Koopman operator theory and deep Koopman neural networks

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Introduction

This project focuses on applying Koopman operator theory to study classical dynamical systems both theoretically and numerically. The brief outline of the project splits mainly into the following two parts,

- **Theory review/application**
  - Koopman theory
  - Existing issue and dilemma
  - Application to DS on finite dimensional space
  - Application to partial differential equation(PDE)
- **Numerical implementations in Python**
  - dlkoopman by Galois Inc.[1]
  - autokoopman by Ethan James Lew[2]
  - Deep-Koopman by Dongyang Kuang[3]

[1] https://github.com/GaloisInc/dlkoopman
[2] https://github.com/EthanJamesLew/AutoKoopman
[3] https://github.com/dykuang/Deep—-Koopman

Koopman operator theory

Setting for the theory

Let's first recall that the setting for the Koopman operator theory can be a continuous dynamical system represented by a system of ordinary differential equations(ODE),

$$\frac{dx}{dt} = F(x), x \in M \subset \mathbb{R}^n \tag{1}$$

where usually the dynamics F is highly nonlinear.
But the setting definitely needs not to be (1). In particular, it can be a more sophisticated dynamical system represented by partial differential equation(PDE) which we shall see later, or a discrete system.

Koopman operator theory

Importance

Let's recall one more time that the Koopman operator provides a way to globally linearize the highly nonlinear dynamics F in (1), and linearization and doing prediction based on the linearized dynamics is our ultimate goal! so this demonstrates the importance of the Koopman operator theory.
Many useful applications based on Koopman operator theory such as DMD and eDMD were created to do prediction and forecasting on dynamical systems.

Space of observable

One of most important concept in the Koopman theory, as we learnt previously, is the so-called space of observable.

Definition: A space of observable, denoted by $\mathcal{F}$, is a function space which consists of all mappings g from the space M to the complex plane $\mathbb{C}$.

Example 1: $\mathcal{F} = C^{\infty}(M)$: The space of all analytic functions
Example 2: $\mathcal{F} = L^2(M)$: The space of all square-integrable functions. This is the space that we will use most often through this whole project! because the Koopman operator defined on it and associated to a dynamical system with conservative quantities(i.e. Hamiltonian system) has nice properties.

We next review the definition of the Koopman operator and its related concepts such as infinitesimal generator and its eigenfunction.

Koopman operator

Definition: The Koopman operator $\mathcal{K}^t$ is a mapping defined on the space of observable $\mathcal{F}$ to $\mathcal{F}$ itself, which satisfies the following condition,

$$[\mathcal{K}^t g](x) \equiv g\left(T^t(x)\right) \tag{2}$$

for any $g \in \mathcal{F}$, and where T^t is the time-t flow for (1).

Definition: The infinitesimal generator of the Koopman operator is a mapping for $\mathcal{F}$ to $\mathcal{F}$itself, which is defined as follow. For any $g \in \mathcal{F}$

$$Ug \equiv \lim_{t \to 0} \frac{\mathcal{K}^t g - g}{t} \tag{3}$$

Based on the above definitions, we have the following lemma which is very useful.

Lemma: For any $g \in \mathcal{F}$,

$$\nabla g \cdot F = Ug \tag{4}$$

Proof.

See lecture slides.

Eigenfunction

Definition: A eigenvalue-eigenfunction pair (λ, ϕ) of the Koopman opertator associated with (1) is defined as follow,

$$\mathcal{K}^t \phi \equiv e^{\lambda t} \phi \tag{5}$$

The following theorem is not hard to prove and it also provides a way to compute the eigenfunction.
Theorem: For each Koopman eigenpair (ϕ, λ),

$$\nabla \phi \cdot F = \lambda \phi \tag{6}$$

Proof.
Use (4) and (5). ■

Eigenvalue/Eigenfunction relation

We review some important relationship between each eigenvalue and its associated eigenfunction. The following two theorems which we had already seen from previous lectures are not hard to prove but keys to demonstrate some Eigenvalue/Eigenfunction relations.

Eigenvalue/Eigenfunction relation

Continued

Theorem

If (ϕ_1, λ_1) *and* (ϕ_2, λ_2) *are two distinct eigenpairs, then* $(\phi_1\phi_2, \lambda_1\lambda_2)$ *is also an eigenpair.*

Proof.

Suppose (ϕ, λ) is a given eigenpair, then observe that

$$\begin{aligned}
\mathcal{K}^t(\phi_1\phi_2)(x) &= (\phi_1\phi_2)(T^t(x)) \\
&= \phi_1(T^t(x))\phi_2(T^t(x)) \\
&= \mathcal{K}^t(\phi_1)(x)\mathcal{K}^t(\phi_2)(x) \\
&= \lambda_1\phi_1(x)\lambda_2\phi_2(x) \\
&= \lambda_1\lambda_2\phi_1(x)\phi_2(x)
\end{aligned}$$

Eigenvalue/Eigenfunction relation

Continued

Theorem

If (ϕ, λ) is an eigenpair, then (ϕ^r, λ^r) is also an eigenpair for any $r \in \mathbb{R}$.

Proof.

Observe that for any $r \in \mathbb{R}$,

$$\begin{aligned}
\mathcal{K}^t \phi^r(x) &= \phi^r(T^t(x)) \\
&= \left(\phi(T^t(x))\right)^r \\
&= \left(\mathcal{K}^t(\phi)(x)\right)^r \\
&= (\lambda \phi(x))^r \\
&= \lambda^r \phi^r(x)
\end{aligned}$$

■

Conjugacy

We note also that conjugacy is an important strategy to compute the eigenfunctions. Let's review the following theorem,

Theorem

Given two dynamical systems $\dot{x} = F(x)$ *and* $\dot{y} = G(y)$ *with respective flow maps* S^t *and* T^t*, if there exists a* C^k *diffeomorphism* h *between the two systems such that* $h(S^t(x)) = T^t(h(x))$ *then* $\phi \circ h$ *is a eigenfunction associated with the system* $\dot{x} = F(x)$ *whenever* ϕ *is a eigenfunction associated with the system* $\dot{y} = G(y)$*.*

We will see an example about using conjugacy to find the Koopman eigenfunction for a nonlinear system based on a linear system where we already know what its eigenfunctions are.

Issue with the spectrum

We have to notice that usually when one tries to compute the Koopman eigenpair (ϕ, λ) for a given system, it is easy to simply treat the eigenvalue λ as a free parameter and hence ignore the fact that only a subset of $\mathbb{C}$ can be the eigenvalues for the Koopman operator.

For most dynamical systems we have encountered, the associated Koopman operator always has a continuous spectrum. For example, the Koopman operator associated with the simple pendulum system which we shall see later only has eigenvalue which lies on the unit circle of the complex plane $\mathbb{C}$. Identifying the continuous spectrum for a given system is a very hard task, but at least this dispels the wrong thought that the Koopman operator only has point spectrum or the entire $\mathbb{C}$ as the eigenvalues.

Issue with the eigenfunction

Besides the issue of the spectrum, the eigenfunction is also sometimes problematic in the sense that for certain dynamical systems, the Koopman eigenfunction may not even exist in a formal sense. In this situation, according to Mezic, we can instead introduce the concept called *eigendistribution/eigenmeasure* as a substitute for the Koopman eigenfunction.

Let's consider the following example which demonstrates such issue with the eigenfunction.

Issue with the eigenfunction

Example

Consider the following dynamical system defined on the action-angle coordinate system $(I, \theta) \in [a, b] \times \mathbb{S}^1$,

$$\begin{aligned} \dot{I} &= 0 \\ \dot{\theta} &= I \end{aligned} \tag{7}$$

We observe first that if a Koopman eigenpair (λ, ϕ) exists for (7), then it has to satisfy

$$\mathcal{K}^t \phi(I, \theta) = \phi(I, \theta + It) = e^{i\omega t} \phi(I, \theta) \tag{8}$$

One may ask why the eigenvalue of $\mathcal{K}^t$ has the form $e^{i\omega t}$, and this is due to the fact that the system (7) preserves the Lebesgue measure μ, and we only restrict the domain of $\mathcal{K}^t$ to $L^2([a, b] \times \mathbb{S}^1, \mu)$!

Issue with the eigenfunction

Example(continued)

It is important to note that the only way to make (8) true is to set $t = 0$, so this means at any other point which lies on the unit circle of the complex plane $\mathbb{C}$, there exists no eigenpair (λ, ϕ).

Now, it is the time to extend the eigenfunction to a much broader scenario.

Eigenmeasure/Eigendistribution

Dirac-delta measure

To define the so-called Koopman eigenmeasure/eigendistribution, we need to understand first the *Dirac-delta "function"*, denoted by $\delta(x)$, which is definied as follow,

$$\delta(x) = \begin{cases} \infty & \text{if } x = 0 \\ 0 & \text{if } x \neq 0 \end{cases} \tag{9}$$

Note that it is not a function in a formal sense because no actual function can satisfy (9), but we can treat it as a measure. Since it is a measure, we can define integral based on it, which has the following properties.

Eigenmeasure/Eigendistribution

Dirac-delta measure(continued)

Property 1: the measure satisfies

$$\int_{-\infty}^{\infty} \delta(dx) = 1 \tag{10}$$

Property 2: For any continuous function f with compact support on $\mathbb{R}$,

$$\int_{-\infty}^{\infty} f(x)\delta(dx) = f(0) \tag{11}$$

Property 3 (Translation): For any continuous function f with compact support on $\mathbb{R}$, and a fixed number $y \in \mathbb{R}$,

$$\int_{-\infty}^{\infty} f(x)\delta(x-y)dx = f(y) \tag{12}$$

Note: The "Property 3" is very useful in many fields of analysis.

Eigenmeasure/Eigendistribution

Definition

Definition: The Koopman eigenmeasure or eigendistribution, associated with the system (7) and denoted by $\phi(I, \theta)$, is defined as the following variant of the Dirac-delta measure. For a constant $c \in \mathbb{R}$,

$$\phi(I, \theta) = e^{i\theta}\delta(I - c) \tag{13}$$

where it must satisfy the following chain of equalities.
For any smooth function $w(I, \theta)$ with compact support in $[a, b] \times \mathbb{S}^1$,

$$\begin{aligned} \int \mathcal{K}^t \phi(I, \theta) w(I, \theta) dI d\theta &= \int \phi(I, \theta + It) w(I, \theta) dI d\theta \\ &= \int e^{i(\theta + It)} \delta(I - c) w(I, \theta) dI d\theta \\ &= e^{ict} \int \phi(I, \theta) w(I, \theta) dI d\theta \end{aligned} \tag{14}$$

Connection to Eigenfunction

For a dynamical system other than (7), we can define the associated Koopman eigenmeasure/eigendistribution similarly as (13), but we have to realize that there is a relationship between it and the Koopman eigenfunction, which is specified by the following lemma.

Lemma

For a given dynamical system, any associated Koopman eigenfunction is also eigenmeasure/eigendistribution.

Proof.

Use the definition of eigenfunction and (14). ■

Note: The converse statement is definitely not true since eigenmeasure/eigendistribution is even not a function in a formal sense as we discussed before.

Examples

Next, we will switch our focus to some examples of dynamical system which can be represented by a system of ODE or PDE, where we actually are able to identify the spectrum of the associated Koopman operator and to compute analytically its eigenfunctions.

Linear system

As a warm-up, we first do a quick review on the linear dynamical system defined on a finite-dimensional state space.
Any continuous linear dynamical system has the following canonical form

$$\dot{x} = Ax \tag{15}$$

where $x \in \mathbb{R}^n$ and A is a $n \times n$ matrix. For simplicity, we assume that the matrix A only has simple eigenvalues.
We have already seen from our homework that its **primary** eigenfunctions are

$$\phi_n(x) = \langle x, w_n \rangle \tag{16}$$

where $\{w_n\}$ is the set of eigenvectors associated with the adjoint matrix A^* of A.
We note that for any linear system, the associated Koopman operator always has a point spectrum which consists of all the eigenvalues of A.

Linear system

Continued

Recall that once in class we were asked if the primary eigenfunctions from Eq. (16) are all the Koopman eigenfunctions for the linear system?
The answer is NO, and it turns out that a linear system can have more eigenfunctions than these presented in Eq. (16). To see this, let us look at the following example.

Linear system

Diagonal A

Consider the example for the continuous linear system where the matrix A in Eq.(15) is diagonal, say $A = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$.
Recall from the previous lecture that the primary eigenfunctions associated with it are simply the coordinate observers, namely

$$\begin{aligned} \phi_{\lambda_1}(x, y) &= x \\ \phi_{\lambda_2}(x, y) &= y \end{aligned} \tag{17}$$

On the other hand, we can obtain the eigenfunctions by solving Eq.(6). Note that we need to impose an initial data curve on (6) to make it become a Cauchy initial value problem. The initial data curve $\Lambda = \{(x, y, z) = (f_1(s), f_2(s), h(s))\}$ has to satisfy the so-called *transverse* property according to the method that we used to solve the Cauchy problem.

Linear system

Continued: Diagonal A

By choosing the initial data curve as $\Lambda = \{(x, y, z) = (s, 1, h(s))\}$, the solution to the Cauchy problem reads

$$\phi_\lambda(x, y) = y^{\frac{\lambda}{\lambda_2}} h\left(\frac{x}{y^{\frac{\lambda_1}{\lambda_2}}}\right) \tag{18}$$

Note that Eq.(18) is only valid for $\lambda = \lambda_1$ and $\lambda = \lambda_2$, and in particular when $\lambda = \lambda_2$, we have that

$$\phi_{\lambda_2}(x, y) = yh\left(\frac{x}{y^{\frac{\lambda_1}{\lambda_2}}}\right) \tag{19}$$

A easy observation is that if we choose the initial data $h = 1$, we obtain

$$\phi_{\lambda_2}(x, y) = y \tag{20}$$

Linear system

Continued: Diagonal A

Eq.(19) actually demonstrates two key points:
1. The primary eigenfunctions(coordinate observers) are not the only components in the eigenspace, and in fact there are uncountably many.
2. Both primary eigenfunctions can be derived from the expression of the general eigenfunction.

Furthermore, we will see how we need to manipulate the Cauchy problem which yields a general solution that can be used to derived the other primary eigenfunction. But the point here is that it is just the business of choosing the initial data distribution.

Linear system

Continued: Diagonal A

We notice that Eq.(19) can somehow only lead one primary eigenfunction which is the second coordinate observer. But, if we change the original initial data curve Λ to $\Lambda = \{(x, y, z) = (1, s, h(s))\}$, then the solution to the corresponding Cauchy problem reads

$$\phi_\lambda(x, y) = x^{\frac{\lambda}{\lambda_1}} h\left(\frac{y}{x^{\frac{\lambda_2}{\lambda_1}}}\right) \tag{21}$$

Similary, Eq.(21) only holds for either $\lambda = \lambda_1$ or $\lambda = \lambda_2$ and if we choose $\lambda = \lambda_1$ and the initial data $h = 1$, we get

$$\phi_{\lambda_1}(x, y) = x \tag{22}$$

Linear system

A with simple eigenvalues

For a general case where the matrix A is not necessarily diagonal but still only has simple eigenvalues, the previous reasoning still applies because of the following theorem,

Theorem

Given two continuous linear dynamical systems,

$$\begin{aligned} \dot{x} &= Wx \\ \dot{y} &= Gy \end{aligned} \tag{23}$$

they are topologically conjugate if and only if there exists an invertible matrix P such that

$$W = PGP^{-1} \tag{24}$$

To illustrate this, we consider another example shown in the following slide.

Linear system

Example

Consider the following linear system

$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= x \end{aligned} \tag{25}$$

According to (16), the eigenfunctions are

$$\begin{aligned} \phi_1(x, y) &= y + x \\ \phi_2(x, y) &= y - x \end{aligned} \tag{26}$$

But, the most general form of the associated eigenfunction should read

$$\phi(x, y) = f\left[(y - x)(y + x)\right](y + x)^{\lambda} \tag{27}$$

where f is any function in the class C^1.
We note that λ in (19) can only be either 1 or -1 because the matrix A only has these two eigenvalues.

Linear system

Example continued

This shows that by taking f from (9) to be any analytic function, we have new eigenfunctions! for instance, we have

$$\phi(x, y) = \tanh(y^2 - x^2)(y + x) \tag{28}$$

or

$$\phi(x, y) = \frac{\sin(y^2 - x^2)}{y + x} \tag{29}$$

as the new candidates for the eigenfunction corresponding to eigenvalue 1 and -1, respectively.

1D nonlinear system

If we are interested in learning the following one-dimensional autonomous system

$$\dot{x} = F(x), x \in M \subset \mathbb{R} \tag{30}$$

In this case, by (6), each Koopman eigenpair (ϕ, λ) simply satisfies

$$\frac{d\phi}{dx} \cdot F(x) = \lambda\phi \tag{31}$$

(8) is easy to solve and its solution reads

$$\boxed{\phi(x) = p \exp\left(\int \frac{\lambda dx}{F(x)}\right)} \tag{32}$$

where p is an arbitrary constant.

Note: (9) has also been derived by Kutz in his paper [1].

Simple pendulum

The simple pendulum is a classic dynamical system which was widely studied long time ago. It can be represented by the following second-order nonlinear differential equation,

$$\ddot{x} + \frac{g}{L}\sin(\omega x) = 0 \tag{33}$$

where g is the magnitude of the gravitational field and L the length of the rod or cord.
In our project, for simplicity, we assume that $\omega = 1$ and $\frac{g}{L} = 1$.
Eq.(33) can be easily written into the following 2D first-order system,

$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= -\sin(x) \end{aligned} \tag{34}$$

Simple pendulum

Spectrum

For the spectrum of the Koopman operator associated with the simple pendulum system, we claim that it must lie on the unit circle of the complex plane $\mathbb{C}$. This is because the simple pendulum system is a Hamiltonian system with the conservative quantity,

$$H(x, y) = \frac{1}{2}y^2 - \cos(x) \tag{35}$$

We notice that any Hamiltonian system preserves the Lebesgue measure μ, namely the dynamics T preserves μ. By results from ergodic theory (See lecture slides), we know the Koopman operator associated with any Hamiltonian system is a unitary operator w.r.t the domain $L^2(M, \mu)$. This shows that the eigenvalues for the Koopman operator associated with the simple pendulum system must be a subset of $\{\lambda = e^{i\omega t} \mid \omega \in \mathbb{R}\}$

Simple pendulum

Issue with the spectrum

Although we have explicitly demonstrated that all eigenvalues of the Koopman operator associated with the simple pendulum system can only lie on the unit circle of the complex plane $\mathbb{C}$, the tricky question is that what the *full spectrum* of the Koopman operator is? This question is essentially important because keep in mind that not all complex numbers on the unit circle are the eigenvalues.

Simple pendulum

Eigenfunction

We have derived the Koopman eigenfunction for the simple pendulum system which reads,

$$\phi(x,y) = f(p)\exp\left(\int \frac{dx}{\sqrt{2\cos(x)+2p}}\right)^{\lambda}\Bigg|_{p=\frac{1}{2}y^2-\cos(x)} \tag{36}$$

Note: We notice that (13) is only valid for some λ which lies on the unit circle of the complex plane $\mathbb{C}$.

Simple pendulum

Prediction

With the eigenpair we have derived from Eq.(36), we know how a given observable g evolves by presenting the following Koopman spectral decomposition

$$\mathcal{K}^t g(x) = \sum_{i=1}^{\infty} e^{\lambda_i t} c_i(g) \phi_i(x) \tag{37}$$

where we call each complex value c_i the Koopman mode.

Now Let's move to the next interesting system which is the Duffing system.

Duffing system

The most general Duffing system is represented by the following second-order ordinary differential equation(ODE),

$$\ddot{x} + \delta\dot{x} + \alpha x + \beta x^3 = \gamma \cos(\omega t) \tag{38}$$

Eq.(38) can be easily rewritten as the following two-dimensional(2D) first-order system of ODE,

$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= -\delta y - \alpha x - \beta x^3 + \gamma \cos(\omega t) \end{aligned} \tag{39}$$

where $\delta, \alpha, \beta, \gamma, \omega$ are all given constants.

Duffing system

Koopman eigenfunction

Suppose we are interested in the undamped autonomous without-force version of (38), namely $\delta = \gamma = 0$, and

$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= -\alpha x - \beta x^3. \end{aligned} \tag{40}$$

Then the Koopman eigenfunction for (12) has the following form,

$$\phi(x, y) = f(p) \exp\left(\int \frac{\lambda dx}{\sqrt{2p - \alpha x^2 - \frac{1}{2}\beta x^4}} \right) \Bigg|_{p=\frac{1}{2}y^2+\frac{1}{2}\alpha x^2+\frac{1}{4}\beta x^4} \tag{41}$$

where f is a C^1 function of a single real variable.

Duffing system

Spectrum of the Koopman operator

Similar to the simple pendulum system, it should not be surprising that the Duffing system also has a continuous spectrum. Moreover, since we restrict our attention to the undamped Duffing without external force (i.e. system (25)), the system is Hamiltonian and hence preserves the Lebesgue measure under the function space $L^2(M, \mu)$. By the similar argument made on the simple pendulum system, we conclude that the spectrum of the associated Koopman operator of the Duffing system is a subset of the complex numbers lying on the unit circle of $\mathbb{C}$.

Duffing system

Hamiltonian quantity

One of the most important quantities for the undamped without-force Duffing system is the Hamiltonian denoted by $H \equiv H(x, y)$, which is the Koopman eigenfunction corresponding to $\lambda = 0$, namely

$$\mathcal{K}^t H = H \tag{42}$$

Or equivalently,

$$\boxed{\nabla H \cdot F = 0} \tag{43}$$

The general solution to (43) reads

$$H(x, y) = f\left(\frac{1}{2}y^2 + \frac{1}{2}\alpha x^2 + \frac{1}{4}\beta x^4\right). \tag{44}$$

Note: Setting f to be the identity map results in the standard Hamiltonian for Duffing system which reads

$$H(x, y) = \frac{1}{2}y^2 + \frac{1}{2}\alpha x^2 + \frac{1}{4}\beta x^4. \tag{45}$$

A particular 2D system

Based on the work on Duffing system, we can also derive the Koopman eigenfunctions for the following type of 2D systems analytically,

$$\begin{aligned} \dot{x} &= f(x)g(y) \\ \dot{y} &= h(x)q(y) \end{aligned} \tag{46}$$

where f, g, h, and q are assumed to be all in the class C^1 to guarantee the system(46) has a unique solution.

The following theorem provides the analytical expression for the Koopman eigenfunctions.

A particular 2D system

Continued

Theorem

The Koopman eigenpair (ϕ, λ) for (16) has the following form,

$$\phi(x,y) = f(p)\exp\left(\int \frac{\lambda dx}{f(x)g\left[T^{-1}\left(p+\int \frac{h(x)}{f(x)}dx\right)\right]}\right)$$

$$\Big|_{p=\int\left(\frac{g(y)}{q(y)}\right)dy-\int\left(\frac{h(x)}{f(x)}\right)dx}$$

where f is in the class of C^1, and $T(y)$ reads

$$T(y) = \int \frac{g(y)}{q(y)}dy \tag{47}$$

Example

Let's look at one toy application of the theorem from the last page. Consider the following 2D nonlinear dynamical system,

$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= y^2 \end{aligned} \tag{48}$$

We compute first

$$T(y) = \int \frac{y}{y^2} dy = \log(y) \implies T^{-1}(y) = e^y \tag{49}$$

and

$$\int \frac{h(x)}{f(x)} dx = \int dx = x \tag{50}$$

Then plugging everything into the expression of $\phi(x, y)$ results in

$$\phi(x, y) = f(\log(y) - x) \exp\left(\frac{\lambda}{y}\right) \tag{51}$$

Exercise: Following the above example, if we take $g(y) = y^n$ and $q(y) = y^{n+1}$, we also will get a closed form for $\phi(x, y)$ without an integral term.

Warning

The theorem is not very useful for the situation when the integral term involved in the expression of $\phi(x, y)$ does not have a closed form (e.g. elliptic integral). In this situation, it almost surely indicates that the system possesses a continuous spectrum which we then need to defined its corresponding eigenmeasure/eigendistribution and the formal eigenfunction will not exist in the formal sense as we discussed before.

Koopman operator for PDE

Now, let us change our focus to dynamical system represented by partial differential equations. Before we actually dig into the Koopman theory for dynamical system on infinite-dimensional state space, we can see some examples.

Linear Diffusion equation

Linear diffusion equation is also known as the heat equation, considered as probably the most classical equation in a undergraduate PDE class. It simply models the transfer of heat on a given object...

The equation is gievn as follow

$$u_t = \alpha u_{xx}. \tag{52}$$

where α is a fixed constant.

Burger's equation

Burger's equation is a nonlinear PDE which is analytically solvable by applying the so-called Hopf-Cole transformation to transform the nonlinear equation into the linear diffusion equation.

For simplicity, we focus on the *viscous* Burger's equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2} \tag{53}$$

Note: There are much more PDEs besides the above two such as wave equation, Schodinger equation... If you are interested in more, simply do a literature review or look them up on Wikipedia.

Infinite-dimensional state space

Based on the linear diffusion equation and Burger's equation, we know most PDEs used to model any real-life phenomenon has the following standard form

$$\frac{\partial u(x,t)}{\partial t} = \mathcal{F}[u(x,t)] \tag{54}$$

where $\mathcal{F}$ represents a time-independent nonlinear operator. Compared with the classical dynamical system represented by ODE $\dot{x} = F(x)$, (39) is nothing but a dynamical system sitting on an infinite-dimensional state space, where in this case $\mathcal{F}$ is the dynamics.

Space of observable

Before we introduce the associated Koopman operator for (34), we first need to understand what our space of observable is in this situation. To this end, We need to introduce first the concept of functional.

Definition

A functional is a mapping from a function space to the complex plane $\mathbb{C}$.

Definition

We defined the space of observable as the functional space, denoted by $\mathcal{B}$, which contains all functionals from the field space to the complex plane $\mathbb{C}$

Examples of functional

1. Let $C[0,1]$ be the space of continuous functions defined on $[0,1]$. We define the functional $\phi : C[0,1] \to \mathbb{C}$ as follow

$$\phi[f] = f(1) \tag{55}$$

for any $f \in C[0,1]$.

2. Another example would be

$$\phi[f] = \int_0^1 f(x)dx \tag{56}$$

for any $f \in C[0,1]$.

Koopman operator

Definition

The associated Koopman operator for the system (54) is the mapping $\mathcal{K}^t : \mathcal{B} \to \mathcal{B}$ such that (2) holds.

As we expect it, the only discrepancy between the definition of the Koopman operator associated with a system represented by PDE and one represented by a ODE is the space of observables. Accordingly, there is some minor modification on the definition of its infinitesimal generator.

Infinitesimal generator

Since, by observation, the family of operators $\{\mathcal{K}^t\}_{t\geq 0}$ is a semigroup, we can define the corresponding infinitesimal generator U as follow.

