property that μ_c is minimal subject to the matrix inequality

$$0 \leq \mathfrak{A}(c)^* H \mathfrak{A}(c) \leq \mu_c \mathfrak{A}(c)^* \mathfrak{A}(c) \quad (10)$$

and that the roots of c have modulus not larger than 1. Again the roots are the approximative eigenvalues and the approximative eigenvectors are determined as before.

3. Taking the trace on both sides and dividing by $n - p + 1$ leads to

$$\langle H^{n-p} c, c \rangle \leq \mu_c \|c\|^2 \quad (11)$$

with the Cesáro means matrix

$$H^{n-p} = \frac{1}{n-p+1} \sum_{j=0}^{n-p} G_{[j:j+p]}^T G_{[j:j+p]} \quad (12)$$

We can show, that these matrices converge for $n \rightarrow \infty$ and a sequence of vectors $c_{[0:p]}$ can be found, so that the roots of the related polynoms converge to the eigenvalues of modulus 1 of the Koopman operator which have only a countable number. Eigenvalues and eigenvectors are determined as before.

4. The following is a Rayleigh like approach. Minimize with respect to λ with $|\lambda| \leq 1$ and α the Rayleigh quotient

$$\max_{b \neq 0} \frac{\left\| G_{[0:p]} \begin{bmatrix} -\lambda \\ 1 \end{bmatrix} * \alpha * b \right\|}{\left\| G_{[0:p-1]} \alpha * b \right\|} \quad (13)$$

If this minimum value is near to 0, α is an eigenvector approximation and λ the eigenvalue. α should be forced in having only roots with modulus less or equal 1. If the minimum reached is near to 0, also the other roots of α are candidates for eigenvalues and can be tested with the same formula. $c = \begin{bmatrix} -\lambda \\ 1 \end{bmatrix} * \alpha$ plays the same role as before.

Conclusions

We show an universal approach for the analysis of iterated data produced by nonlinear operators. What eigenvectors of the Koopman operator mean for the special physical setting is a question for the different application domains. We can show relations to Fourier analysis and Ergodic theory. As the spectrum of operators on infinite dimensional spaces is typically not discrete, the question arises, who to handle the continuous part. This part is related to a partial sequence of the given sequence which is disappearing, if the time step is going to ∞ . How this continuous part appears in the results of proposed algorithms, is still not clear. Also not clear is, how accurate eigenvalues with modulus less than 1 are calculated. The algorithms are delivering these, different to Fourier analysis.

An analysis program has been developed to calculate approximative eigenvectors of fluid flow simulations.

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References

- [1] M. Budišić, R. Mohr, and I. Mezić. Applied koopmanism. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 22(4):047510, 2012.
- [2] K. K. Chen, J. H. Tu, and C. W. Rowley. Variants of dynamic mode decomposition: Boundary condition, koopman, and fourier analyses. *Journal of Nonlinear Science*, 22(6):887–915, Dec 2012.
- [3] T. Eisner, B. Farkas, M. Haase, and R. Nagel. *Operator Theoretic Aspects of Ergodic Theory*. Springer International Publishing, Cham, 2015.
- [4] B. Koopman. Hamiltonian systems and transformation in hilbert space. *Proceedings of the National Academy of Sciences of the United States of America*, 17(5):315–318, May 1931.
- [5] P. J. Schmid. Dynamic mode decomposition of numerical and experimental data. *Journal of Fluid Mechanics*, 656:5–28, 2010.
- [6] E. Schröder. Ueber iterirte functionen. *Mathematische Annalen*, 3(2):296–322, Jun 1870.