Definition

For any functional $g \in \mathcal{B}$,

$$Ug[u] = \lim_{t\to 0} \frac{\mathcal{K}^t g[u] - g[u]}{t}$$
$$\boxed{= \int_0^L \mathcal{F}\{u(x)\} \frac{\delta g[u(x)]}{\delta u(x)} dx} \tag{57}$$

where $\dfrac{\delta g[u(x)]}{\delta u(x)}$ denotes the *functional derivative*.

We will introduce briefly the functional derivative which is an important concept in *Calculus of Variation*.

Infinitesimal generator

Functional derivative

For a given smooth functional $g[u]$, we define its derivative as follow.

Definition

$$\lim_{t\to 0} \frac{g[u+t\eta]-g[u]}{t} = \int \frac{\delta g[u]}{\delta u(x)}\eta(x)dx \tag{58}$$

where $\eta(x) \in C_c^\infty(\mathbb{R})$ is an arbitrary test function.

With all these prerequisite knowledge, we are now ready to define the so-called Koopman eigenfunctional.

Eigenfunctional

The eigenfunctional is defined in a similar fashion as the eigenfunction that we discussed a while ago.

Definition

The eigenfunctional $\phi[u]$ is a special functional in $\mathcal{B}$ such that

$$\mathcal{K}^t \phi_\lambda[u] = e^{\lambda t} \phi_\lambda[u] \tag{59}$$

The following theorem demonstrates the relationship between the eigenfunctional and the generator U.

Theorem

The eigenfunctional $\phi[u]$ *satisfies*

$$U\phi[u] = \lambda \phi[u] \tag{60}$$

Next, we will see an important theorem which can tell us all the eigenfunctionals in closed form for any system represented by (35) where the dynamics $\mathcal{F}$ is linear.

Eigenfunctional for linear $\mathcal{F}$

Assume that the dynamics $\mathcal{F}$ in (39) is linear, and $w(x)$ the eigenfunction of the adjoint operator of $\mathcal{F}$, namely

$$\mathcal{F}^*\{w(x)\} = \lambda w(x) \tag{61}$$

Theorem

The eigenfunctional for the system (35) reads

$$\phi_\lambda[u] = \int_0^L u(x)\overline{w(x)}dx \tag{62}$$

The theorem is not hard to prove and we can do it in the next slide.

Proof of the theorem

Proof.

Observe that by (43),

$$
\begin{aligned}
U\phi[u] &= \int_0^L \left(\mathcal{F}(u(x))\right) \frac{\delta\phi[u]}{\delta u(x)} dx \\
&= \lim_{\epsilon\to 0} \frac{\phi[u + \epsilon\left(\mathcal{F}(u(x))\right)] - \phi[u]}{\epsilon} \\
&= \lim_{\epsilon\to 0} \frac{\int_0^L [u(x) + \epsilon\left(\mathcal{F}(u(x))\right)]\overline{w_\lambda(x)}dx - \int_0^L u(x)dx}{\epsilon} \\
&= \int_0^L \left(\mathcal{F}(u(x))\right) \overline{w_\lambda(x)} dx \\
&= \int_0^L u(x)\overline{\mathcal{F}^*(w(x))} dx \\
&= \overline{\lambda} \int_0^L u(x)\overline{w(x)} dx = \overline{\lambda}\phi[u]
\end{aligned}
$$

Diffusion equation

Basic setting

Let's now discuss the application of the theorem (62) to some well-known PDEs. The first one we will see is the diffusion equation. For simplicity, we assume the coefficient $\alpha = 1$, so the equation is $u_t = u_{xx}$. We also assume the solution $u(x,t) \in L^2([0,L] \times \mathbb{R}_+)$ satisfies the Neumann boundary condtions which read

$$\frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(L,t) = 0 \tag{63}$$

We observe first that the dynamics operator $\mathcal{F}$ is

$$\mathcal{F} = \frac{\partial^2}{\partial x^2} \tag{64}$$

and it is not hard to show $\mathcal{F}$ is self-adjoint via integration by parts, so $\mathcal{F} = \mathcal{F}^*$.

Diffusion equation

Eigenfunctional

To find the eigenfunctional, we compute first the solution to the following eigenvalue problem of the adjoint dynamics operator $\mathcal{F}^*$ which reads

$$\frac{\partial^2 w}{\partial x^2} = \bar{\lambda} w \tag{65}$$

By the standard ODE solving technique together with the boundary conditions (63), the solution reads

$$w(x) = cos\left(\frac{n\pi x}{L}\right) \tag{66}$$

where $n = 1, 2, ...$

Finally, by Eq.(62), we know the eigenfunctionals associated with the diffusion equation have the form

$$\boxed{\phi_n[u] = \int_0^L u(x) cos\left(\frac{n\pi x}{L}\right) dx} \tag{67}$$

Exercise: Derive the eigenfunctionals of the diffusion equation with the *Dirichlet boundary conditions*.

Burger's equation

Basic setting

The next example we will see is the viscous Burger's equation which is a nonlinear PDE. Although it is nonlinear, but it is topologically conjugate with the linear diffusion equation so that if we can compute the associated homeomorphism mapping, we are guaranteed to obtain all its eigenfunctionals.
First, let us assume the setting is that we have the viscous Burger's equation and its solution $u(x,t) \in L^2([0,L],\mathbb{R}_+)$ satisfies the Dirichlet boundary conditions which read

$$u(0,t) = u(L,t) = 0 \tag{68}$$

Burger's equation

Cole-Hopf transformation

The Burger's equation and the diffusion equation is closely related by the so-called Cole-Hopf transformation

$$u(x,t) = -2\frac{1}{v(x,t)}\frac{\partial}{\partial x}v(x,t) \tag{69}$$

where $v(x,t)$ satisfies

$$v(x,t) = c(t)\exp\left(\int_0^x u(y,t)dy\right) \tag{70}$$

and $c(t)$ needs to be chosen so that $v(x,t)$ satisfies the diffusion equation with the Neumann boundary conditions, namely

$$\frac{\partial v}{\partial x}(0,t) = \frac{\partial v}{\partial x}(L,t) = 0 \tag{71}$$

This means $v(x,t)$ solves the diffusion equation with Neumann boundary conditions if and only if $u(x,t)$ solves the viscous Burger's equation with Dirichlet boundary conditions.

Burger's equation

Continued

To find the eigenfunctional for Burger's equation, we compute first the expression for $c(t)$. To this end, with the boundary conditions, if we substitute Eq. (55) into the diffusion equation, we have

$$\frac{d}{dt}\ln\left(c(t)\right) = \frac{1}{2}\left(-\frac{\partial u(x,t)}{\partial x}\right)\Bigg|_{x=0} \tag{72}$$

Then, we can create the following candidate for $c(t)$ which reads

$$\boxed{c(t) = \left(\int_0^L \exp\left(-\frac{1}{2}\int_0^x u(y,t)dy\right)dx\right)^{-1}} \tag{73}$$

Burger's equation

Eigenfunctional

Now let us recall the conjugacy theorem which tells us that $\phi^D \circ h$ is the eigenfunctional for the Burger's equation, where ϕ^D denotes the eigenfunctional of the diffusion equation, and h the homeomorphism mapping which is the Hopf-Cole transformation. Using this fact, we eventually know the eigenfunctional ϕ^B for the Burger's equation reads

$$\phi^B[u] = \int_0^L \left[c[u] \exp\left(-\frac{1}{2} \int_0^x u(y)dy \right) - \frac{1}{L} \right] \times \cos\left(\frac{n\pi x}{L} \right) \quad (74)$$

where

$$c[u] = \left(\int_0^L \exp\left(-\frac{1}{2} \int_0^x u(y)dy \right) dx \right)^{-1} \quad (75)$$

and $n = 1, 2, ...$

References

[1] Morrison, Megan Kutz, J.. (2022). Solving nonlinear ordinary differential equations using the invariant manifolds and Koopman eigenfunctions. 10.48550/arXiv.2208.08529.
[2] Hiroya Nakao, Igor Mezić; Spectral analysis of the Koopman operator for partial differential equations. Chaos 1 November 2020; 30 (11): 113131.

Numerical implementation

Now we have finished the theory part of this project, and let us turn to see how we can numerically use Koopman theory to train a neural network.

Quick review of DMD

Given some trajectory data $\mathbf{x_k}, \quad k = 0, \ldots, K$, we might make the assumption that there is some linear transformation of the first $K-1$ terms that gives us the last $K-1$ terms, with a residual term re_{K-1} left over, where $e_{K-1} = \{0, 0, \ldots, 1\}^T$. This relationship can be denoted as

$$\mathbf{x}_K = A\mathbf{x}_{K-1} + re_{K-1}$$

where $\mathbf{x}_{K-1}$ denotes the last $K-1$ terms of the trajectory, and $\mathbf{x}_{K-1}$ denotes the first $K-1$ terms.

Quick review of DMD

With dynamic mode decomposition (DMD), we make the assumption the residual can be safely ignored without too much error. Then, we can simply solve for A via the calculation

$$A = \mathbf{x}_K \mathbf{x}_{K-1}^{\dagger}$$

where $\dagger$ denotes the Moore-Penrose pseudo-inverse.

Quick review of DMD

In terms of Koopman theory, this is equivalent to approximating the infinite dimensional Koopman operator $\mathcal{K}$ associated with the observable $g(\mathbf{x}) = \mathbf{x}$ by a finite dimensional Koopman matrix A. The eigenvalues and eigenvectors of A are approximately the eigenvalues and modes of $\mathcal{K}$.

Quick review of SVD

Actually calculating A is often far too costly, considering it is $(K-1) \times (K-1)$. Luckily, we can capture the most "important" features via Singular Value Decomposition (SVD). Any $m \times n$ matrix can be factored into a product of a $m \times m$ complex unitary matrix U, an $m \times n$ diagonal matrix Σ with non-negative entries, and the transpose V^* of a complex $n \times n$ unitary matrix V.

Quick review of SVD

The diagonal matrix Σ in the SVD contains the singular values of your original matrix. The SVD is not unique, most software implementations will provide the SVD where Σ has the diagonal entries in decreasing order.

Quick review of SVD

The diagonal matrix Σ in the SVD contains the singular values of your original matrix. The SVD is not unique, most software implementations will provide the SVD where Σ has the diagonal entries in decreasing order. SVD may result in some zero entries in Σ, which gives us a dimensionality reduction of our original matrix.

Quick review of SVD

The diagonal matrix Σ in the SVD contains the singular values of your original matrix. The SVD is not unique, most software implementations will provide the SVD where Σ has the diagonal entries in decreasing order.

Using SVD and DMD

If we substitute in the SVD of $\mathbf{x}_{K-1}$ and rearrange the equation, we can find the matrix $S = U^* \mathbf{x}_K V \Sigma^{-1}$. It turns out that the eigenvalues of S are precisely the DMD eigenvalues. For the DMD modes, we calculate Ue_i, where e_i is the i-th eigenvector of S.

Using SVD and DMD

To save computational cost, we can truncate the SVD of $\mathbf{x}_{K-1}$ by sizing down the matrices in the SVD primarily by only taking a subset of the largest diagonal entries of Σ.

EDMD

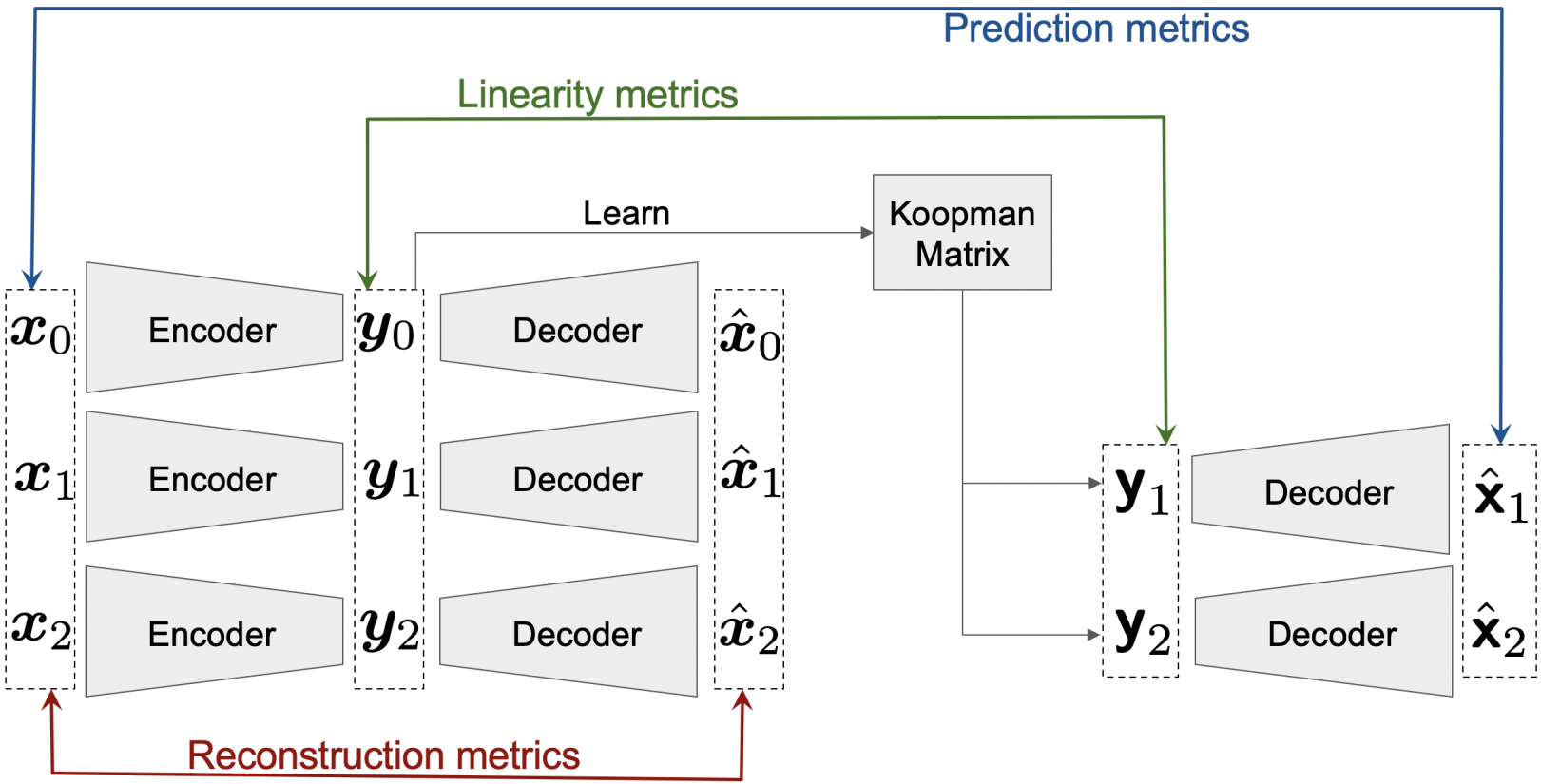
For Koopman theory, we are interested in the eigenvalues and Koopman modes of all sorts of observables. Extended DMD (EDMD) runs the same process just outline, except now we run the algorithm on $g(\mathbf{x}_K = \{g(x_2), \ldots, g(x_K)\}$ and $g(\mathbf{x}_{K-1} = \{g(x_1), \ldots, g(x_{K-1})\}$.

Observables

Often, we might not have any good *a priori* ideas about observables to pick. This is where neural networks come in. Using a well-designed autoencoder will allow us to find data-driven nonlinear observables that hopefully lead to a very good approximation of the Koopman operator.

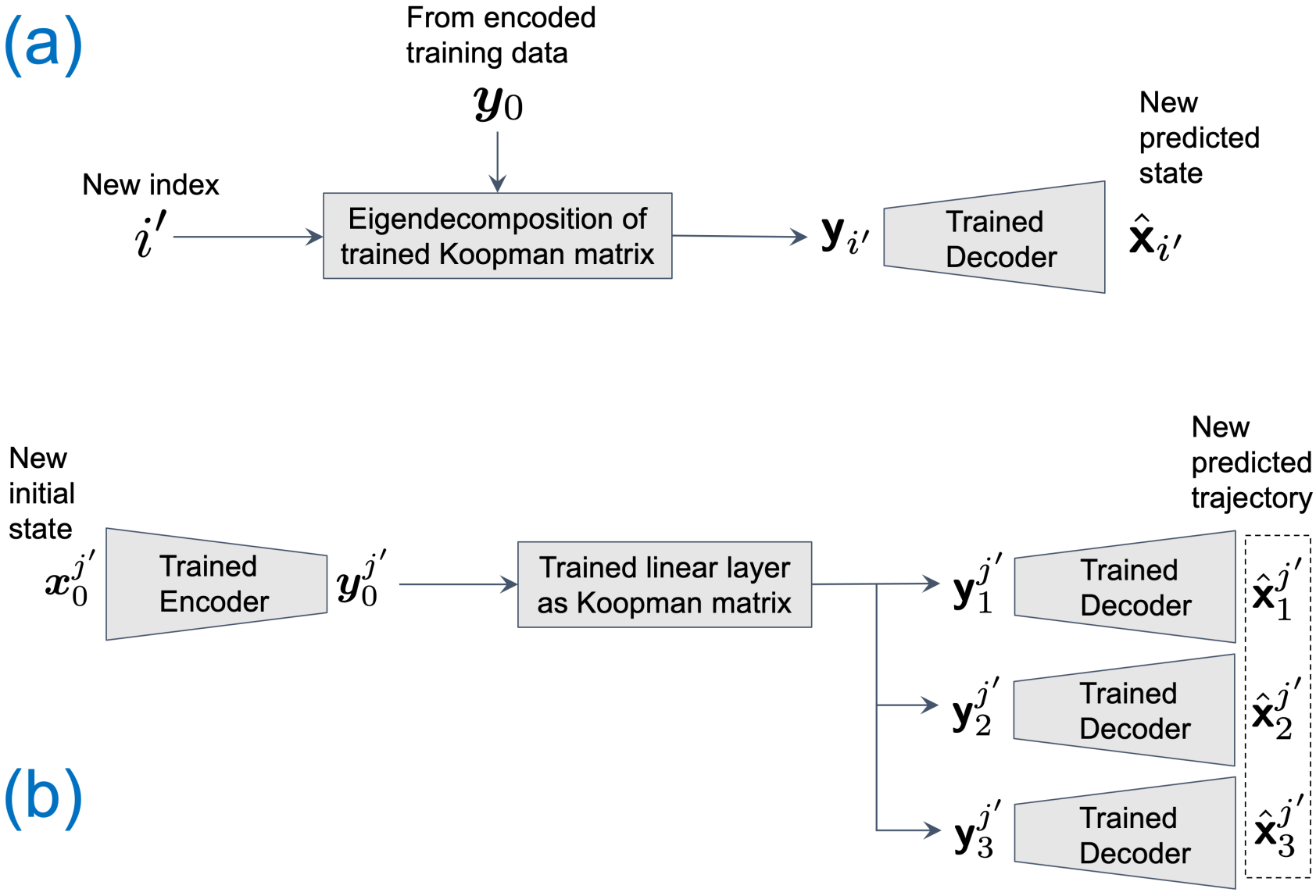
Koopman based learning

dlkoopman training architecture



Koopman based learning

dlkoopman prediction architecture



For trajectory prediction, we would take the new initial condition, encode it through the trained autoencoder layer, advance it in time through the trained Koopman linear layer, and then decode the result for the prediction.

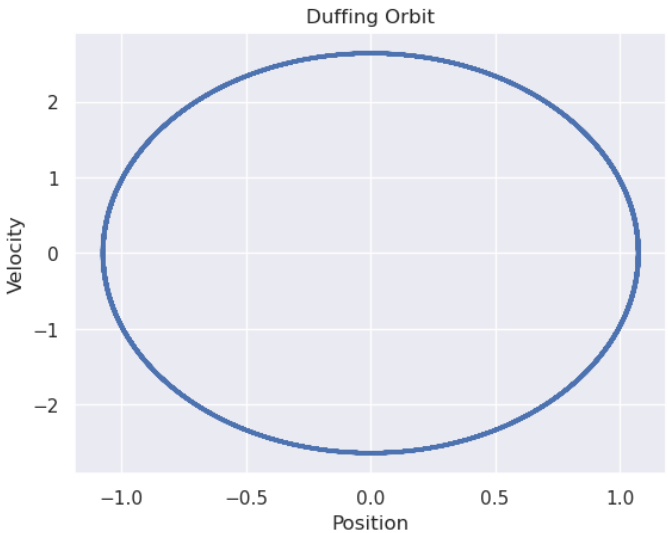
For this project, we tested three different implementations of Koopman neural networks on the Duffing system

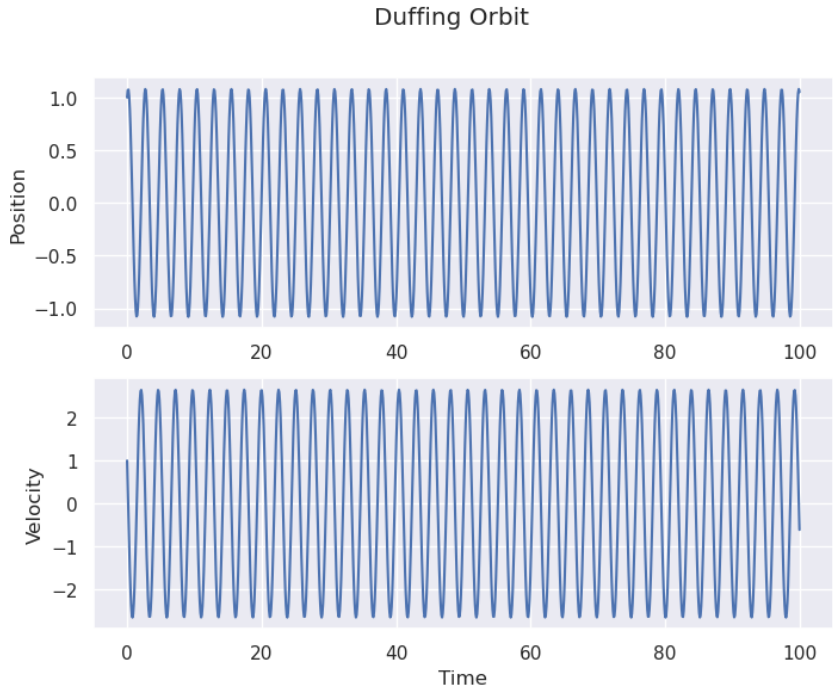
- autokoopman by Ethan James Lew[4]
- dlkoopman by Galois Inc.[5]
- variant of Deep-Koopman by Dongyang Kuang[6]

[4] https://github.com/EthanJamesLew/AutoKoopman
[5] https://github.com/GaloisInc/dlkoopman
[6] https://github.com/dykuang/Deep—-Koopman

Duffing System

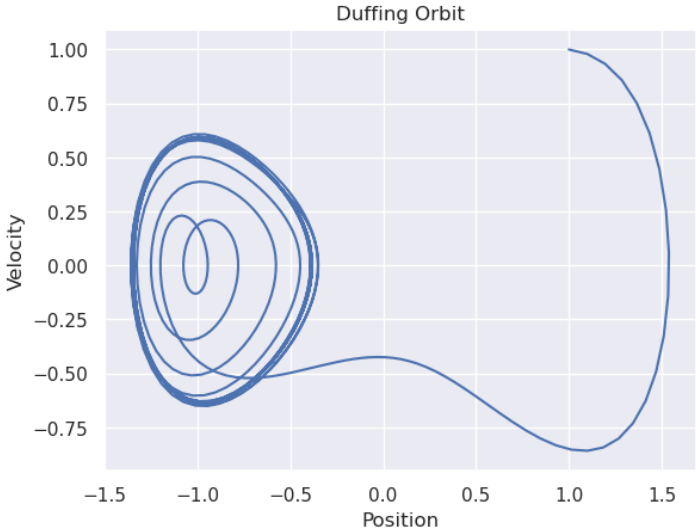
$\alpha = 1, \quad \beta = 0.4, \quad \delta, \gamma = 0$

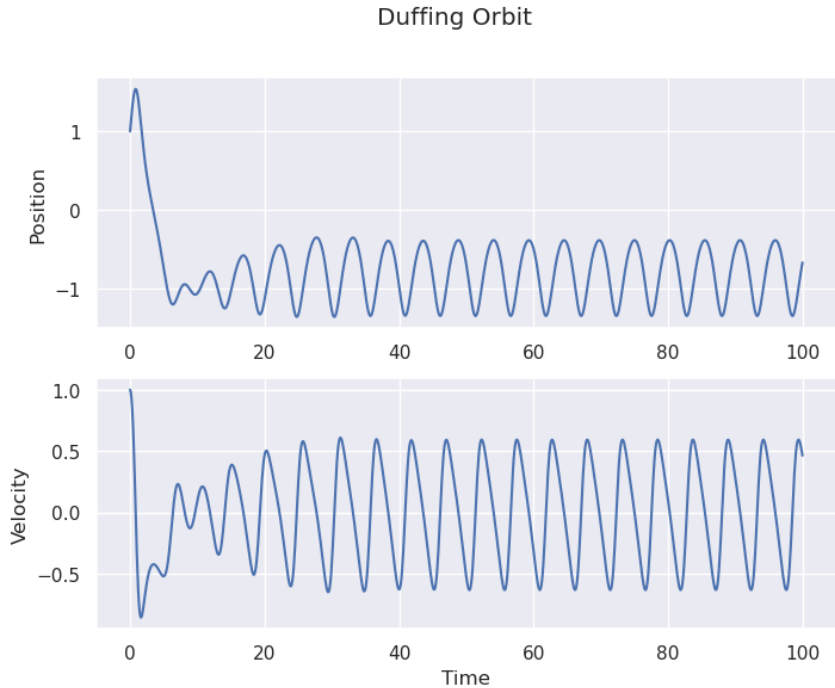




Duffing System

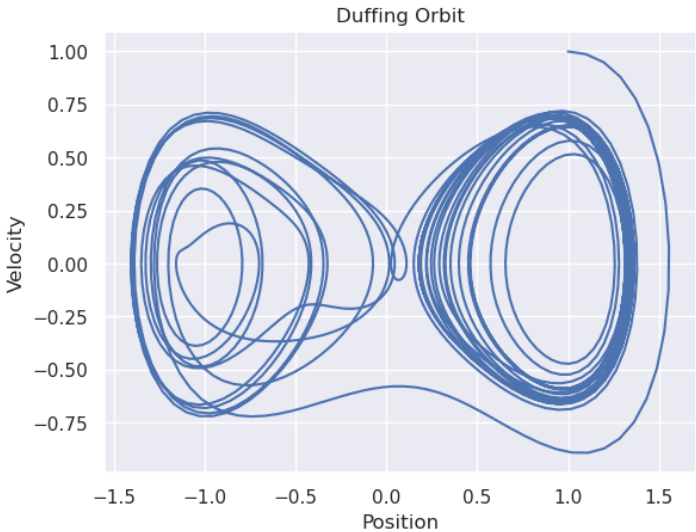
$\gamma = 0.2$

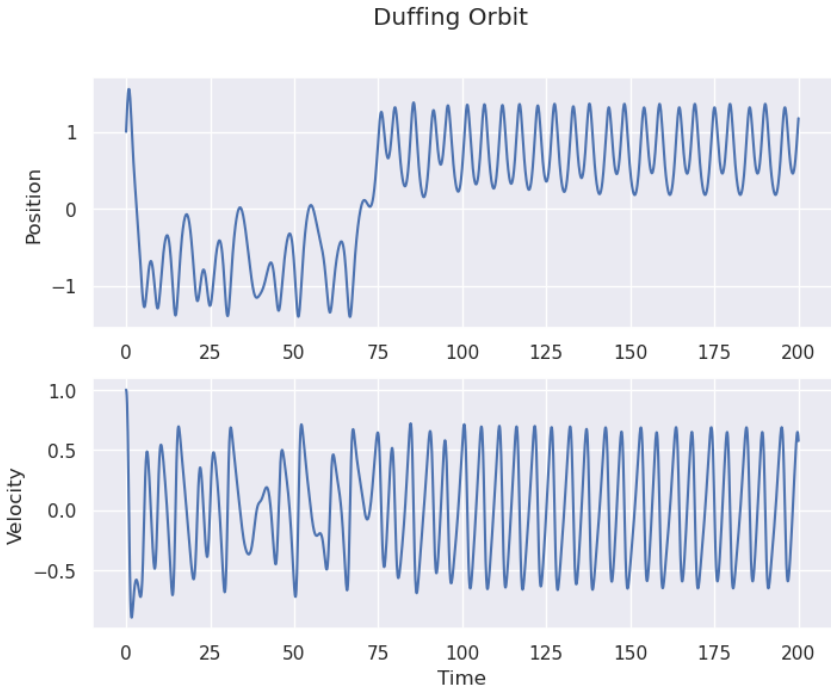




Duffing System

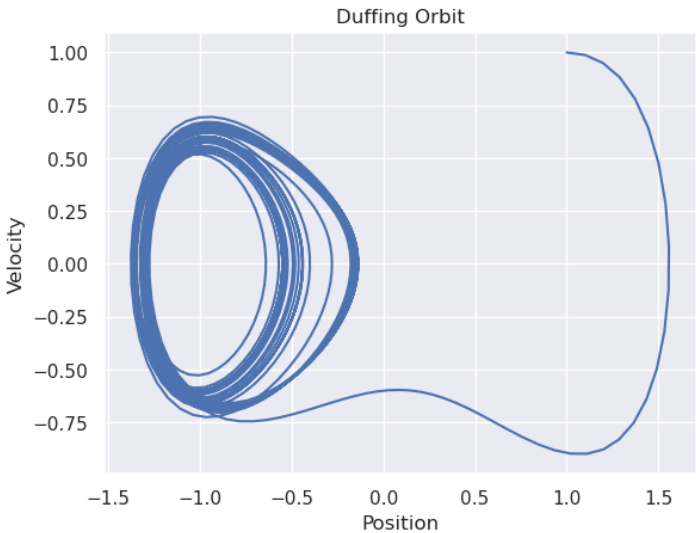
$\gamma = 0.28$

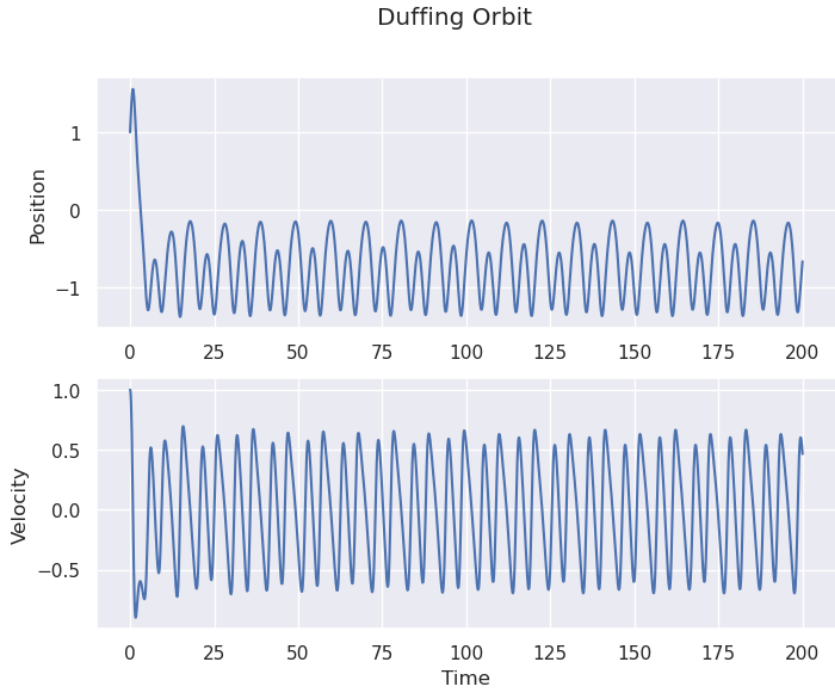




Duffing System

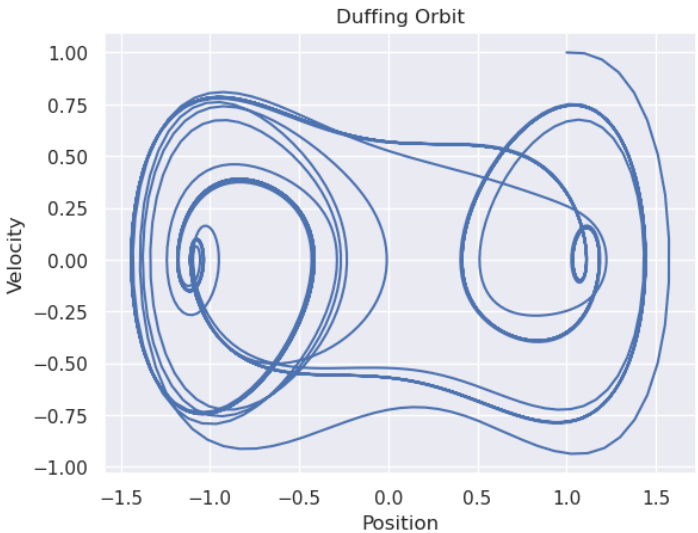
$\gamma = 0.29$

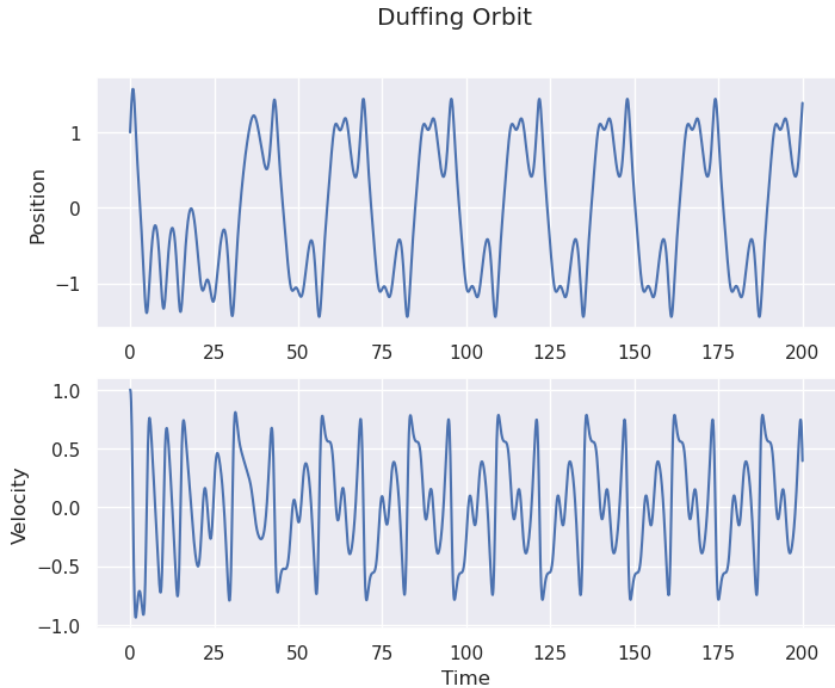




Duffing System

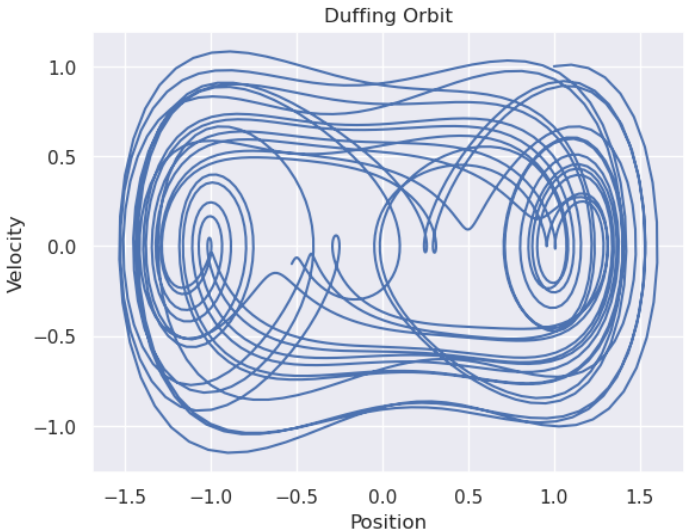
$\gamma = 0.37$

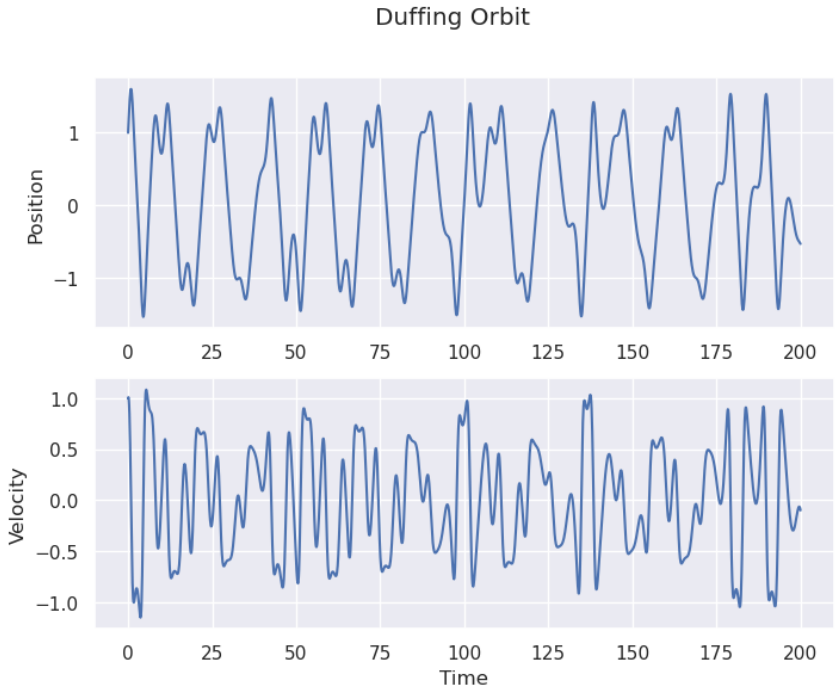




Duffing System

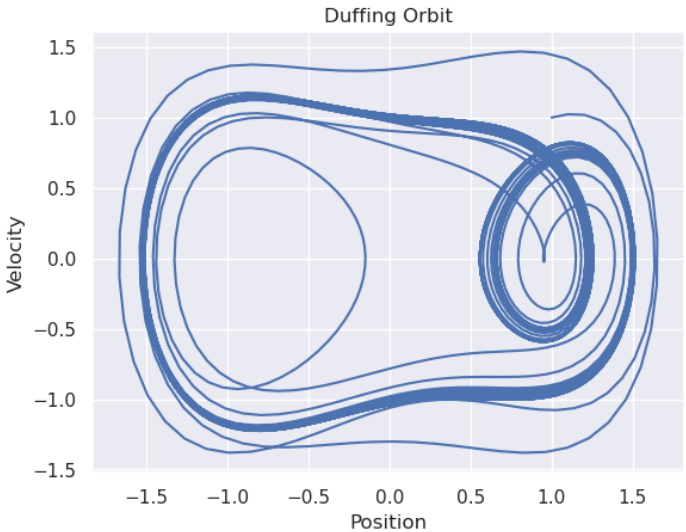
$\gamma = 0.5$

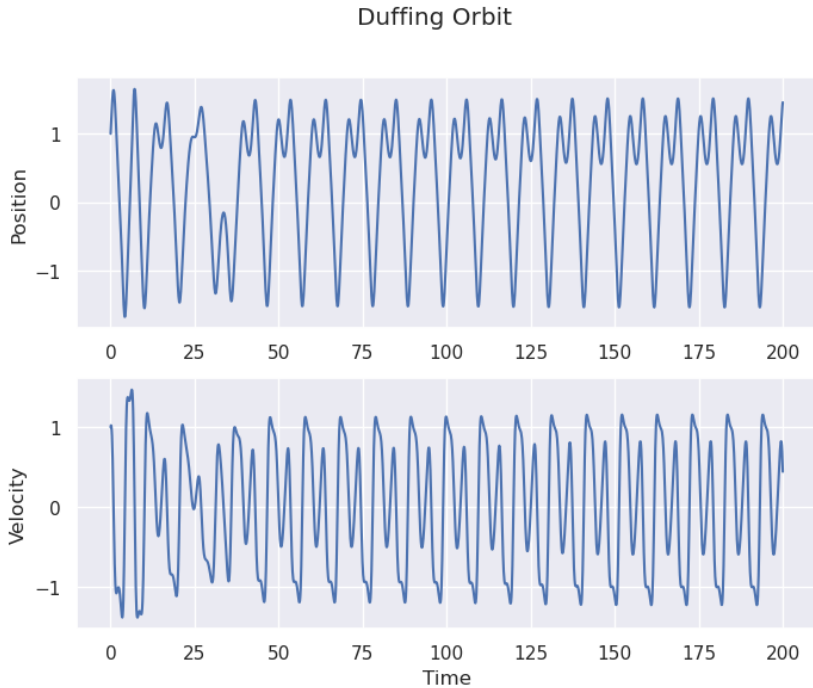




Duffing System

$\gamma = 0.65$





autokoopman

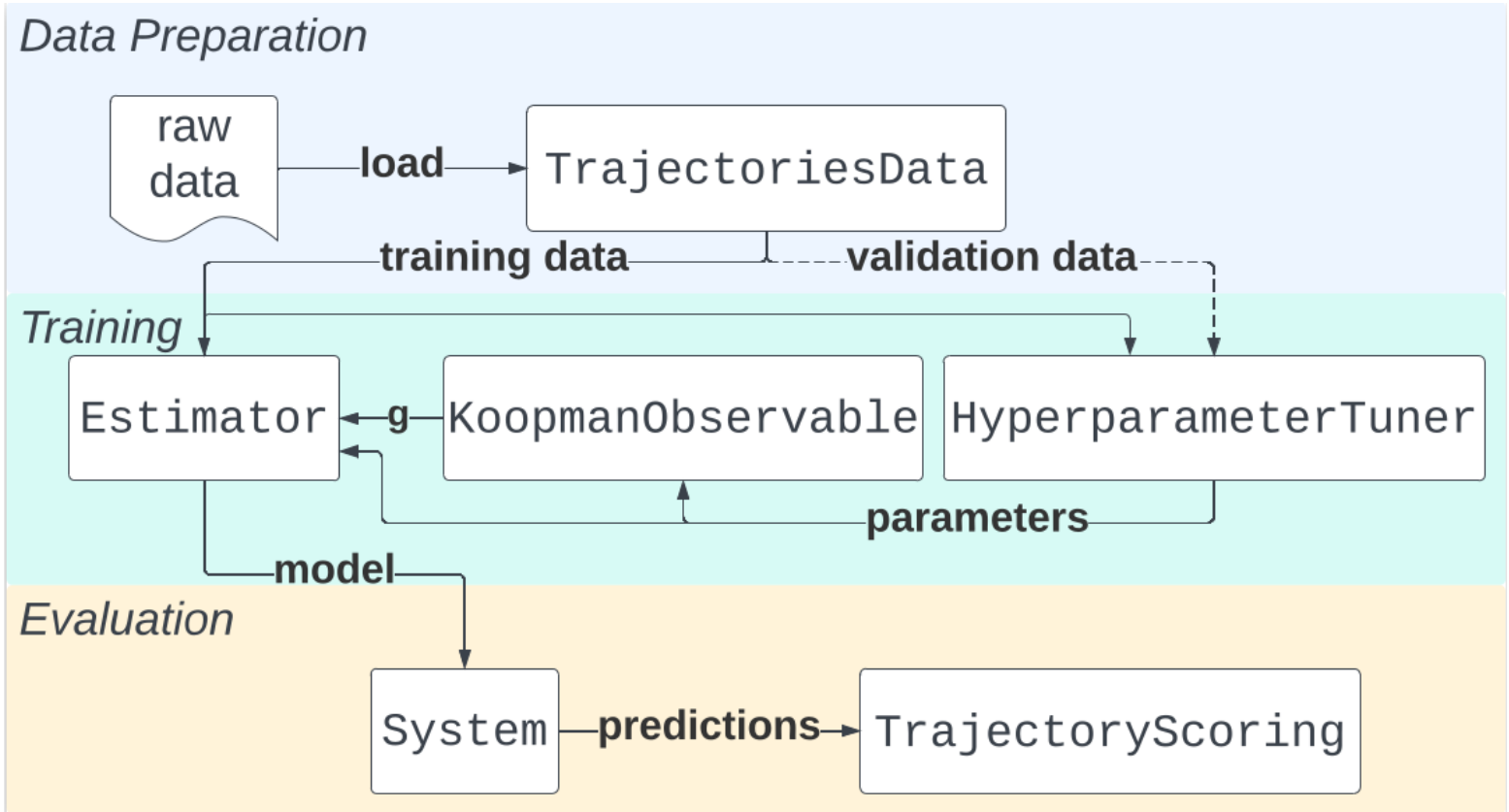
The autokoopman package does not necessarily rely on deep Koopman learning to create a model, it may use SINDy or some other method depending on what the user specifies.

autokoopman

Note: Unfortunately, the autokoopman package is not well-documented, I could not figure out how to access the eigenvalues/modes from the trained Koopman matrix, however, it ended up being the easiest to ask to predict a new initial condition, and have a reasonable answer.

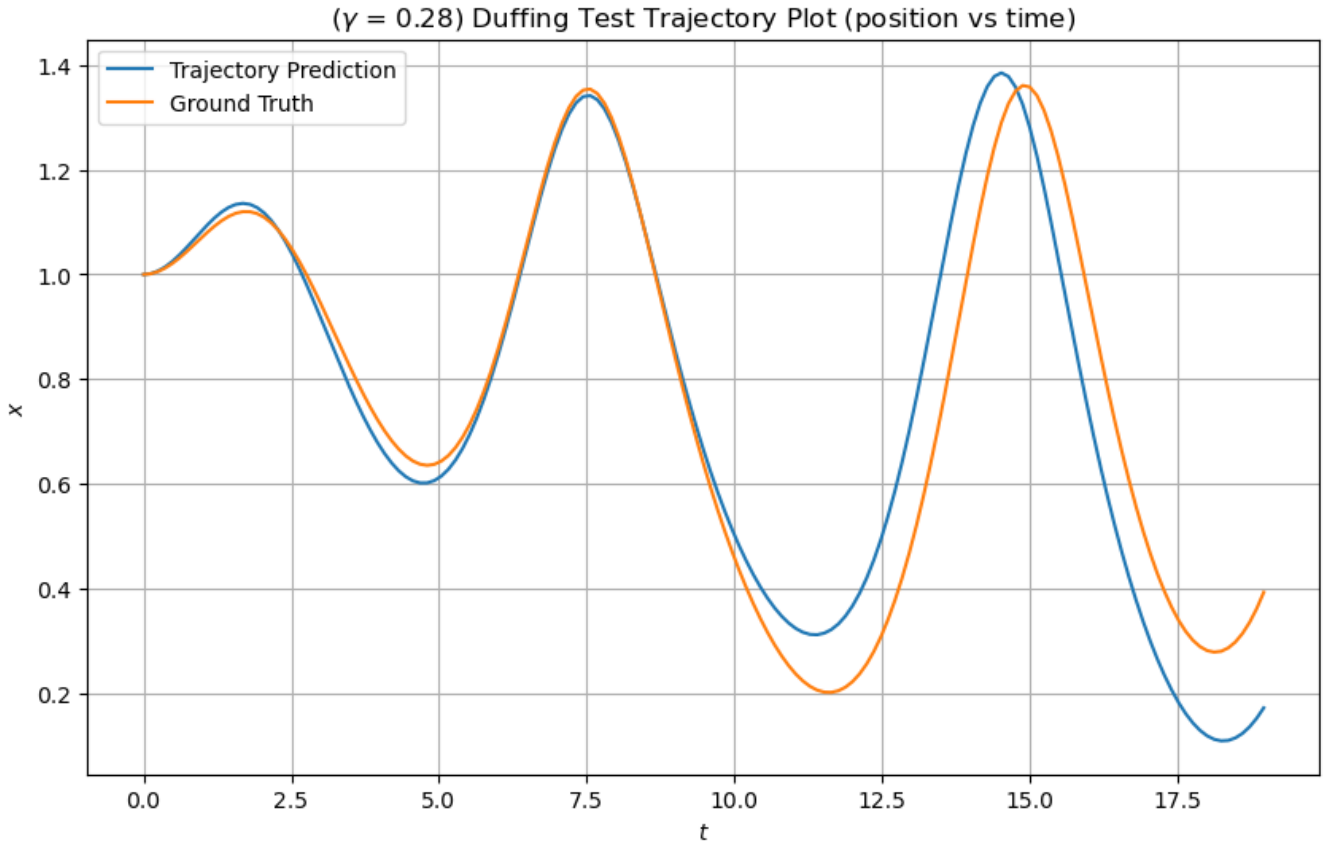
Koopman based learning

autokoopman training architecture



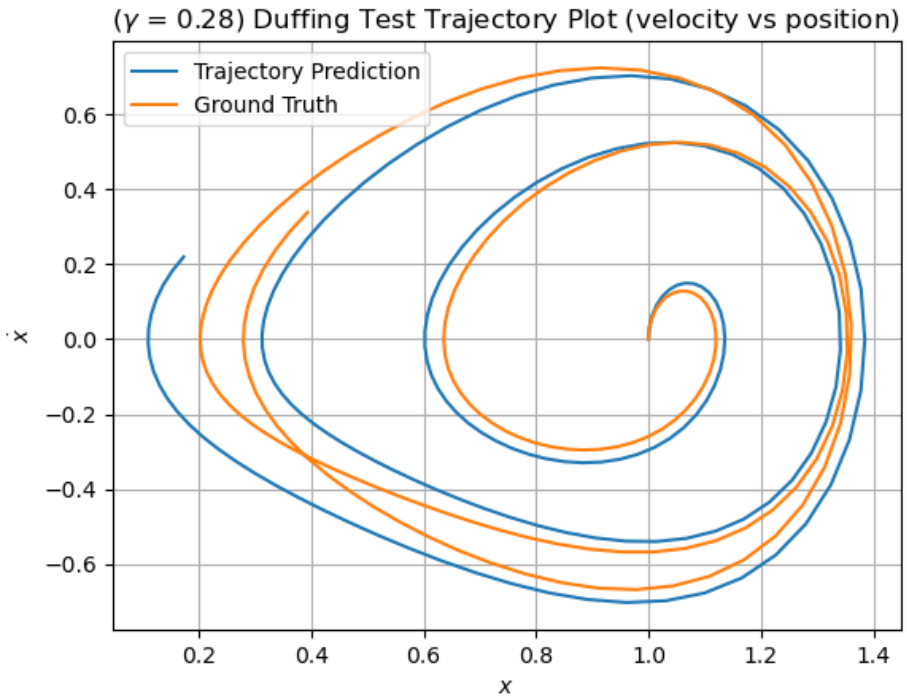
Duffing system

Simulations with autokoopman



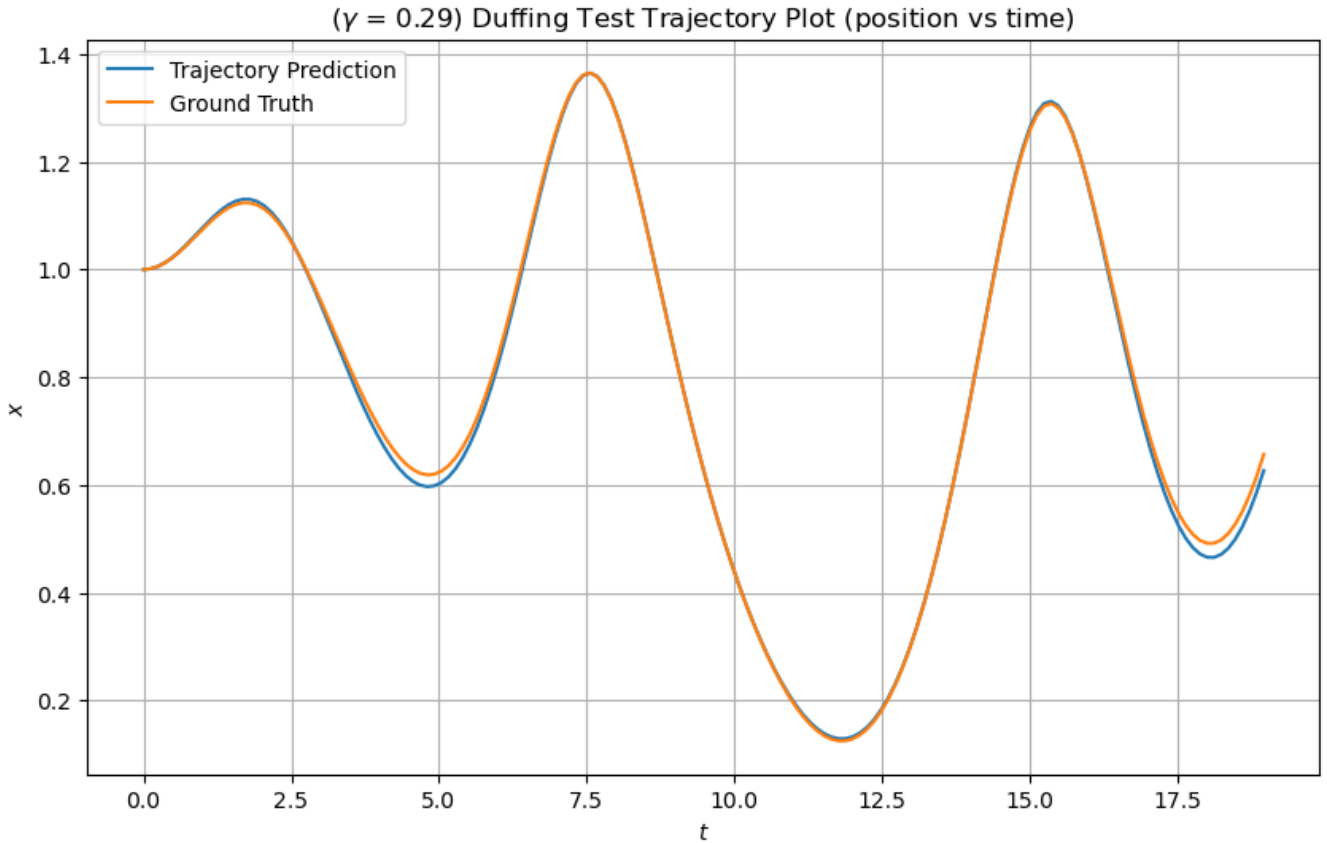
Duffing system

Simulations with autokoopman



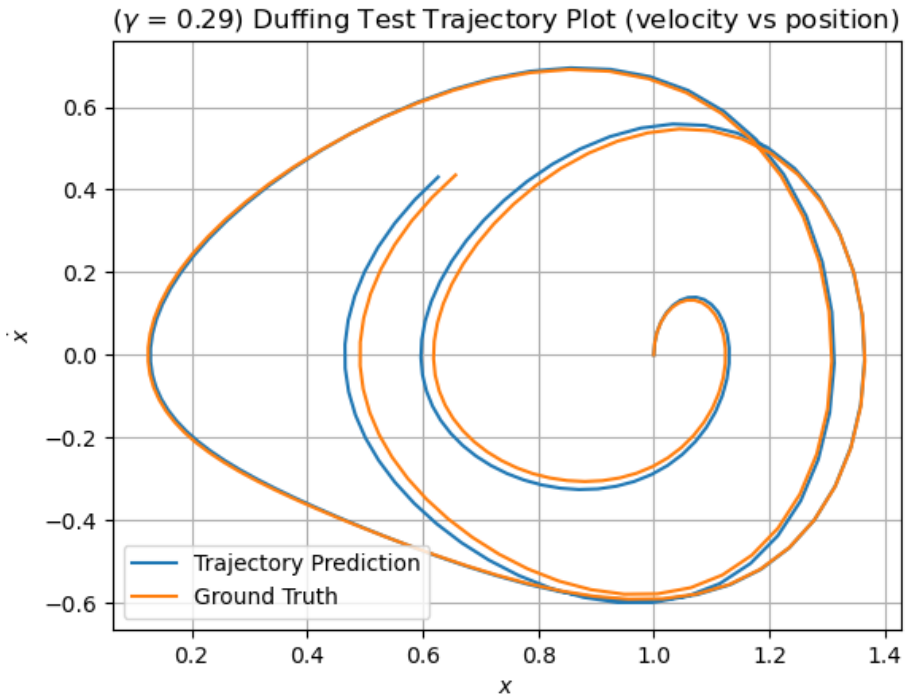
Duffing system

Simulations with autokoopman



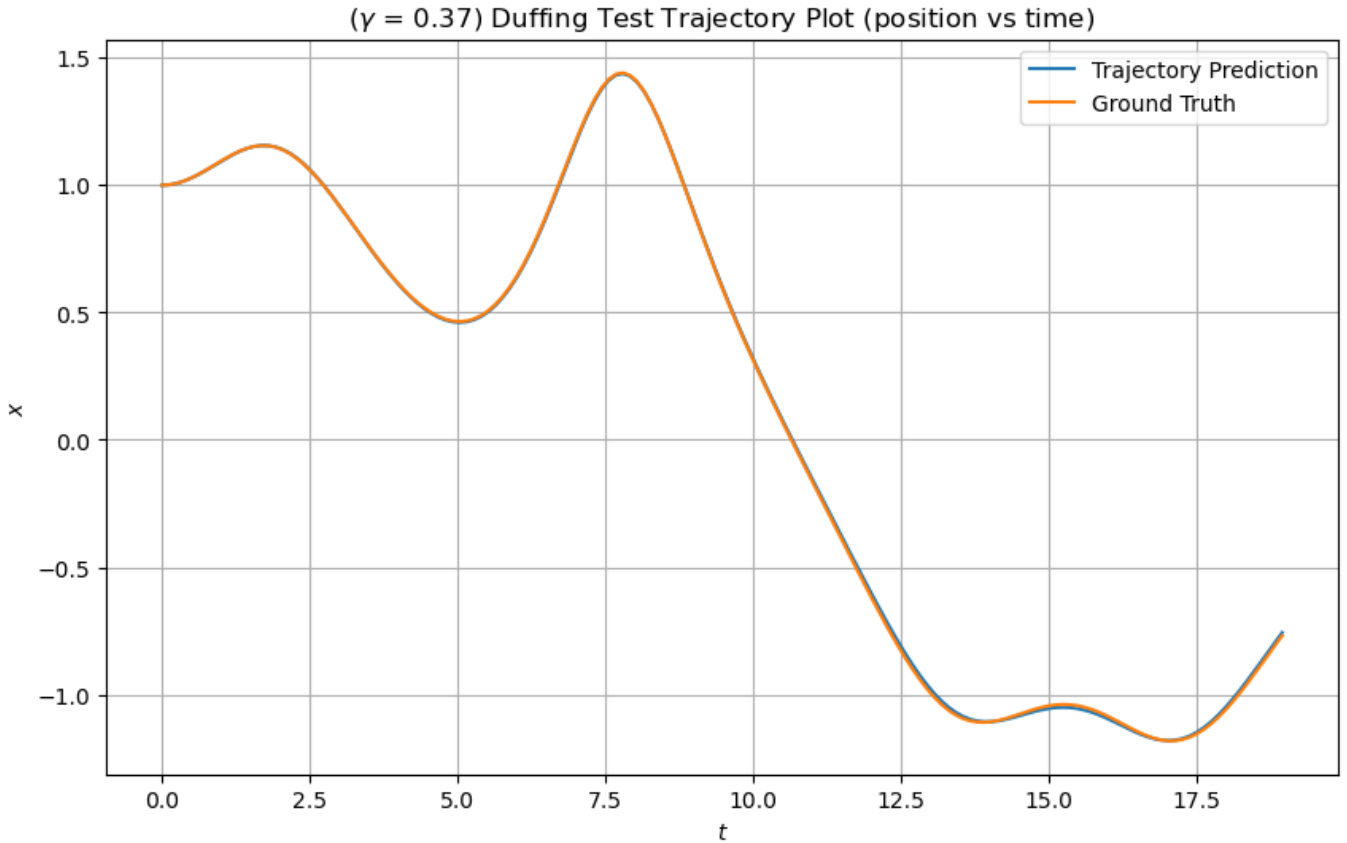
Duffing system

Simulations with autokoopman



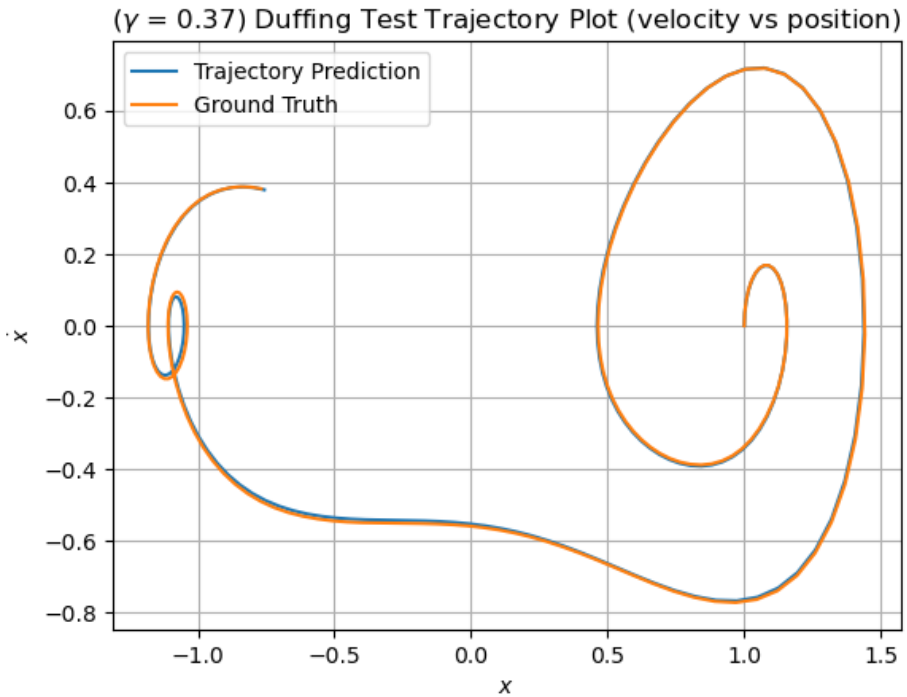
Duffing system

Simulations with autokoopman



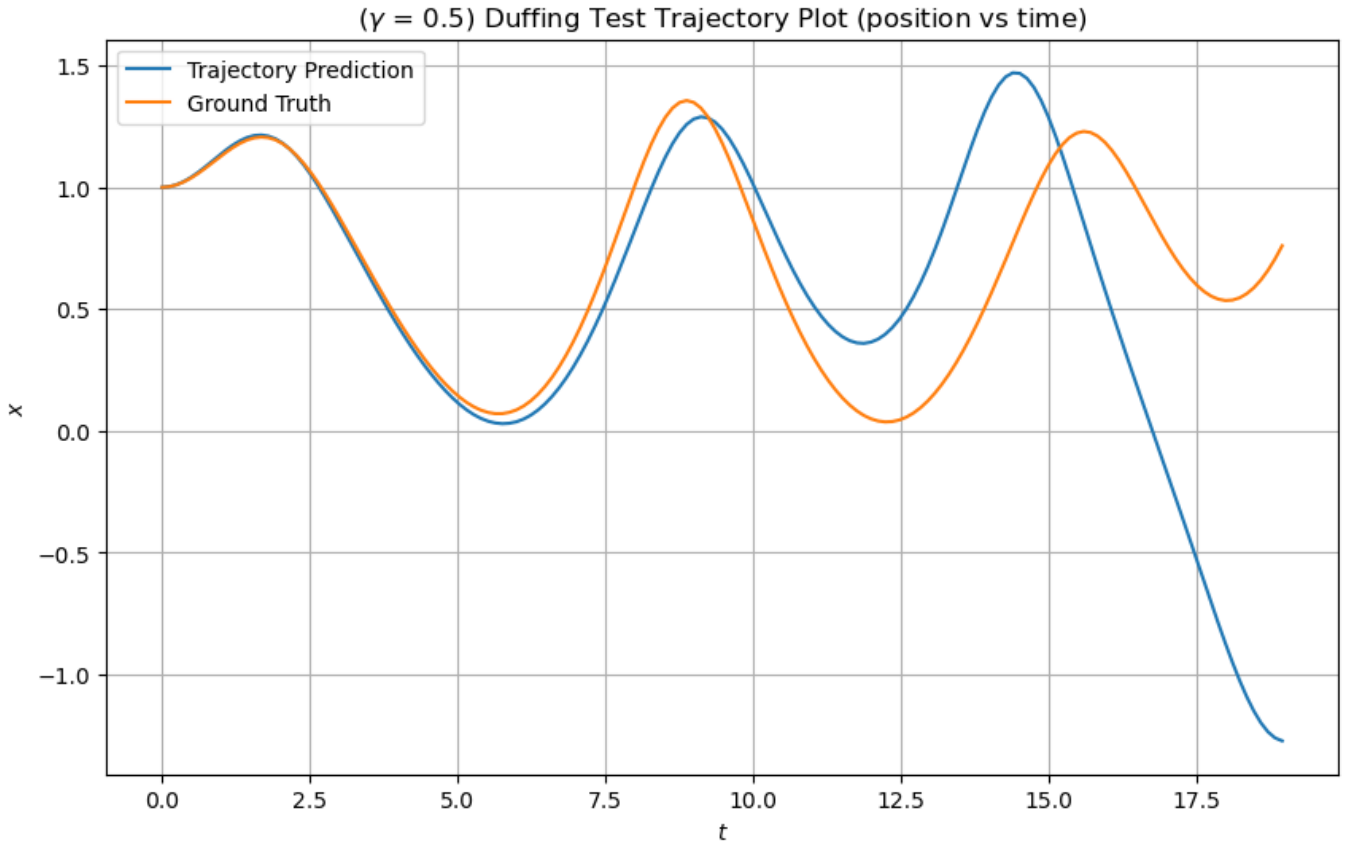
Duffing system

Simulations with autokoopman



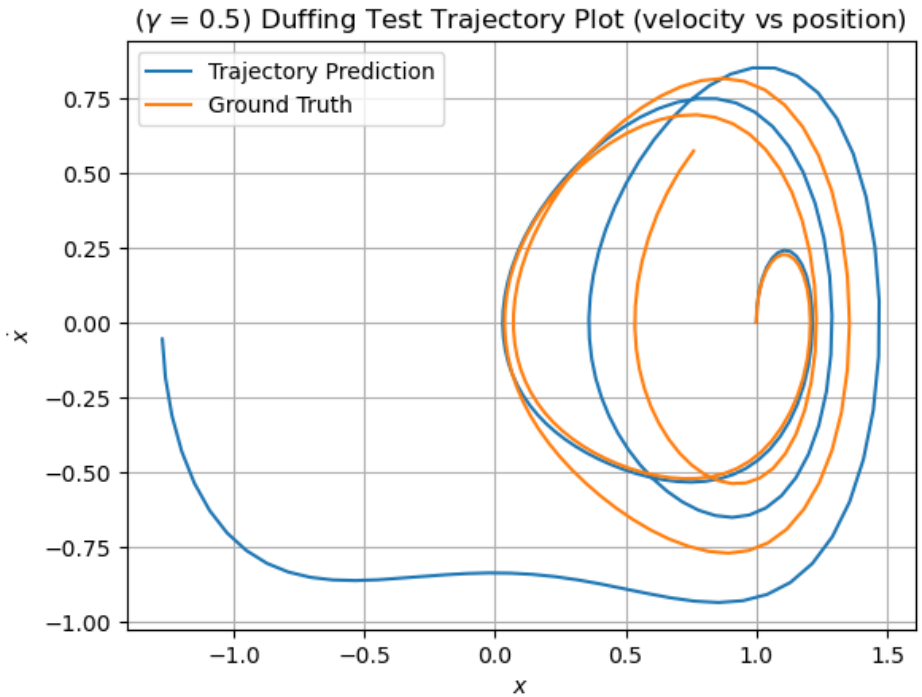
Duffing system

Simulations with autokoopman



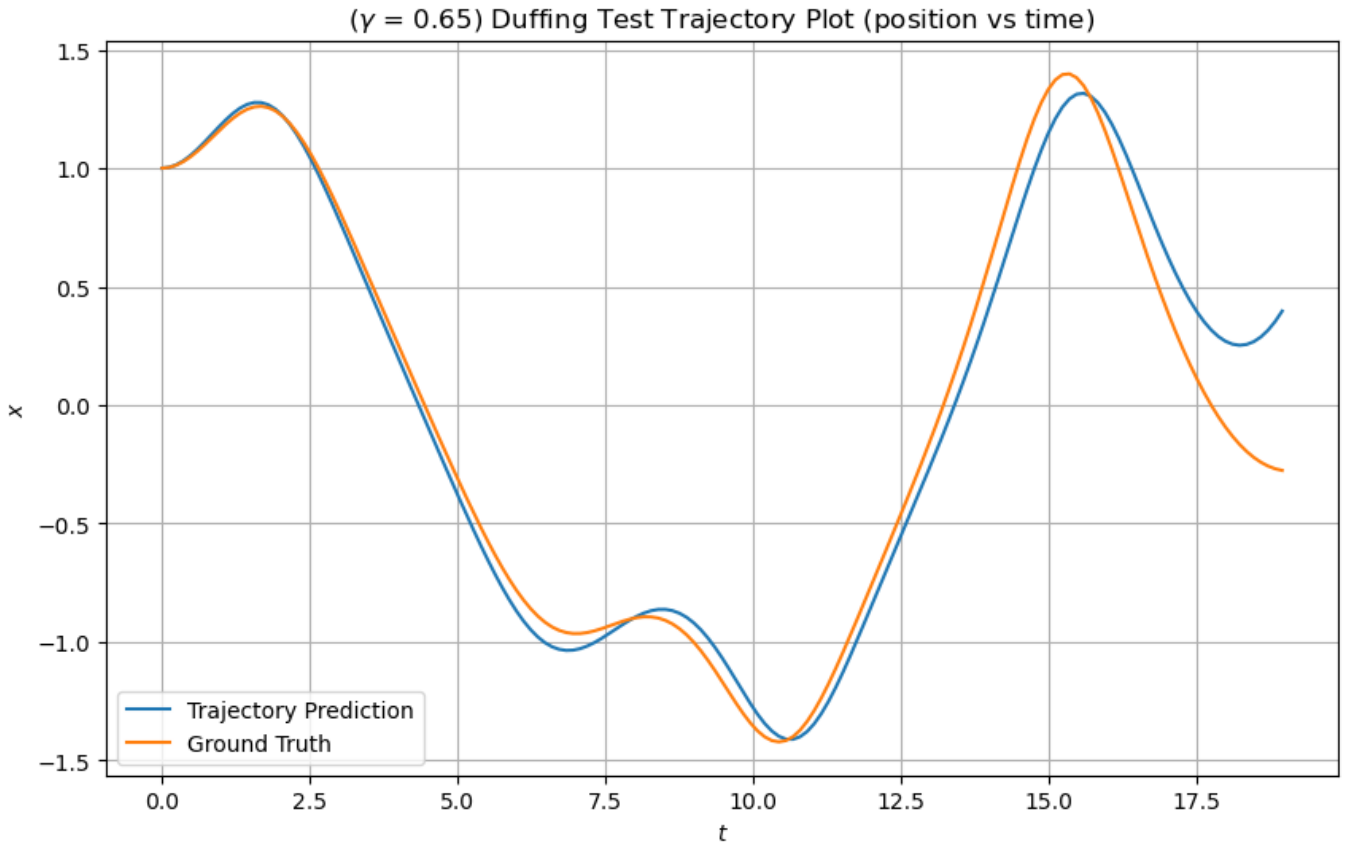
Duffing system

Simulations with autokoopman



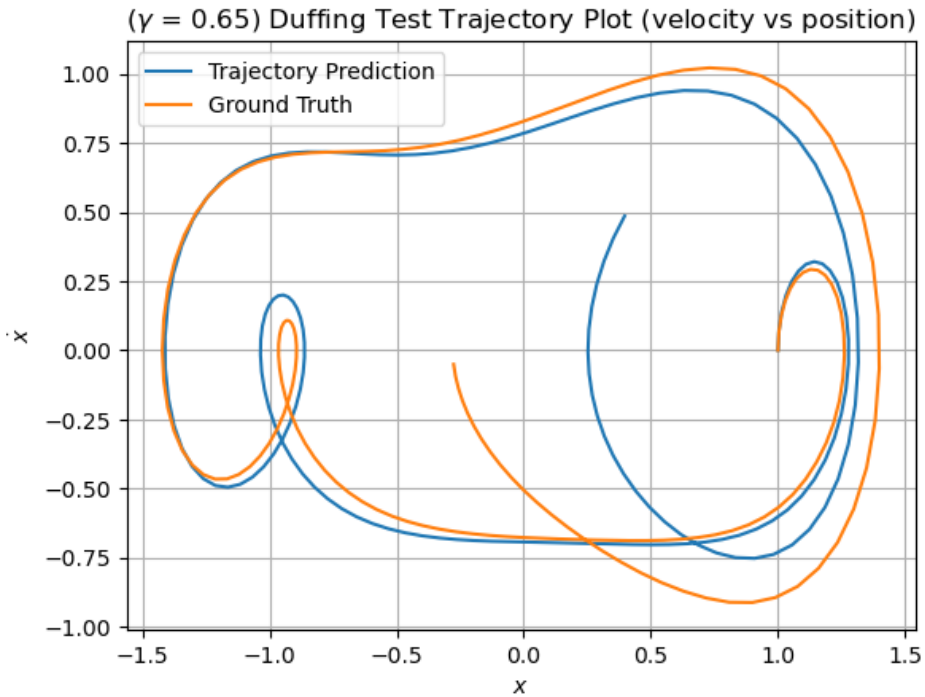
Duffing system

Simulations with autokoopman



Duffing system

Simulations with autokoopman



Deep Koopman

The Deep Koopman implementation used here is a variant of Dongyang Kuang's package, which is itself a modification of Bethany Lusch's implementation. [7][8]

[7] https://github.com/BethanyL/DeepKoopman

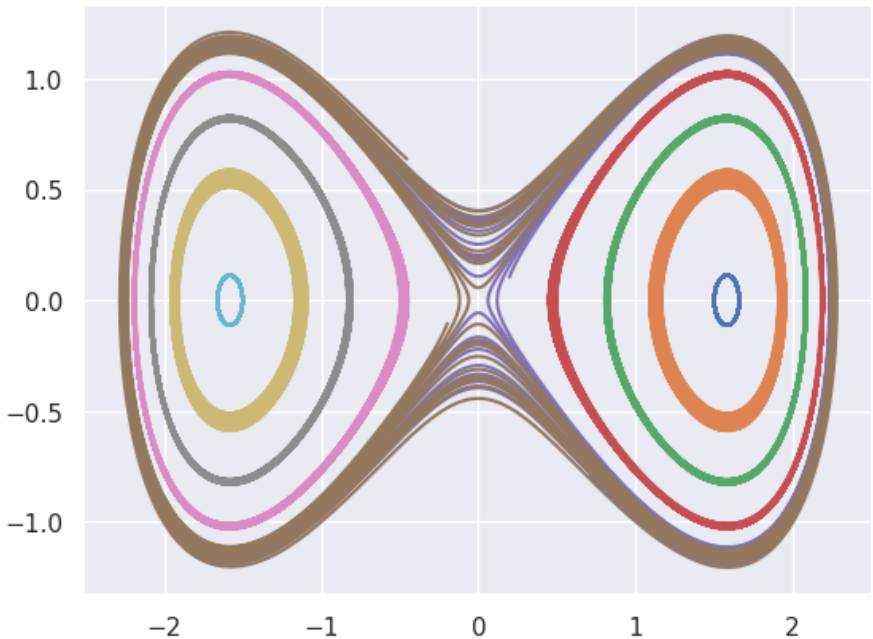
[8] Lusch, B., Kutz, J.N. Brunton, S.L. Deep learning for universal linear embeddings of nonlinear dynamics. Nat Commun 9, 4950 (2018). https://doi.org/10.1038/s41467-018-07210-0

Deep Koopman

$\alpha = 1, \quad \beta = 0.4, \quad \delta, \gamma = 0$

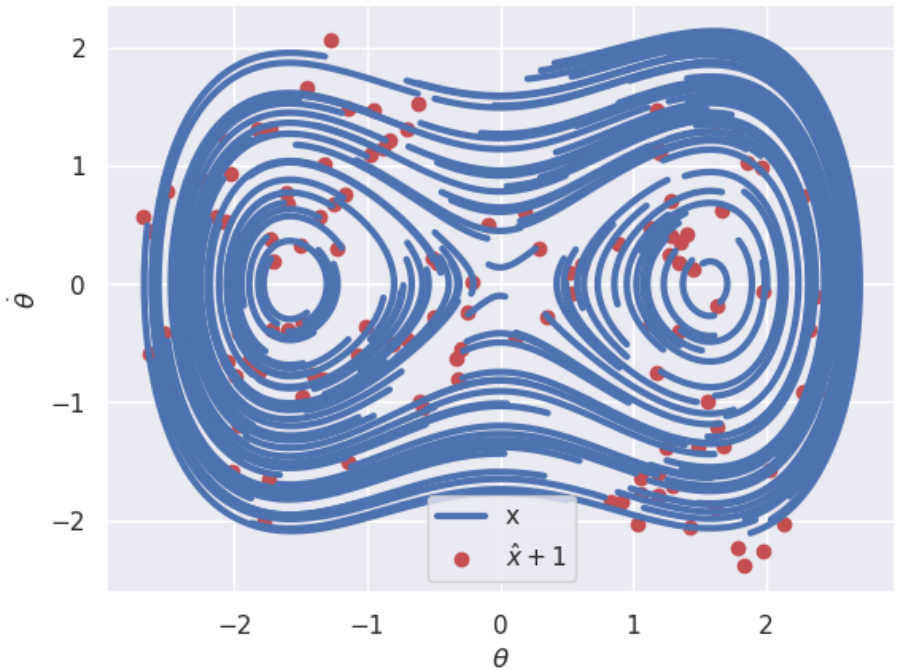
Deep Koopman

$\alpha = 1, \quad \beta = 0.4, \quad \delta, \gamma = 0$



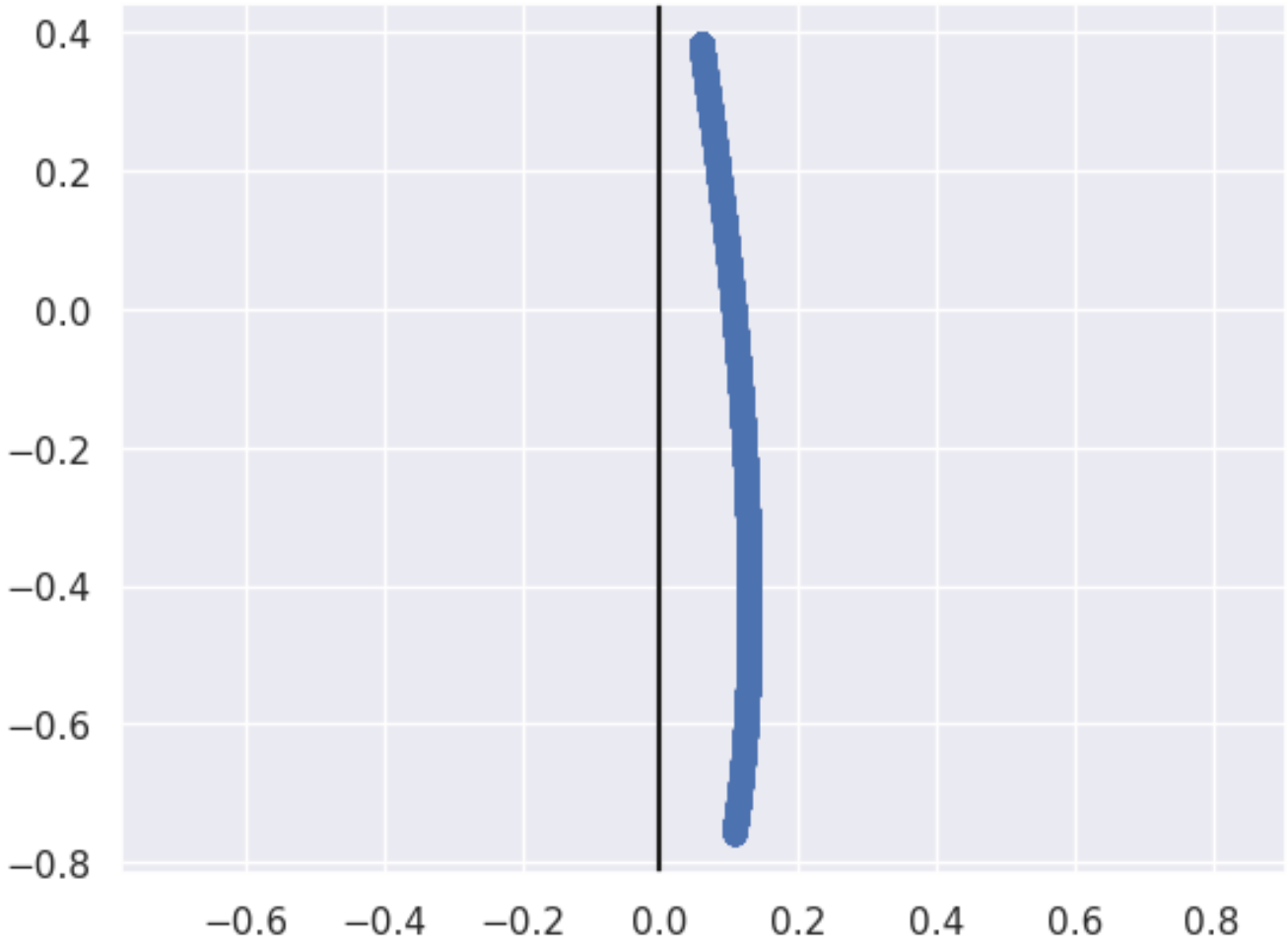
Deep Koopman

$\alpha = 1, \quad \beta = 0.4, \quad \delta, \gamma = 0$



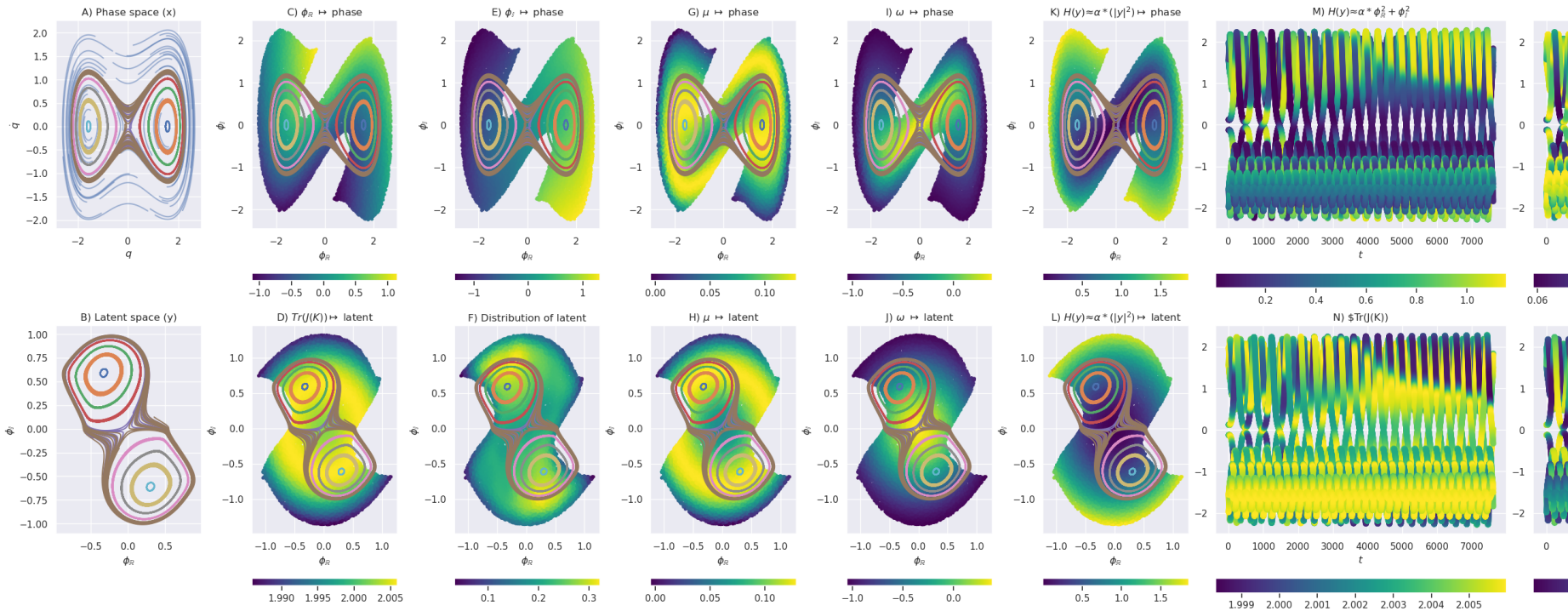
Deep Koopman

$\alpha = 1, \quad \beta = 0.4, \quad \delta, \gamma = 0$



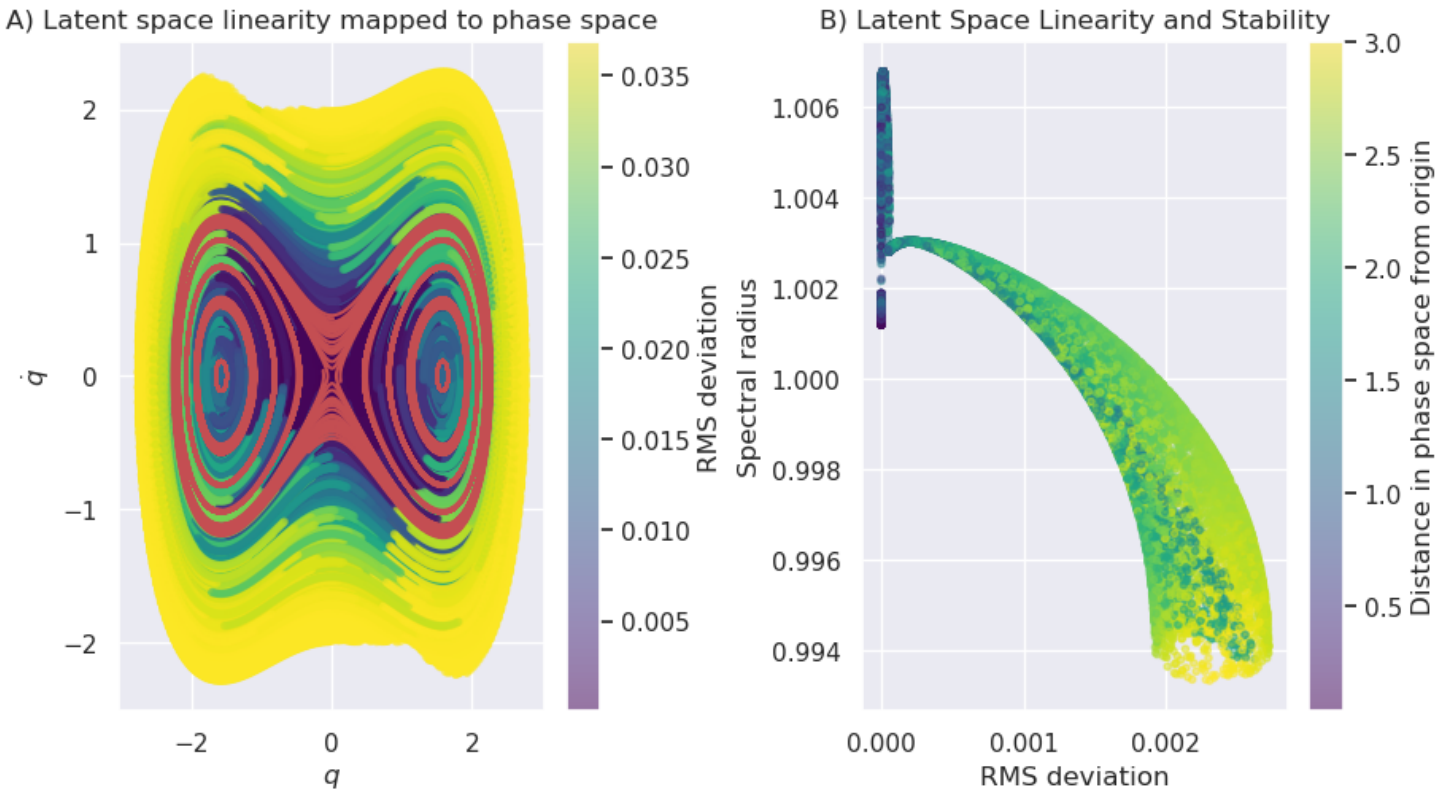
Deep Koopman

$\alpha = 1, \quad \beta = 0.4, \quad \delta, \gamma = 0$



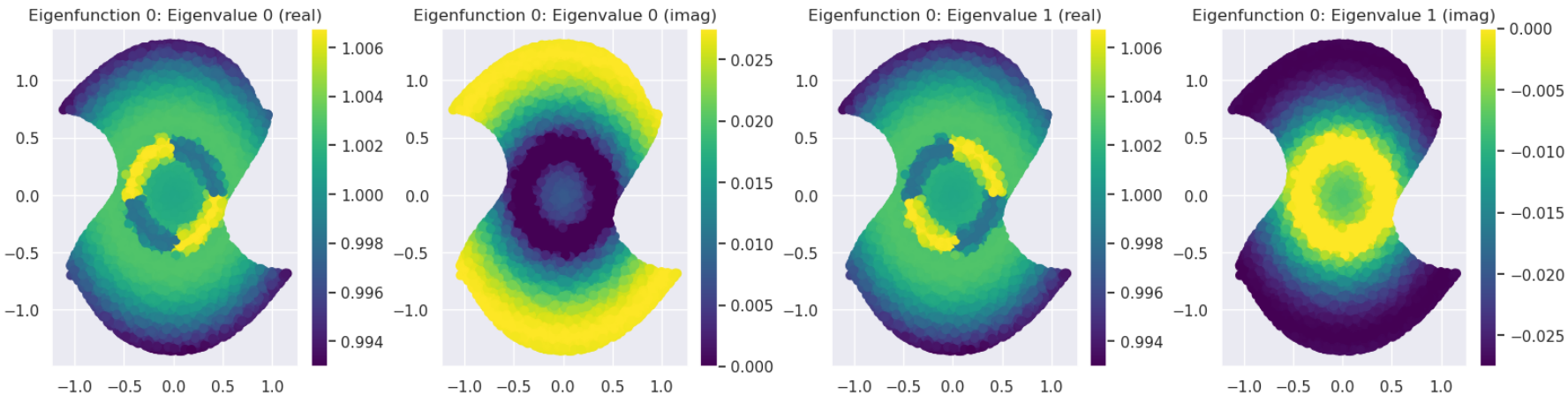
Deep Koopman

$\alpha = 1, \quad \beta = 0.4, \quad \delta, \gamma = 0$



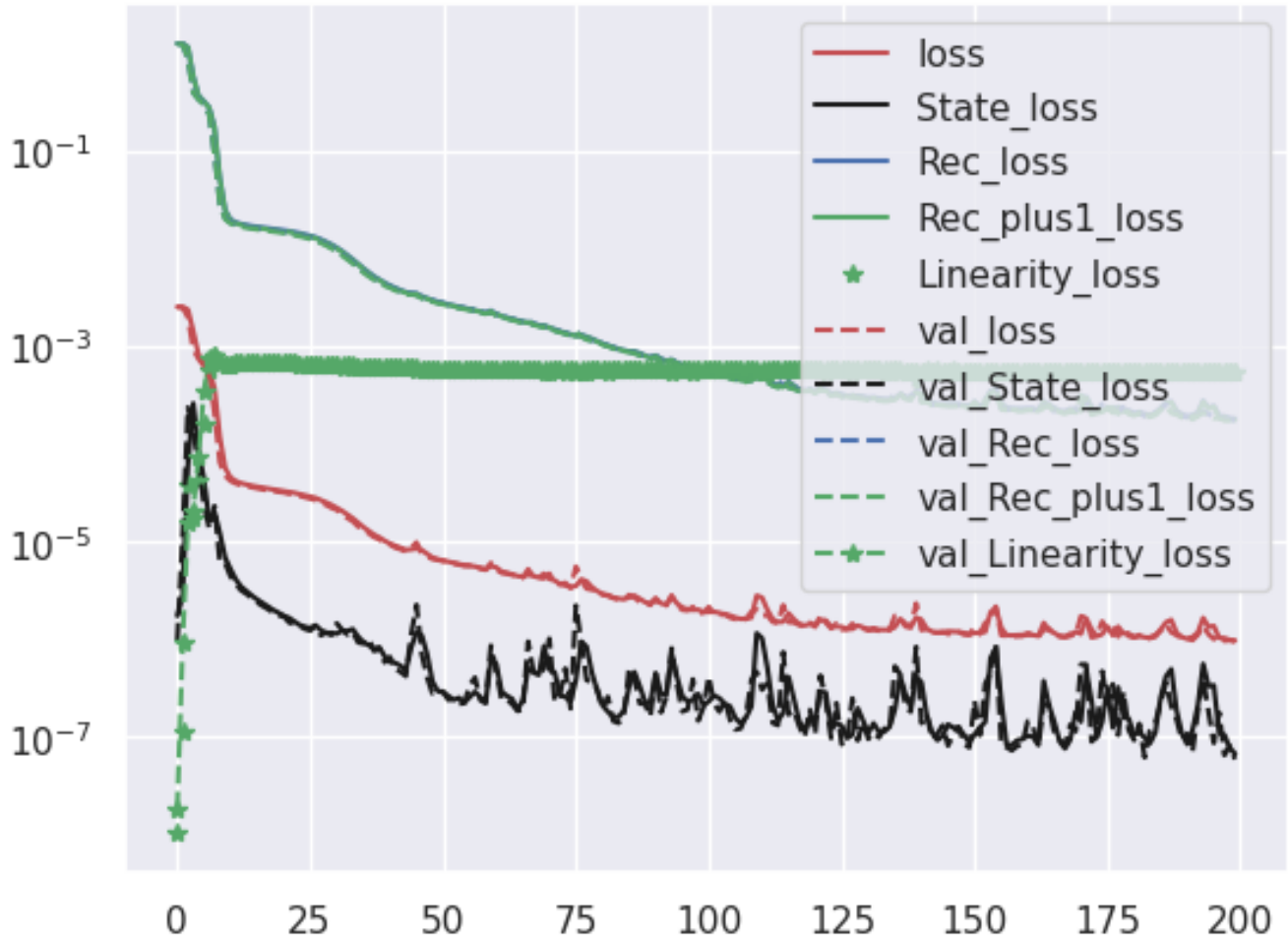
Deep Koopman

$\alpha = 1, \quad \beta = 0.4, \quad \delta, \gamma = 0$



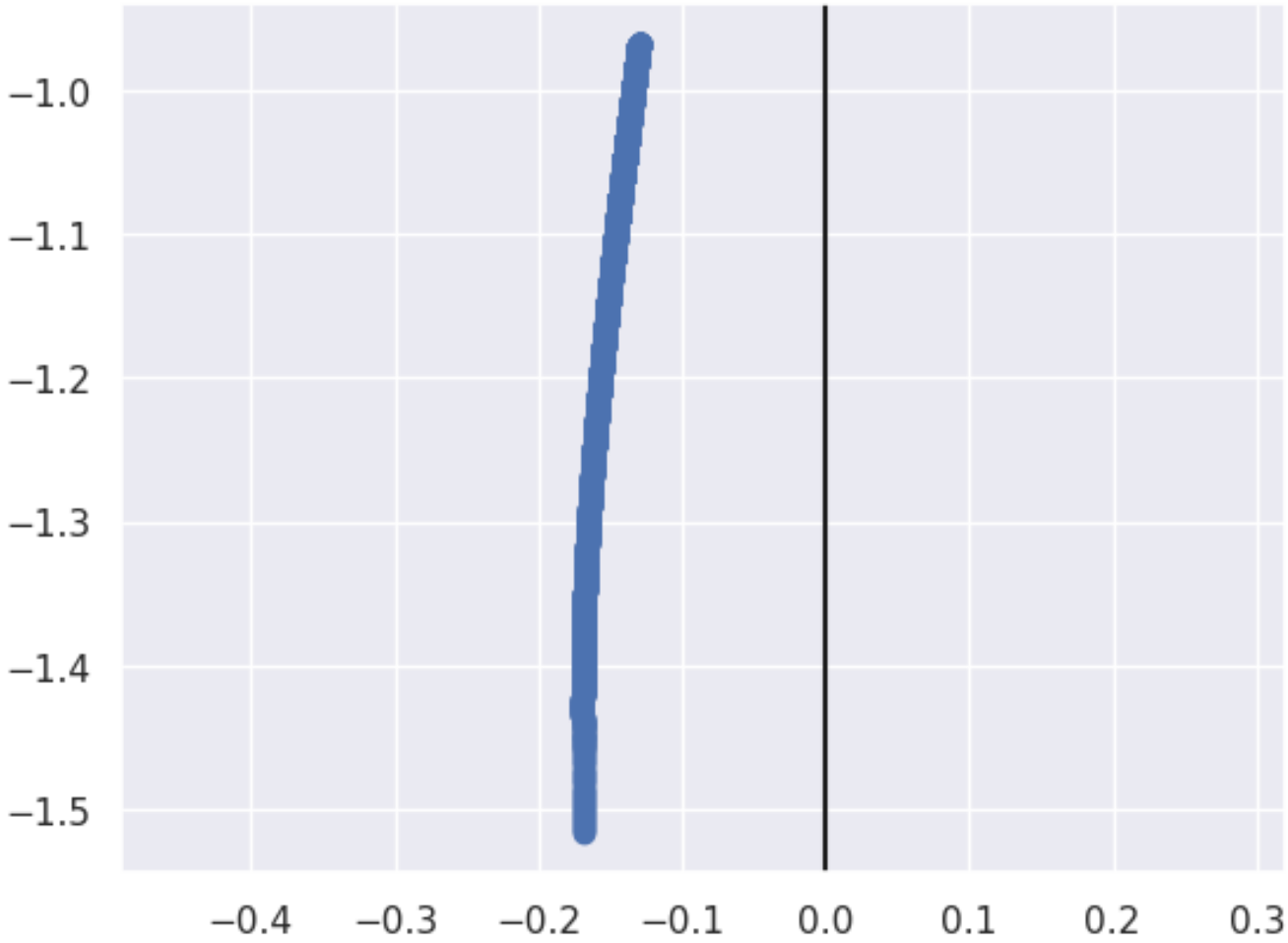
Deep Koopman

$\gamma = 0.2$



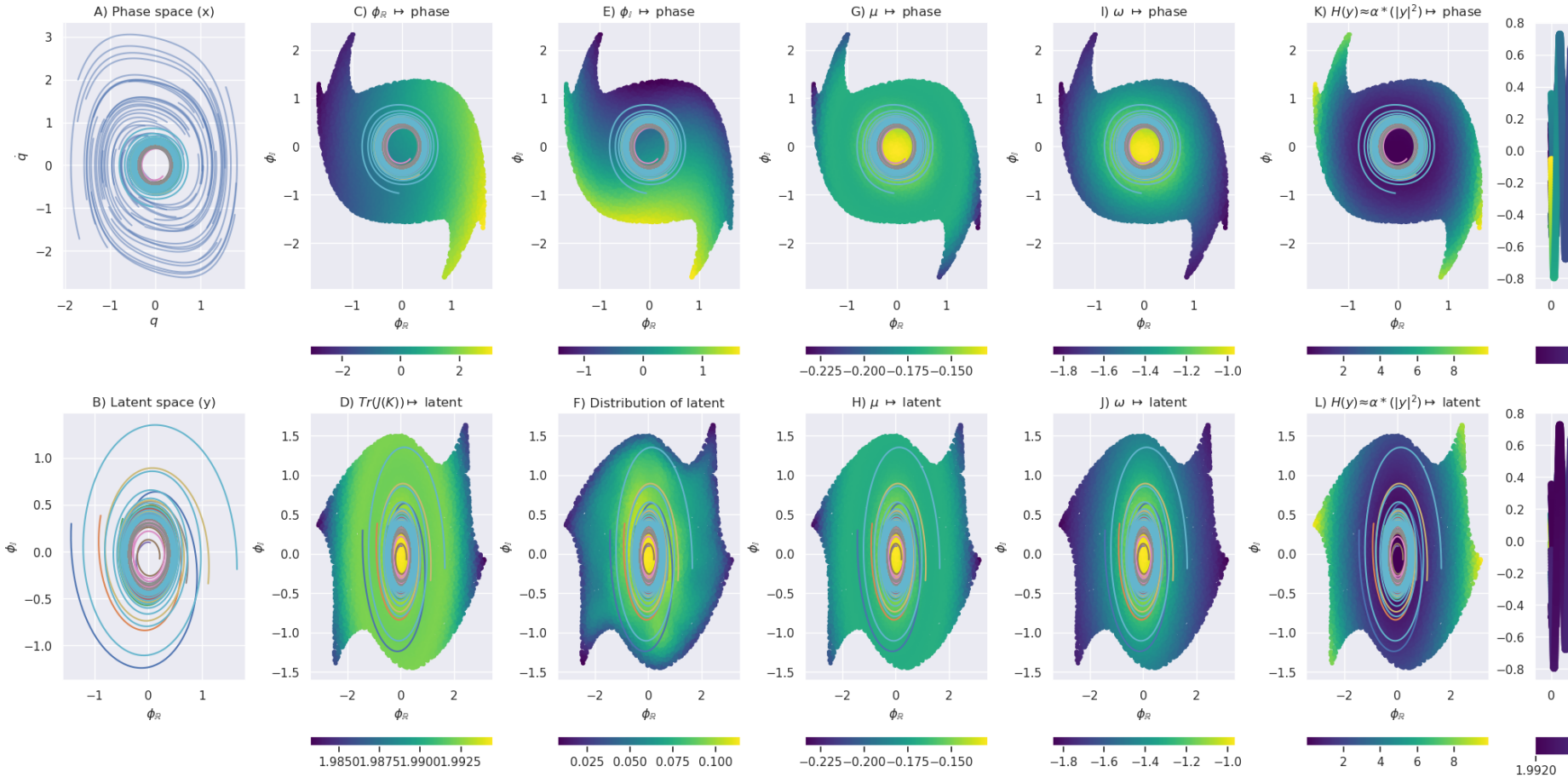
Deep Koopman

$\gamma = 0.2$



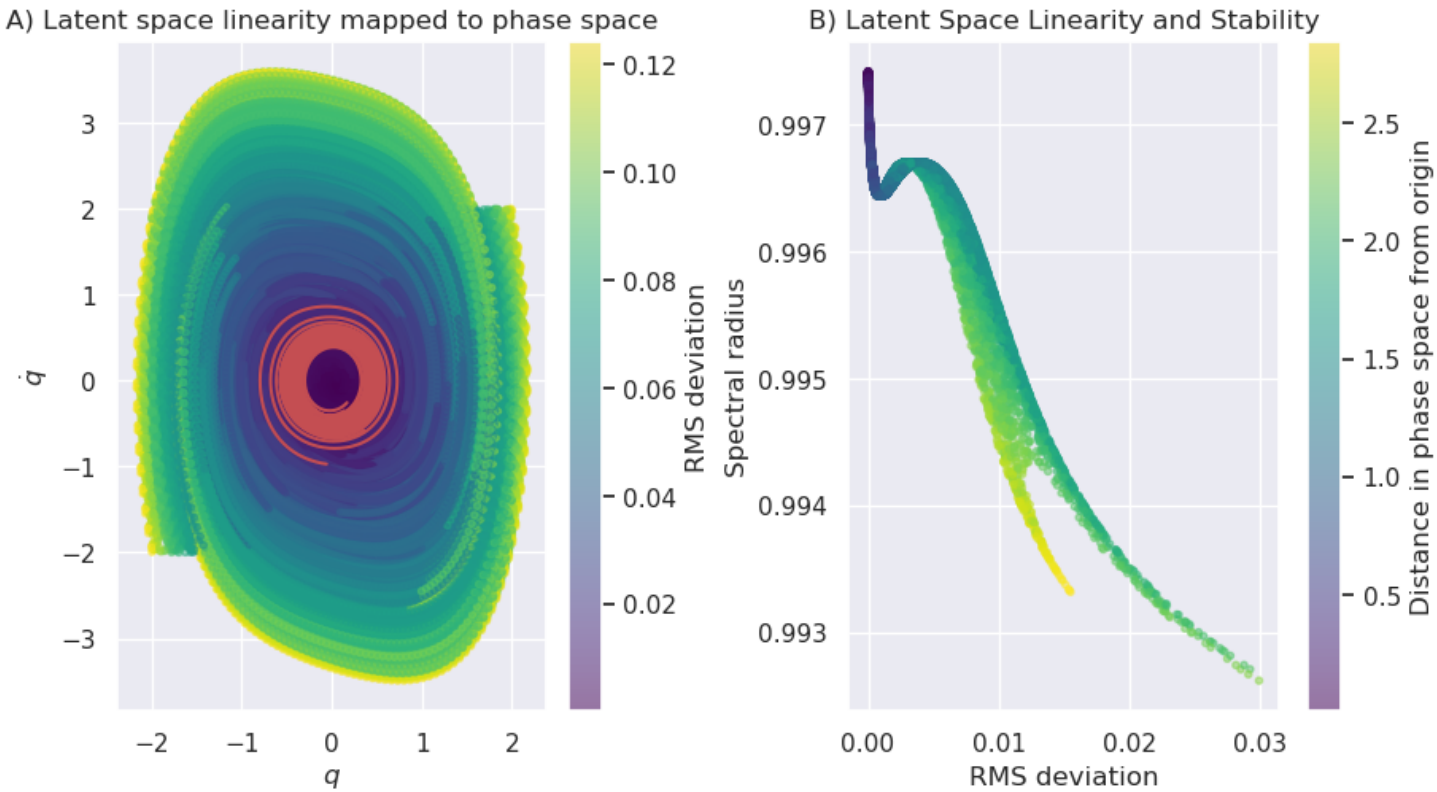
Deep Koopman

$\gamma = 0.2$



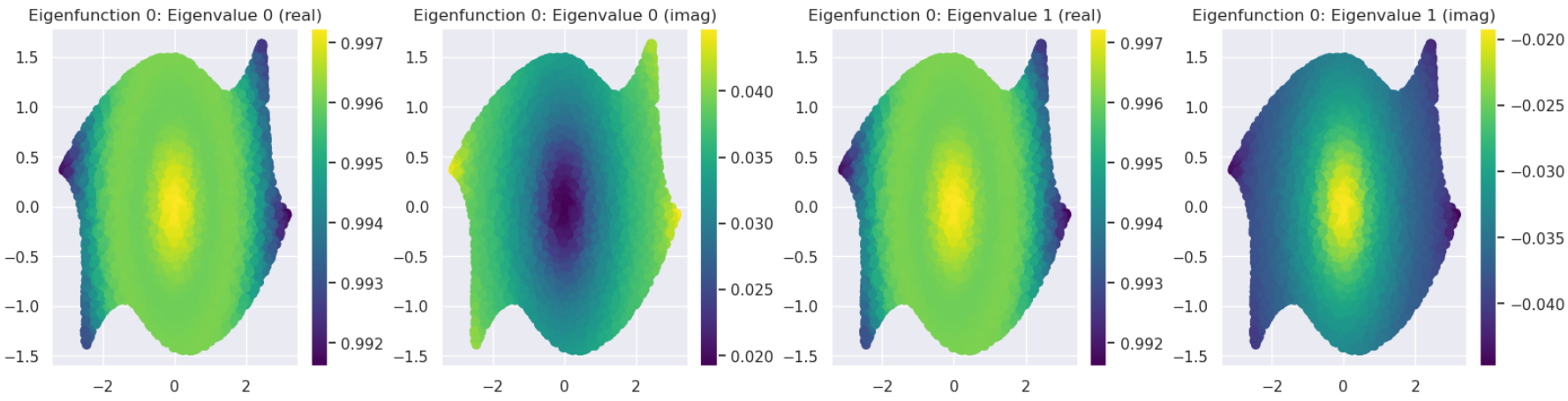
Deep Koopman

$\gamma = 0.2$



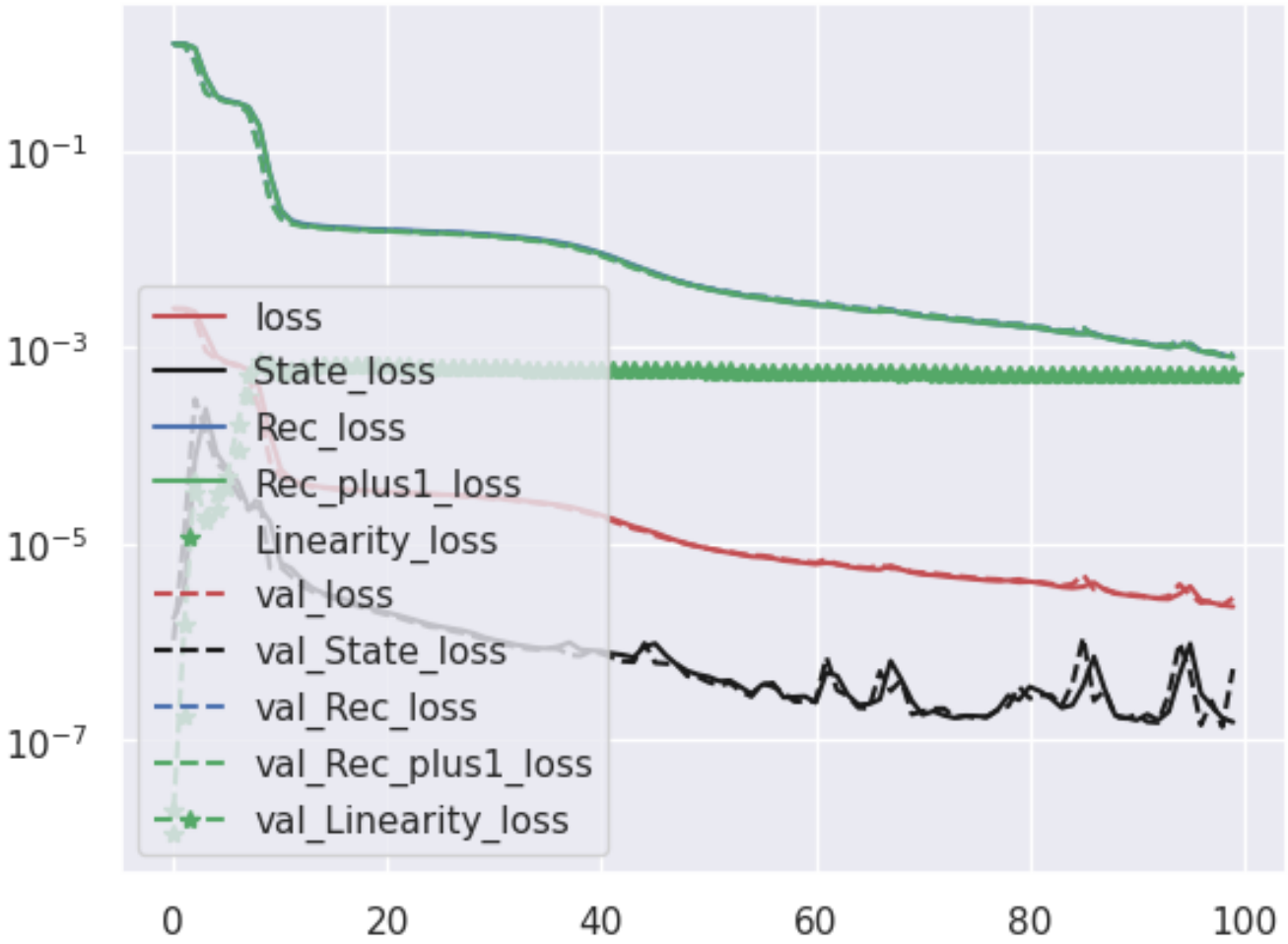
Deep Koopman

$\gamma = 0.2$



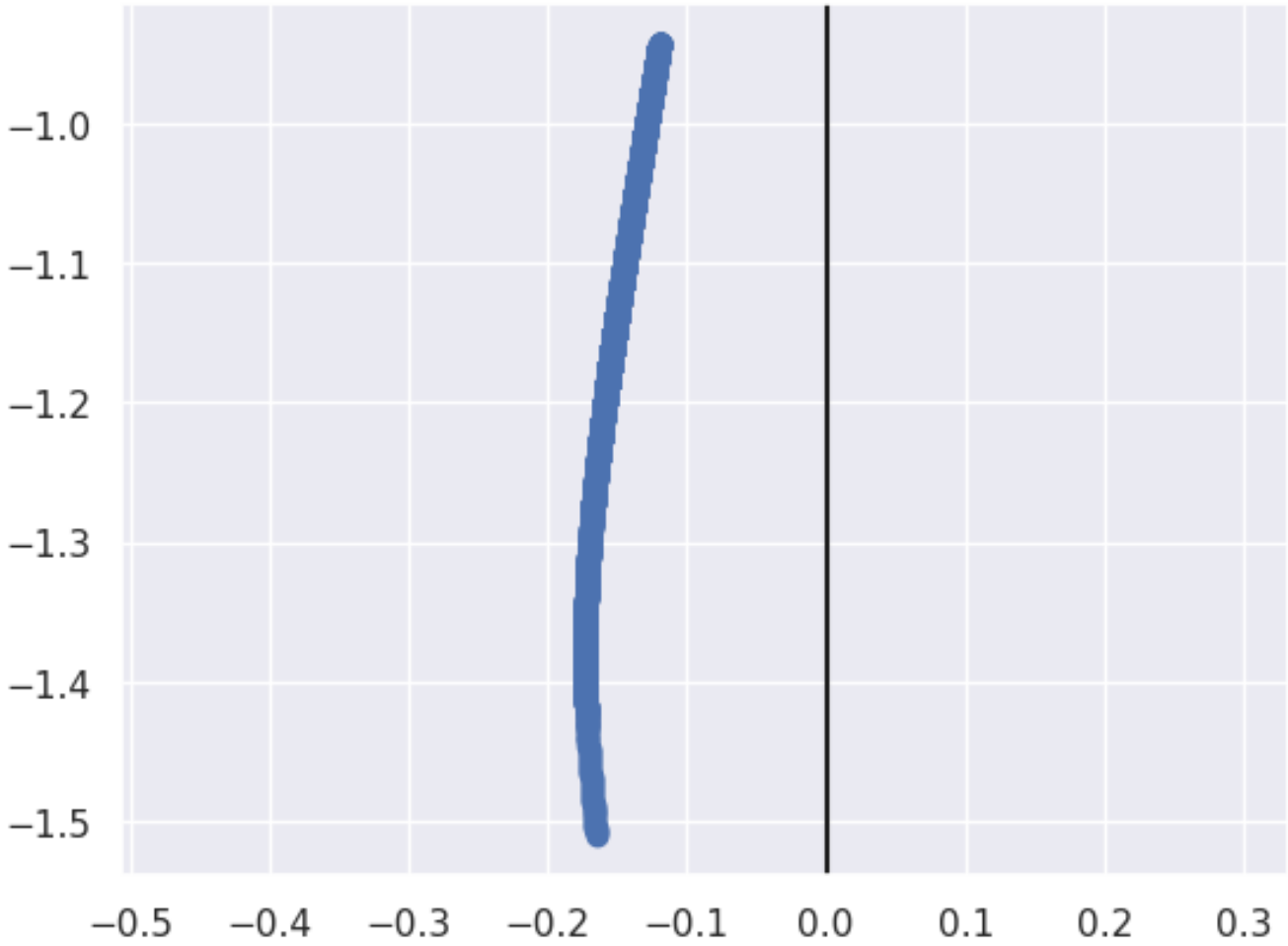
Deep Koopman

$\gamma = 0.28$



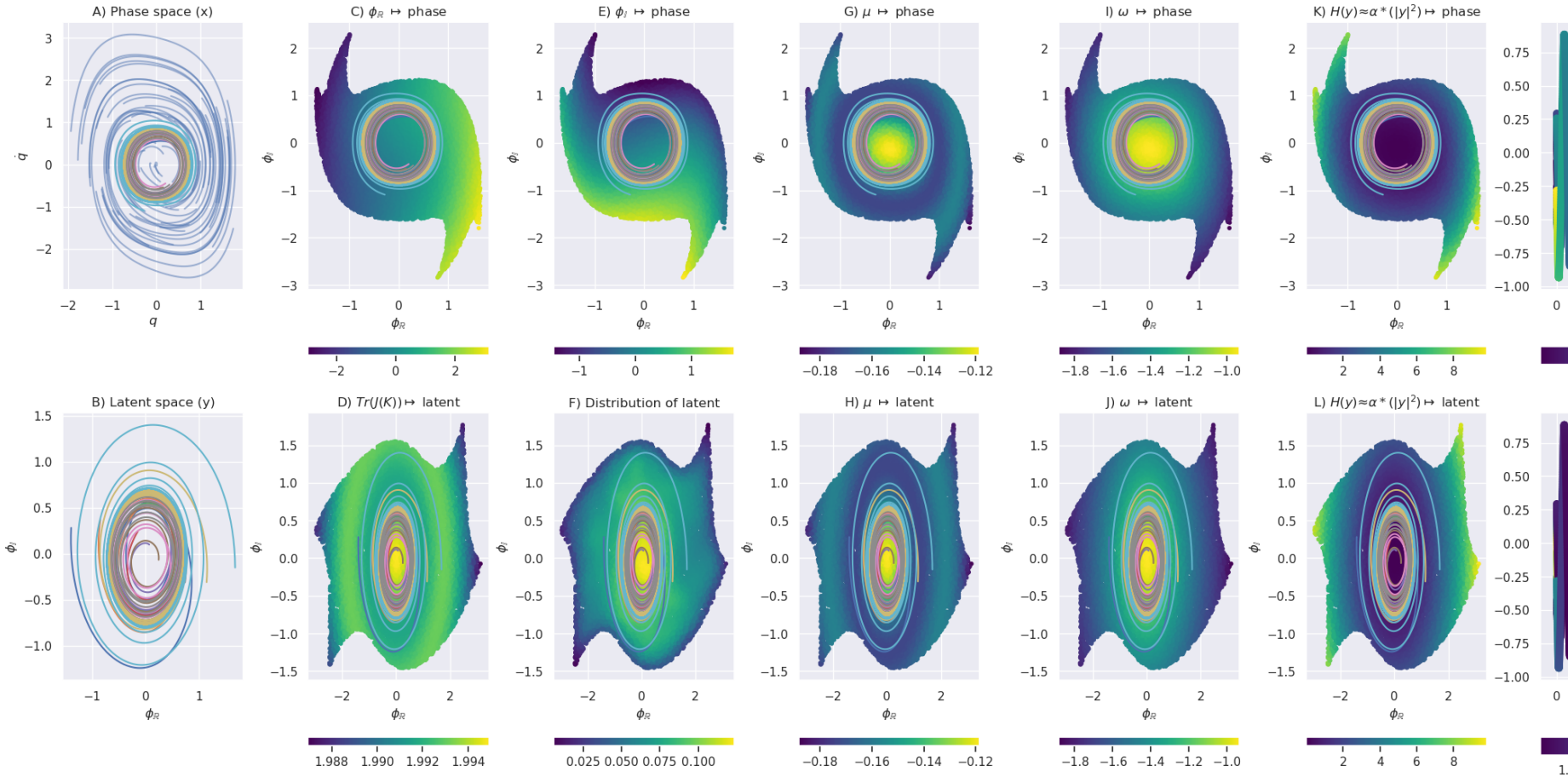
Deep Koopman

$\gamma = 0.28$



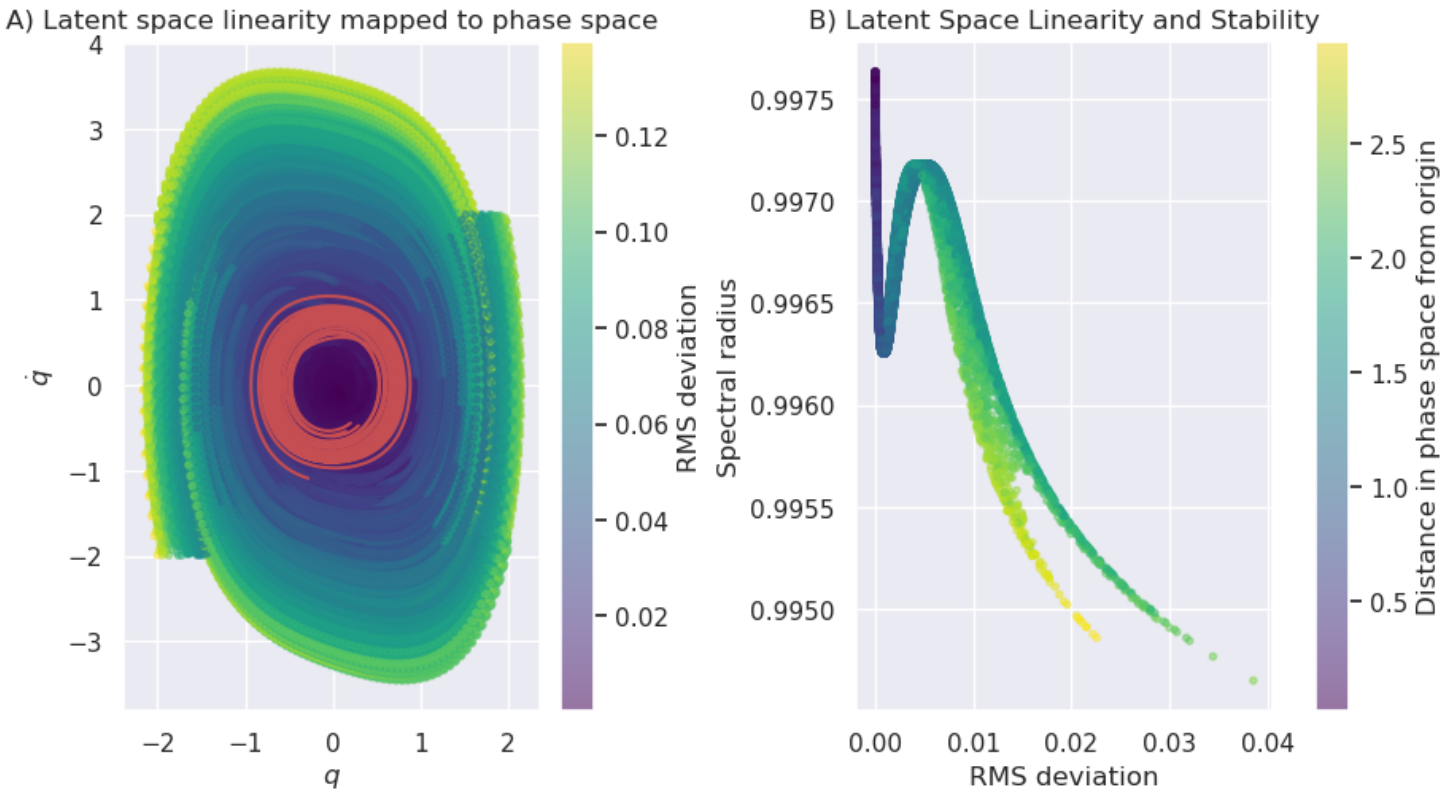
Deep Koopman

$\gamma = 0.28$



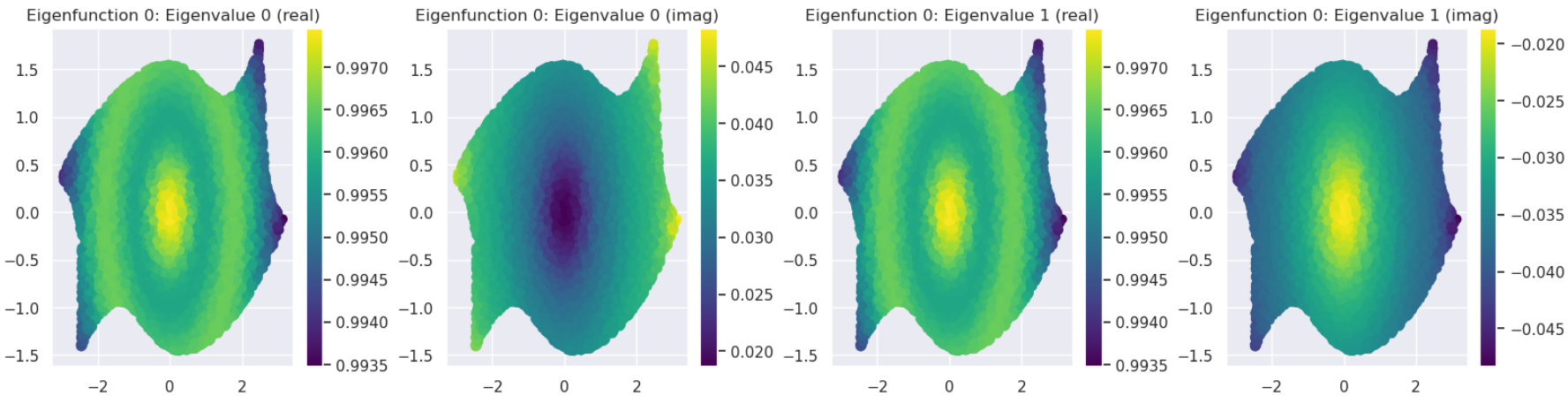
Deep Koopman

$\gamma = 0.28$



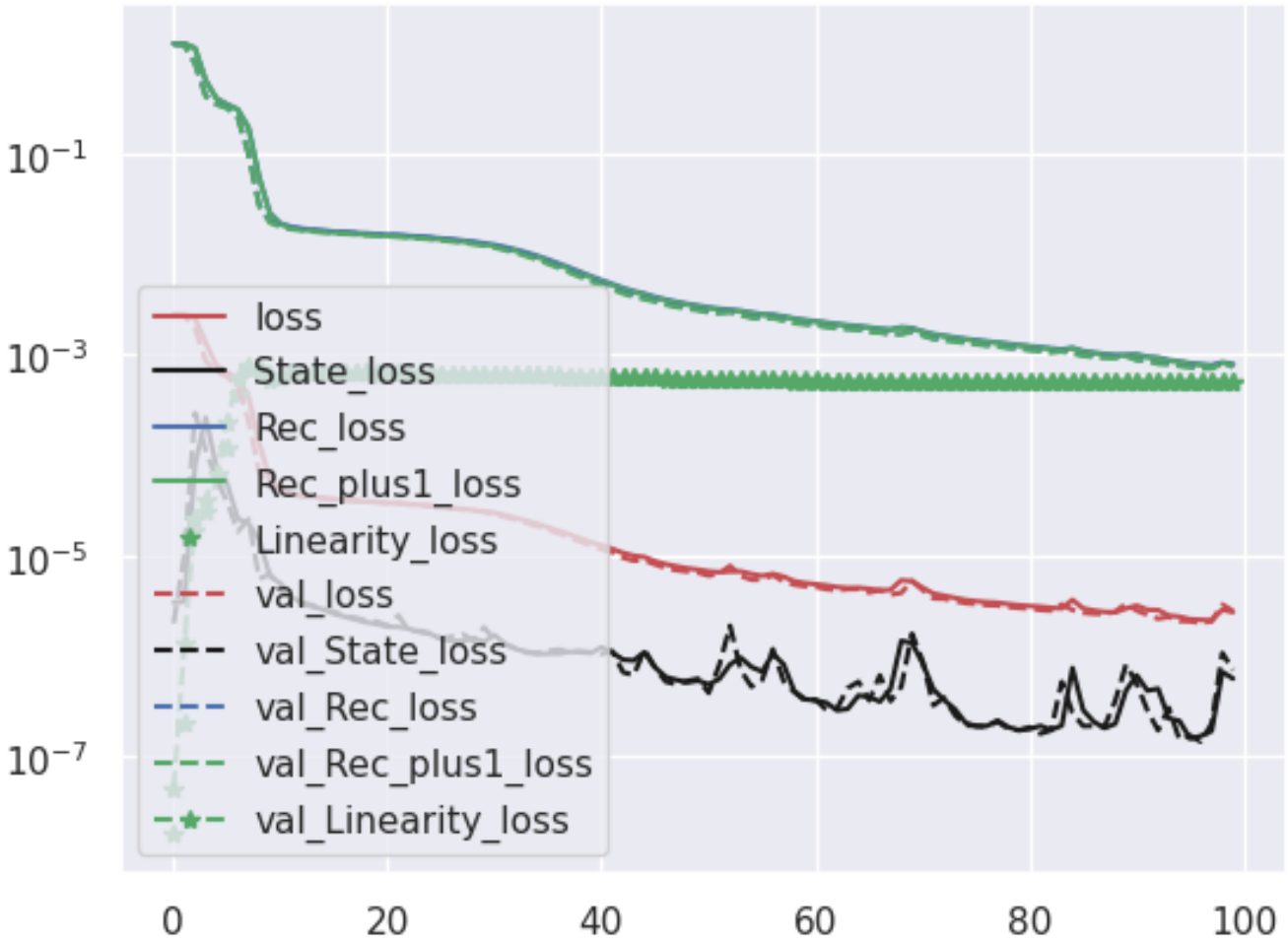
Deep Koopman

$\gamma = 0.28$



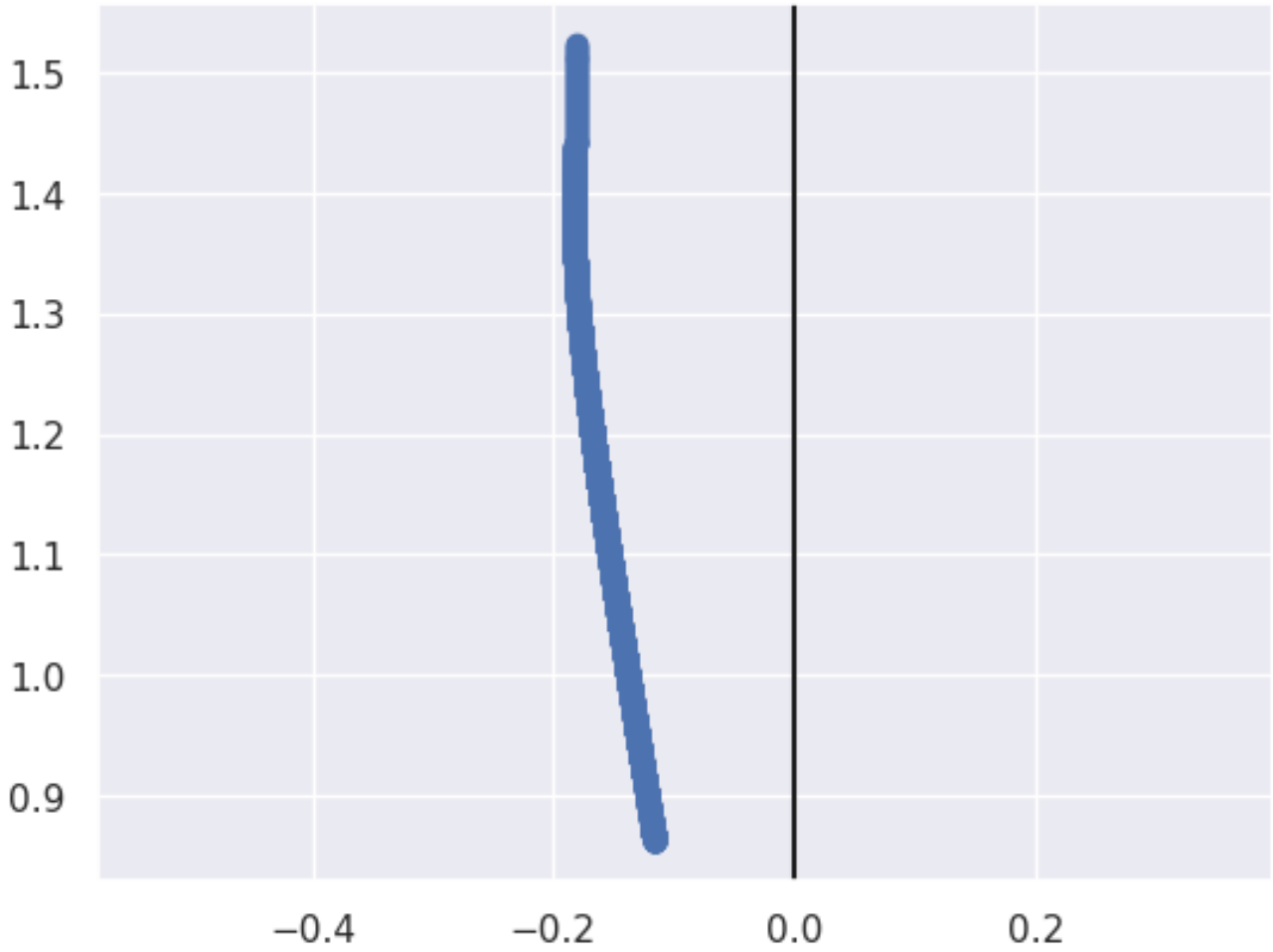
Deep Koopman

$\gamma = 0.29$



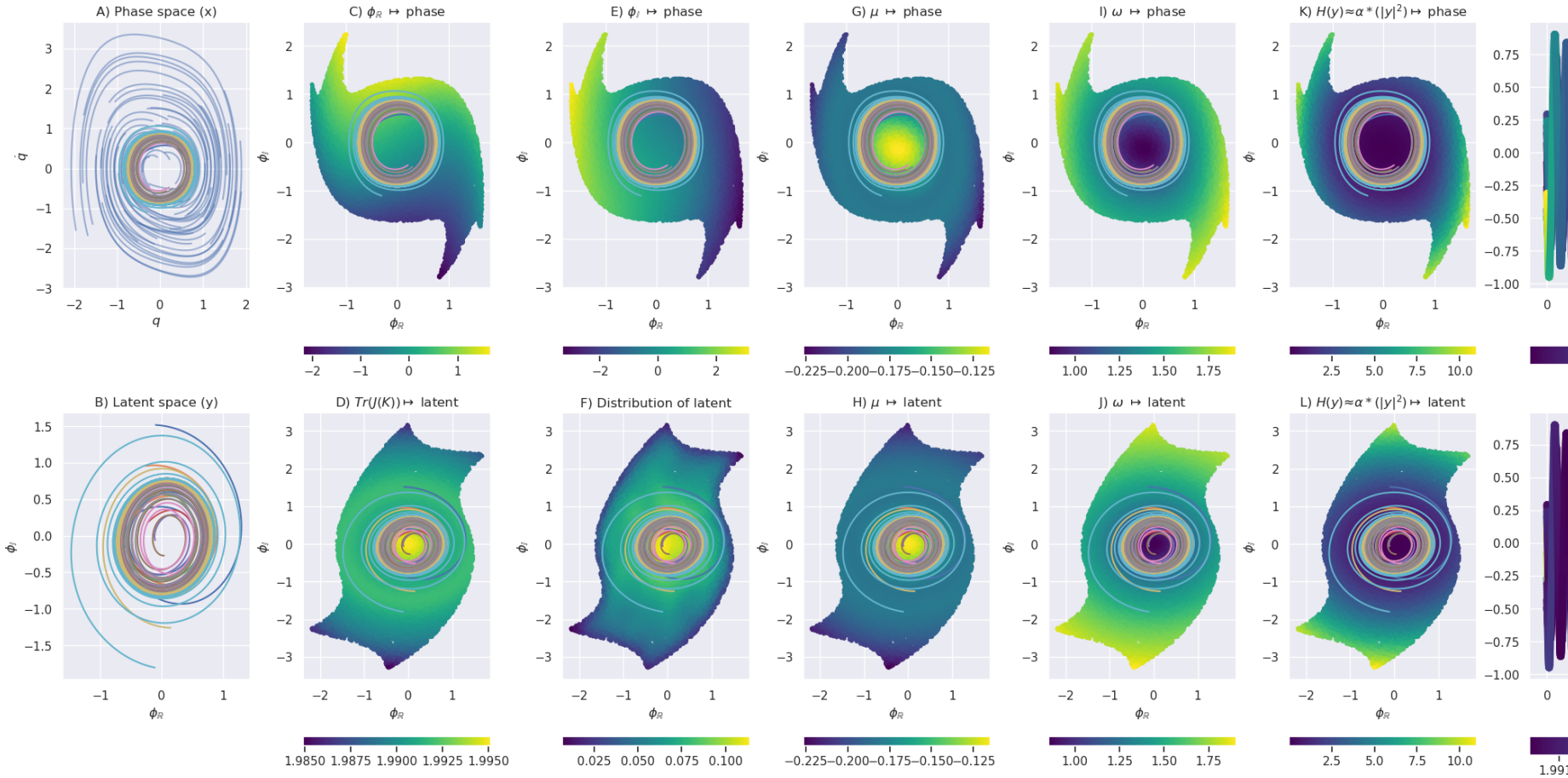
Deep Koopman

$\gamma = 0.29$



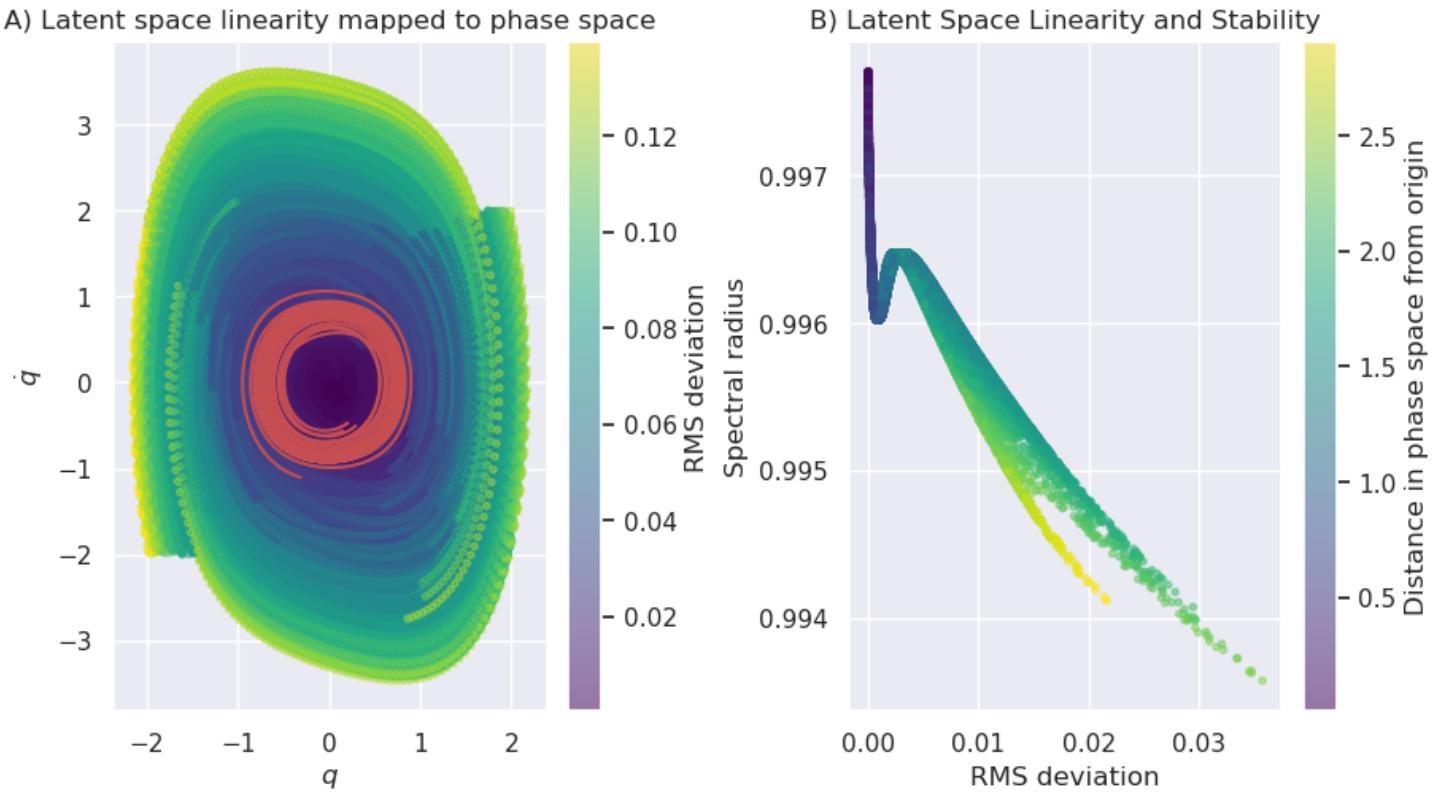
Deep Koopman

$\gamma = 0.29$



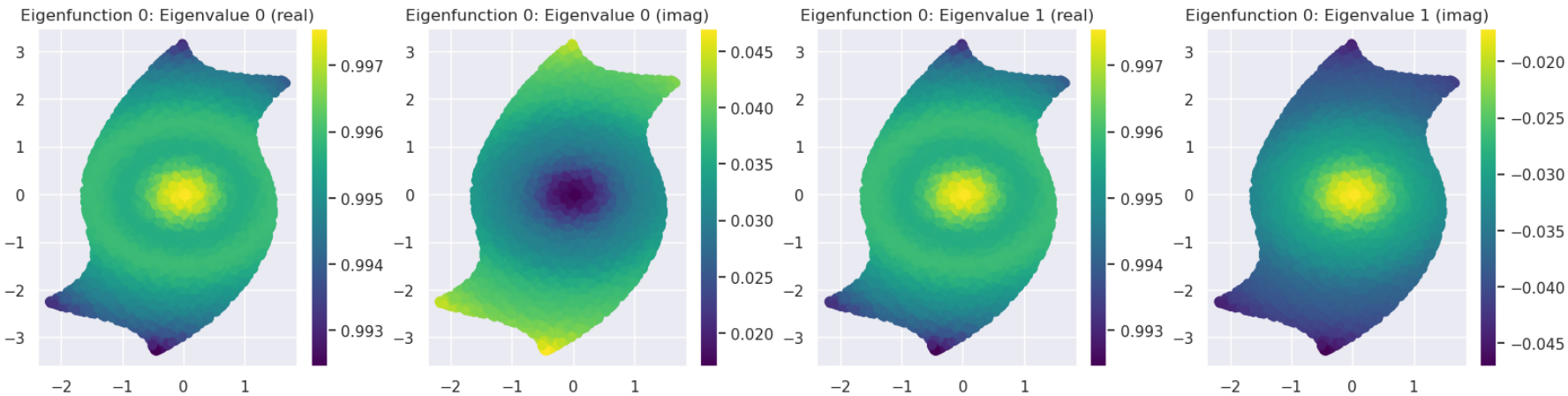
Deep Koopman

$\gamma = 0.29$



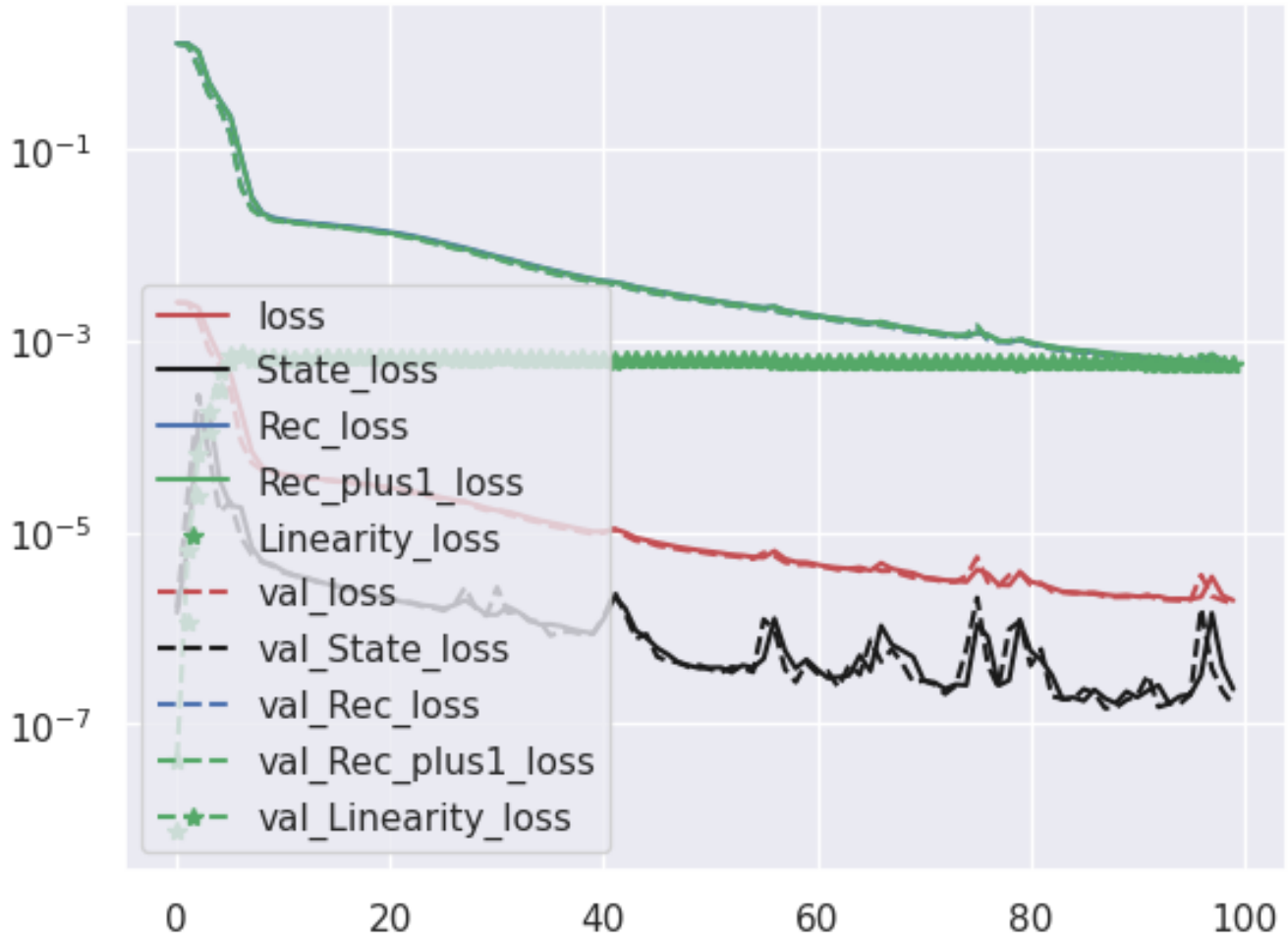
Deep Koopman

$\gamma = 0.29$



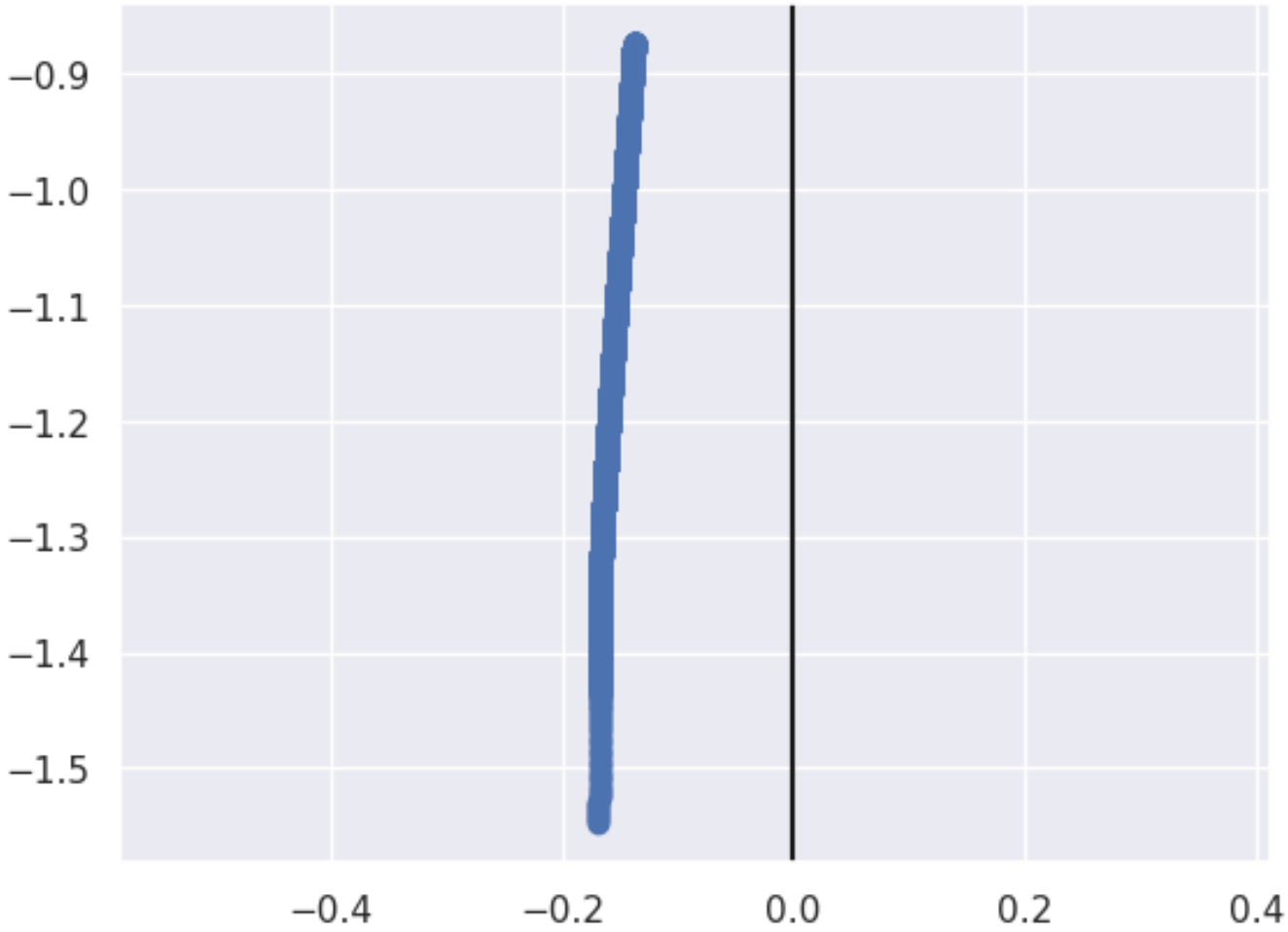
Deep Koopman

$\gamma = 0.37$



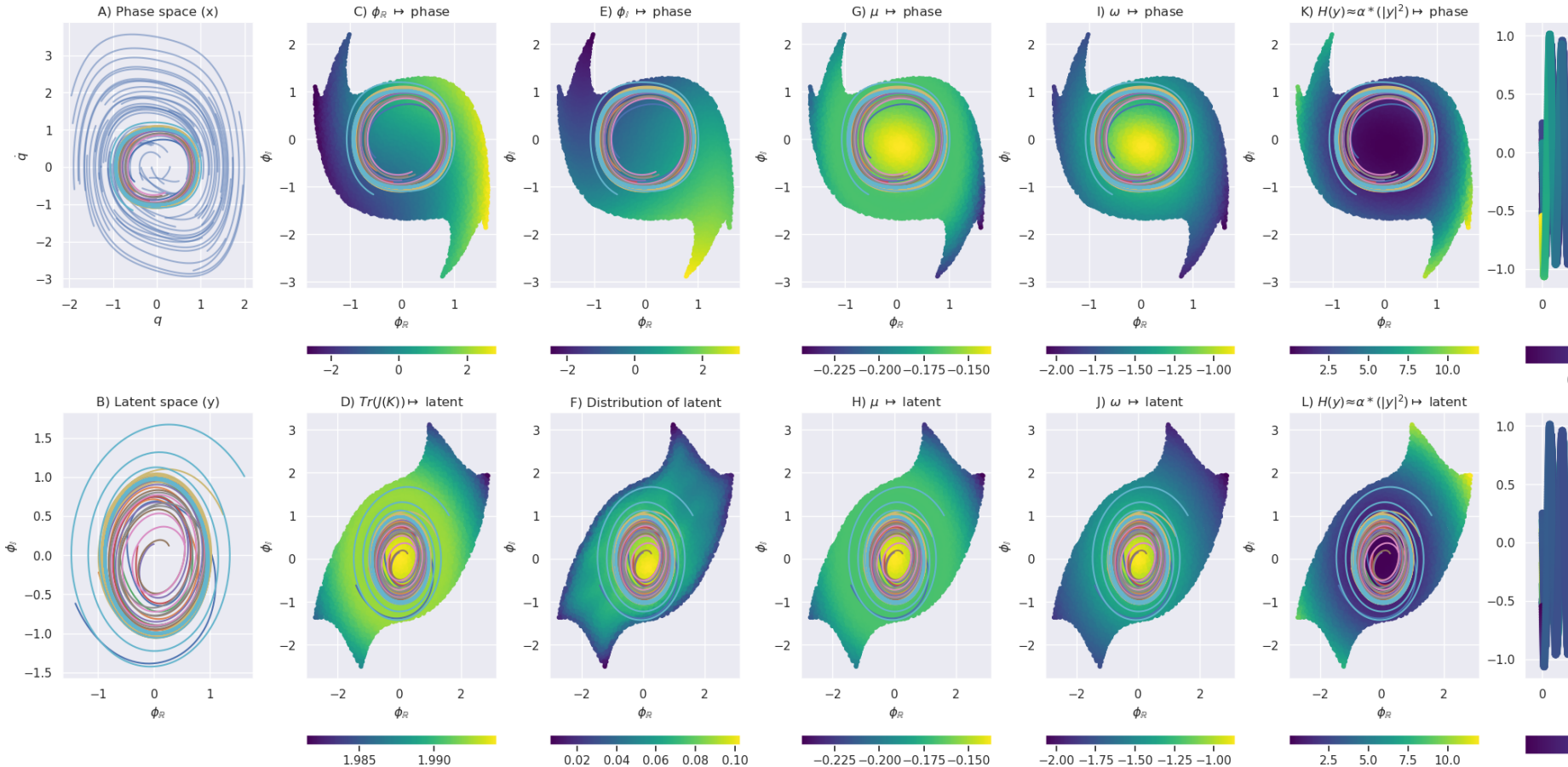
Deep Koopman

$\gamma = 0.37$



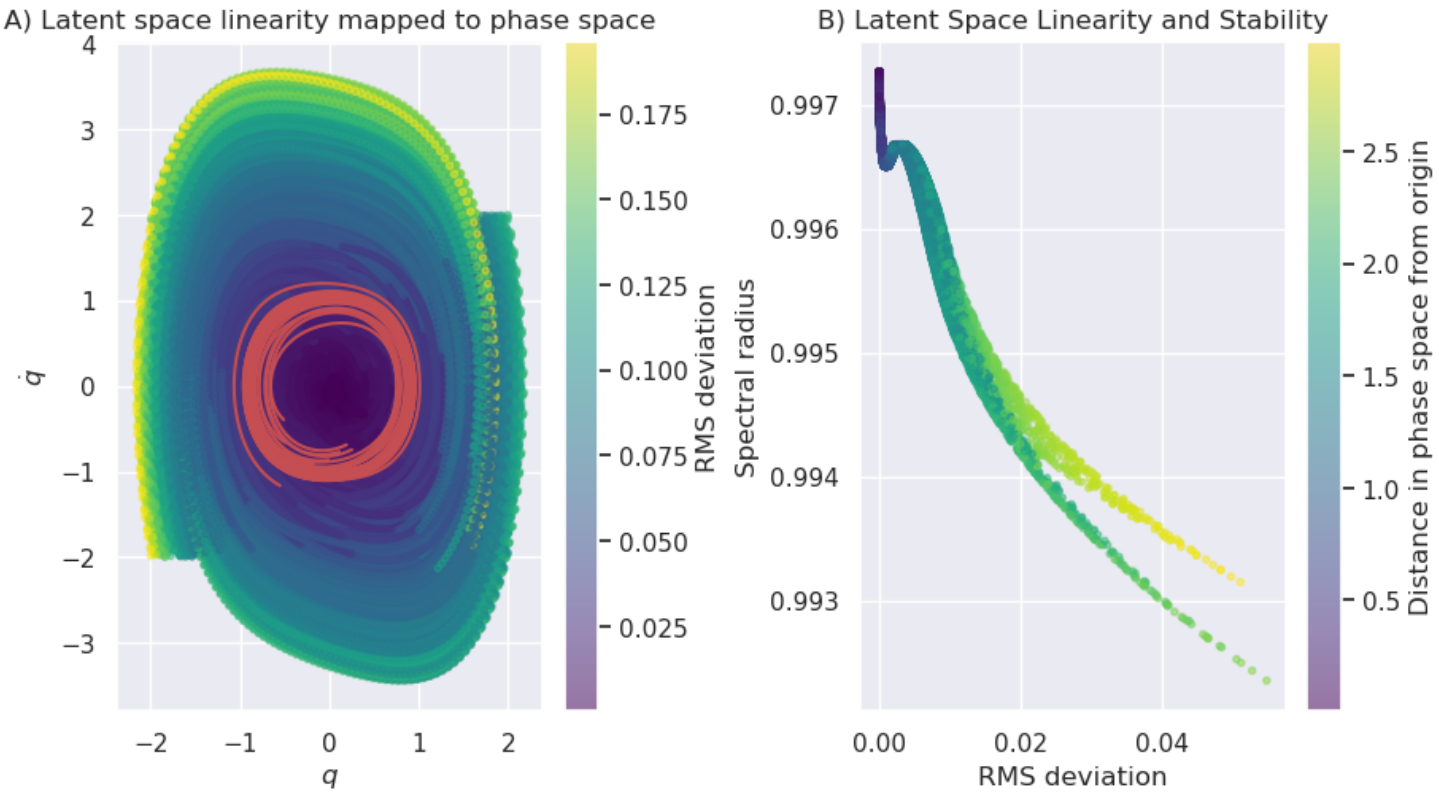
Deep Koopman

$\gamma = 0.37$



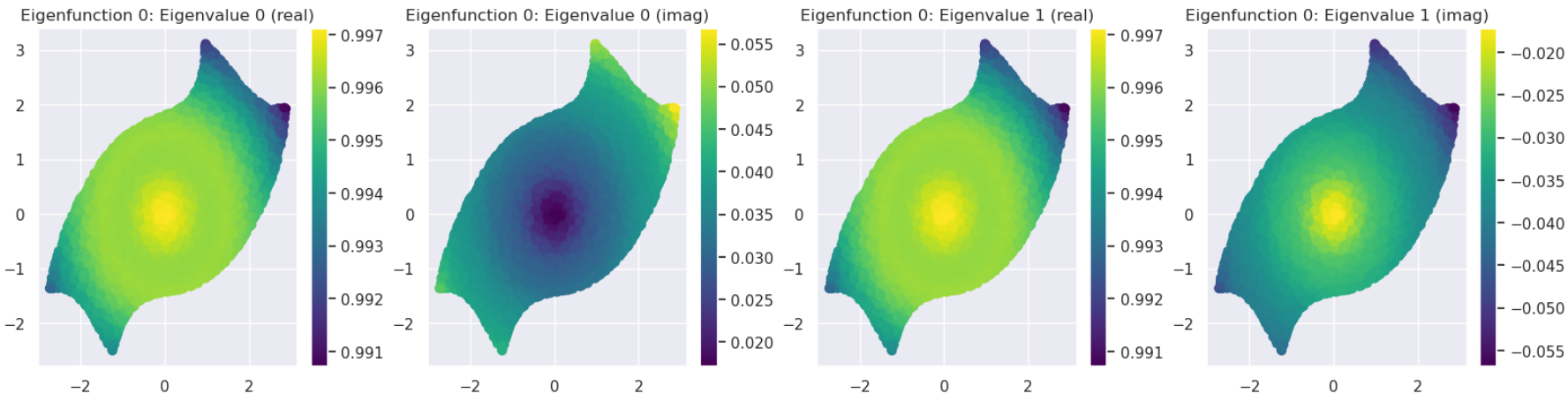
Deep Koopman

$\gamma = 0.37$



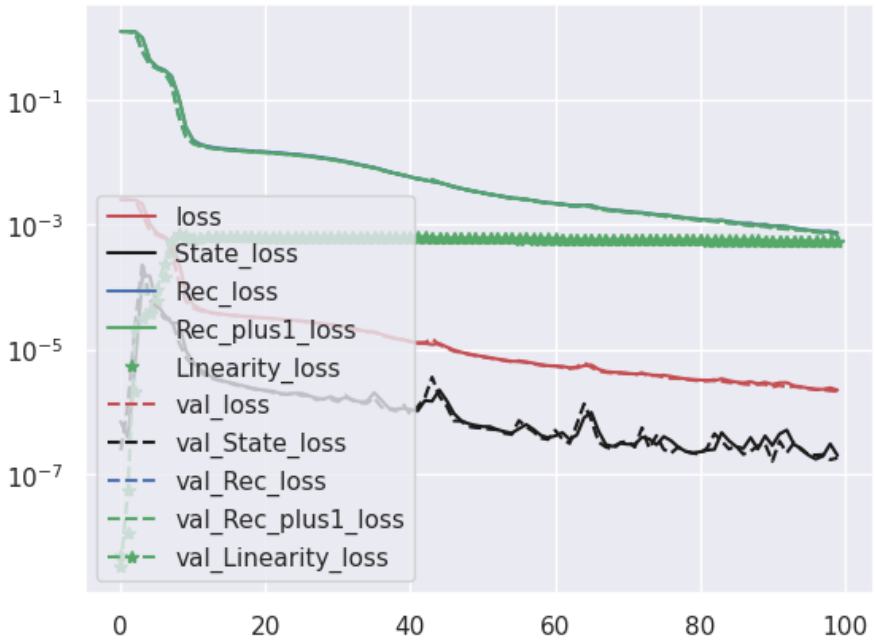
Deep Koopman

$\gamma = 0.37$



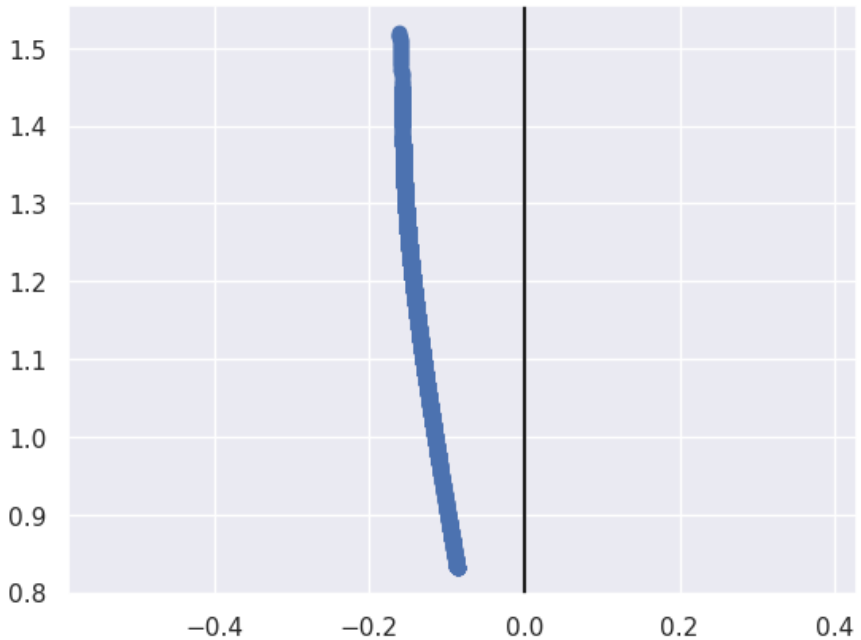
Deep Koopman

$\gamma = 0.5$



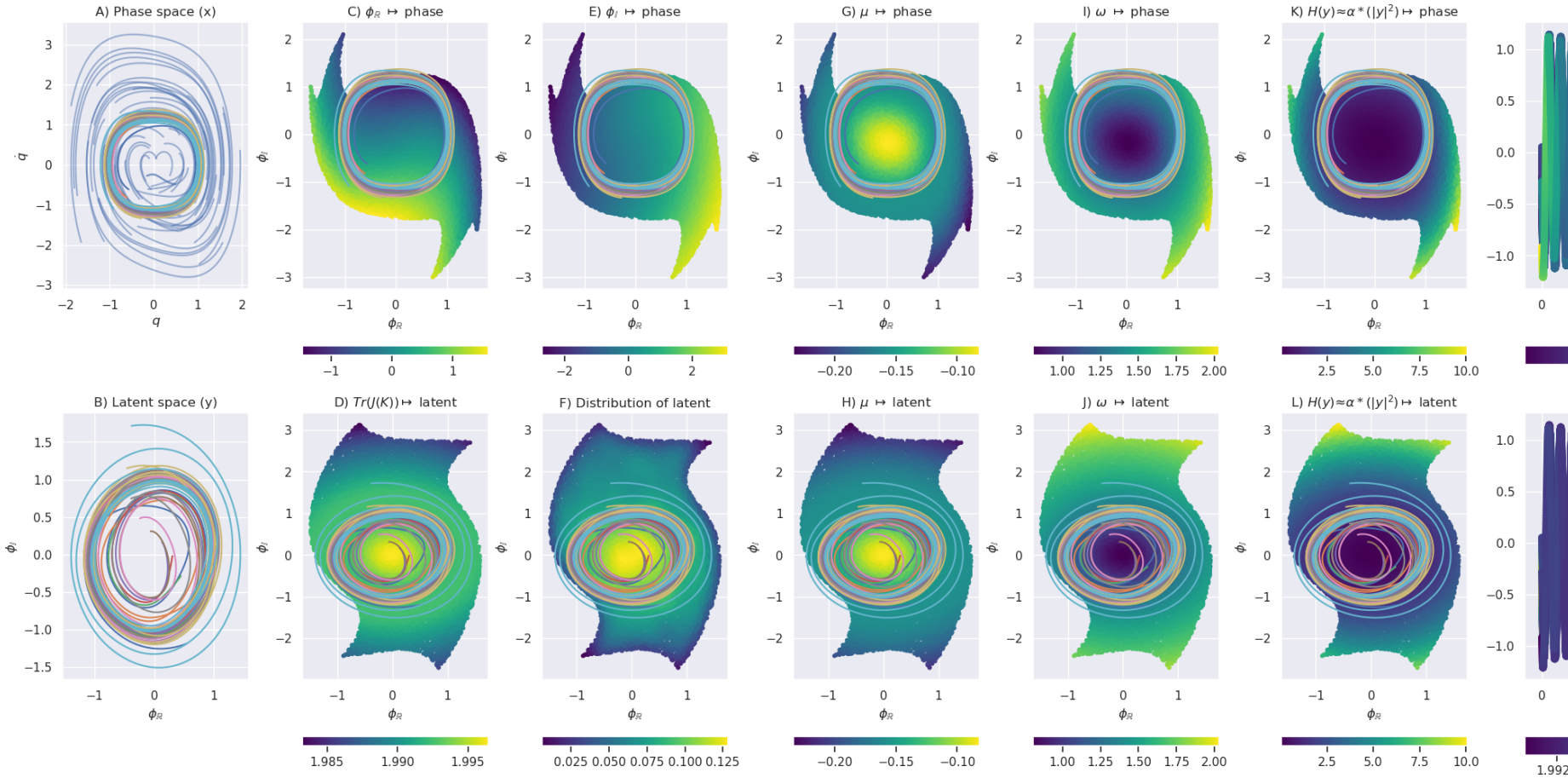
Deep Koopman

$\gamma = 0.5$



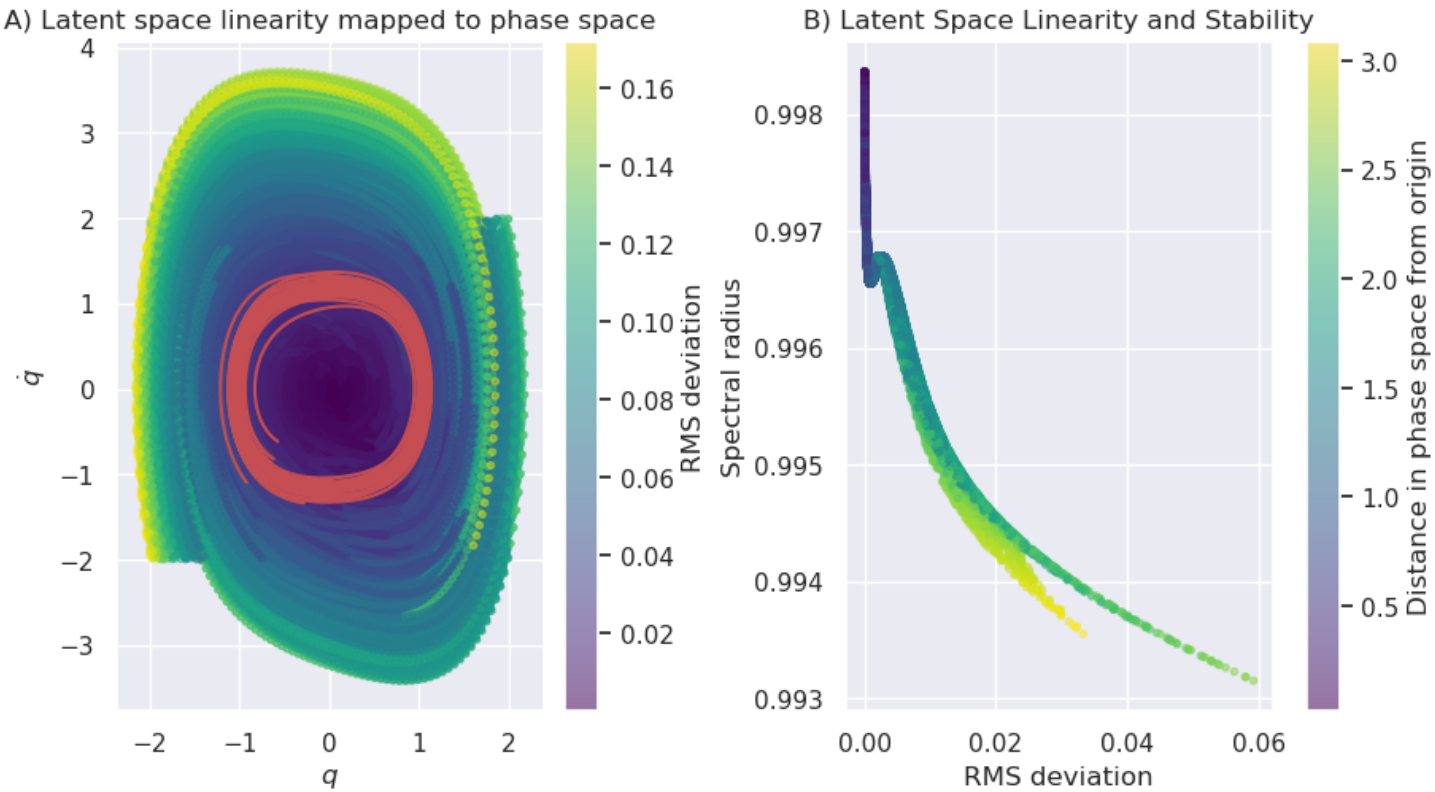
Deep Koopman

$\gamma = 0.5$



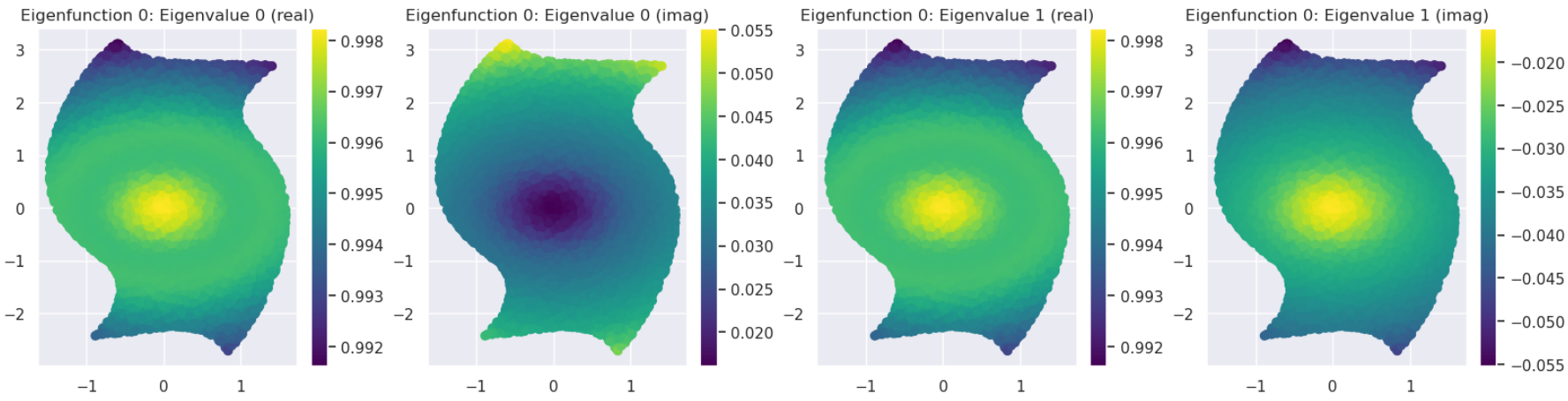
Deep Koopman

$\gamma = 0.5$



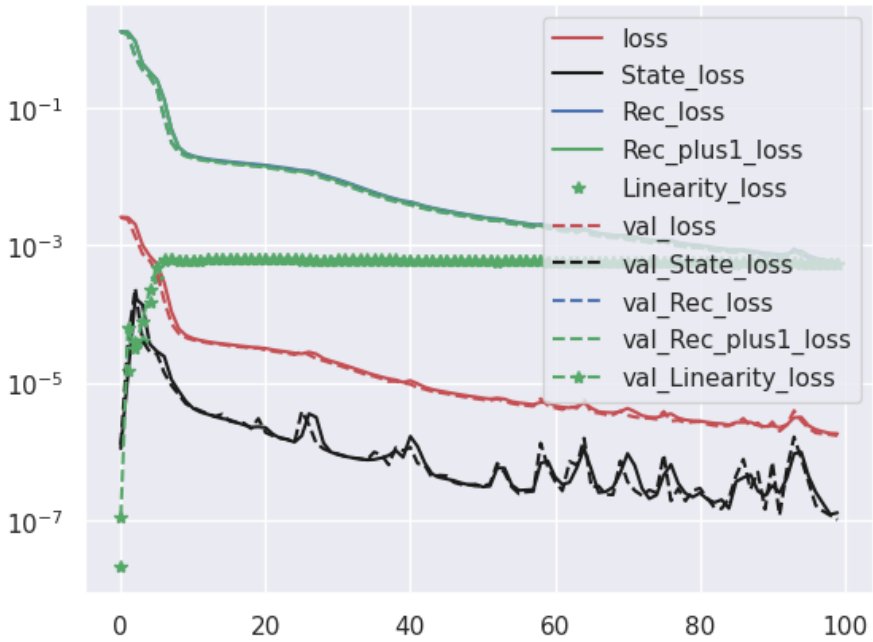
Deep Koopman

$\gamma = 0.5$



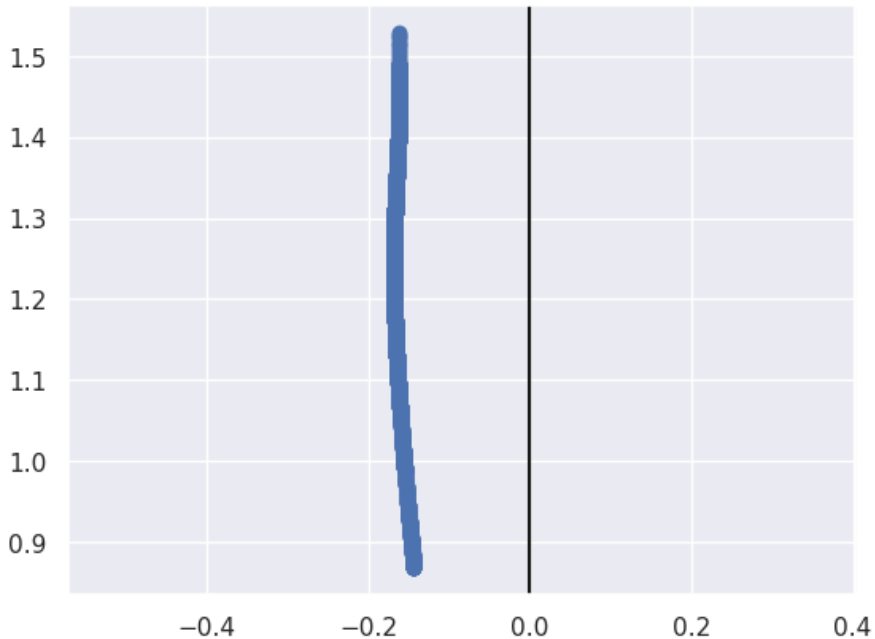
Deep Koopman

$\gamma = 0.65$



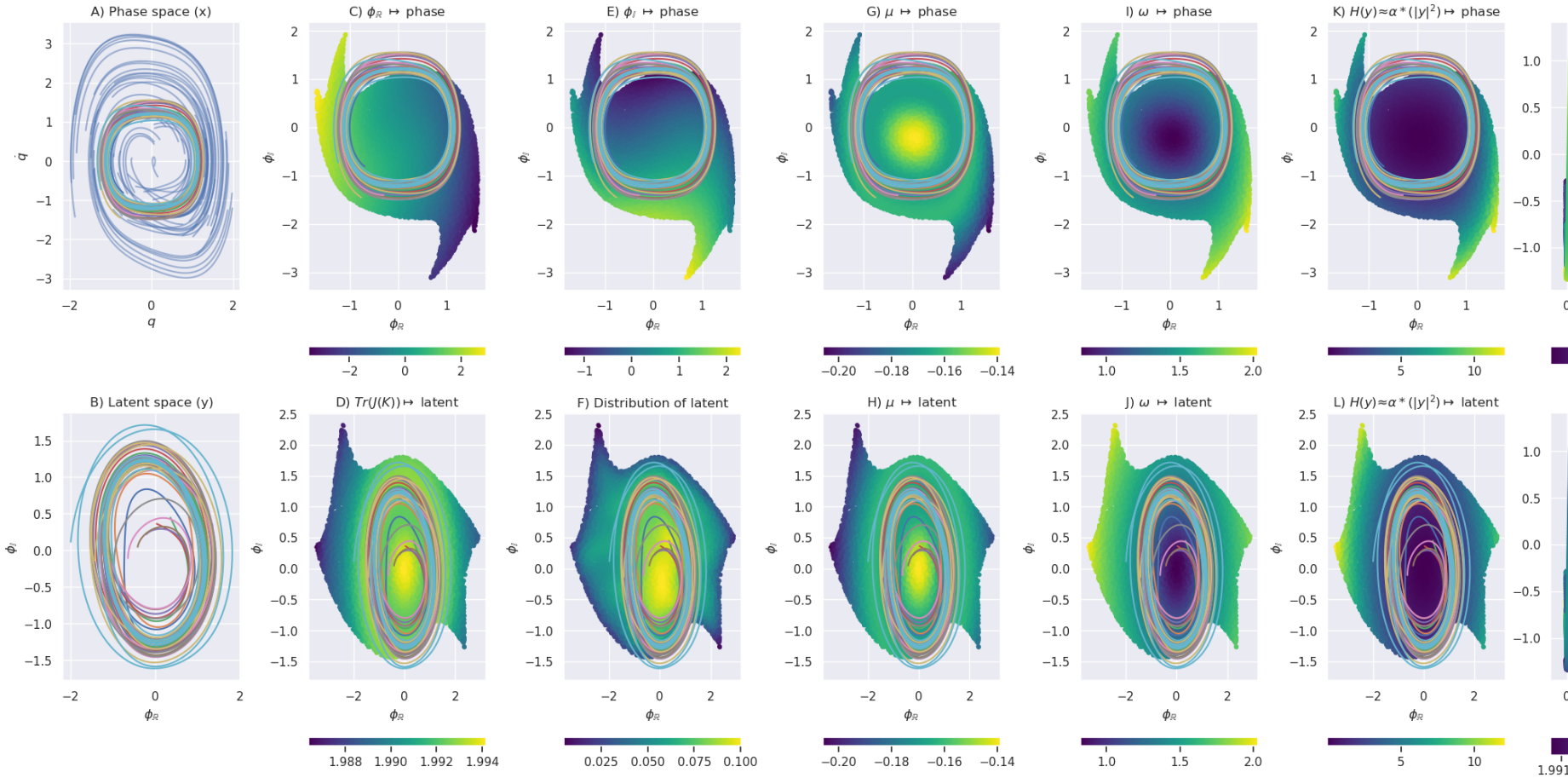
Deep Koopman

$\gamma = 0.65$



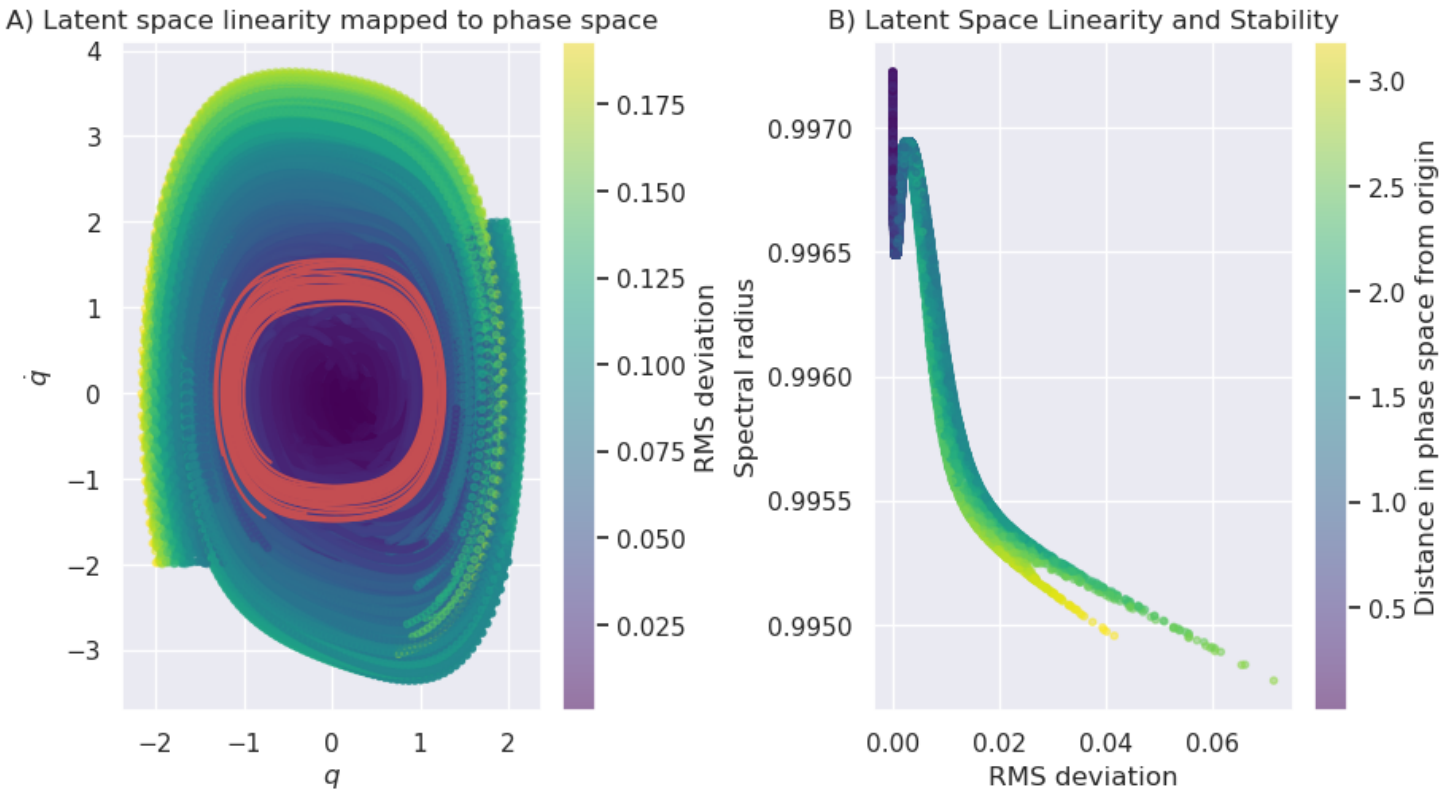
Deep Koopman

$\gamma = 0.65$



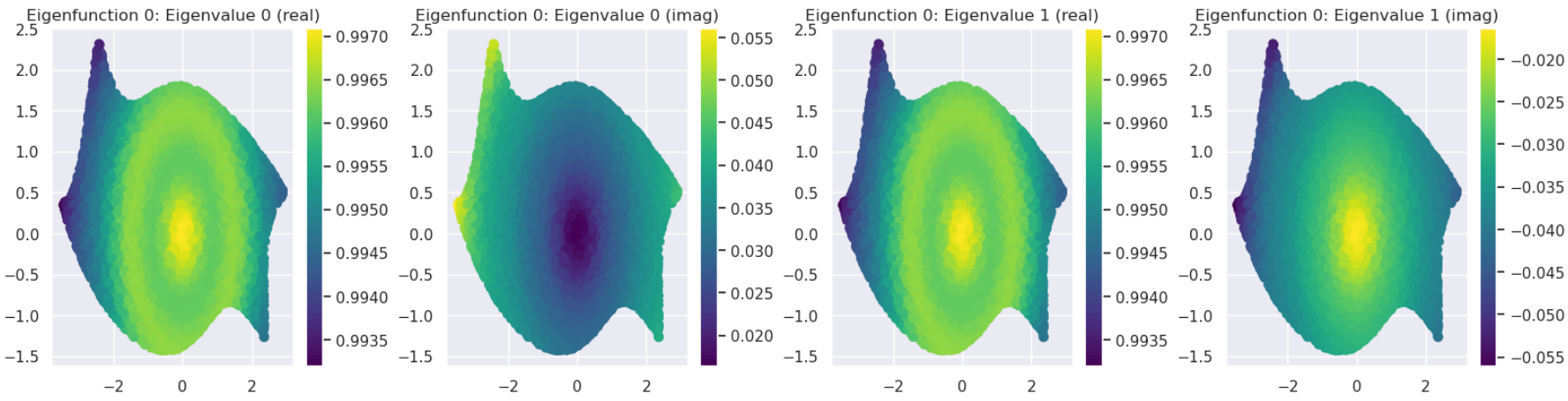
Deep Koopman

$\gamma = 0.65$



Deep Koopman

$\gamma = 0.65$



What about dlkoopman? Well...

dlkoopman

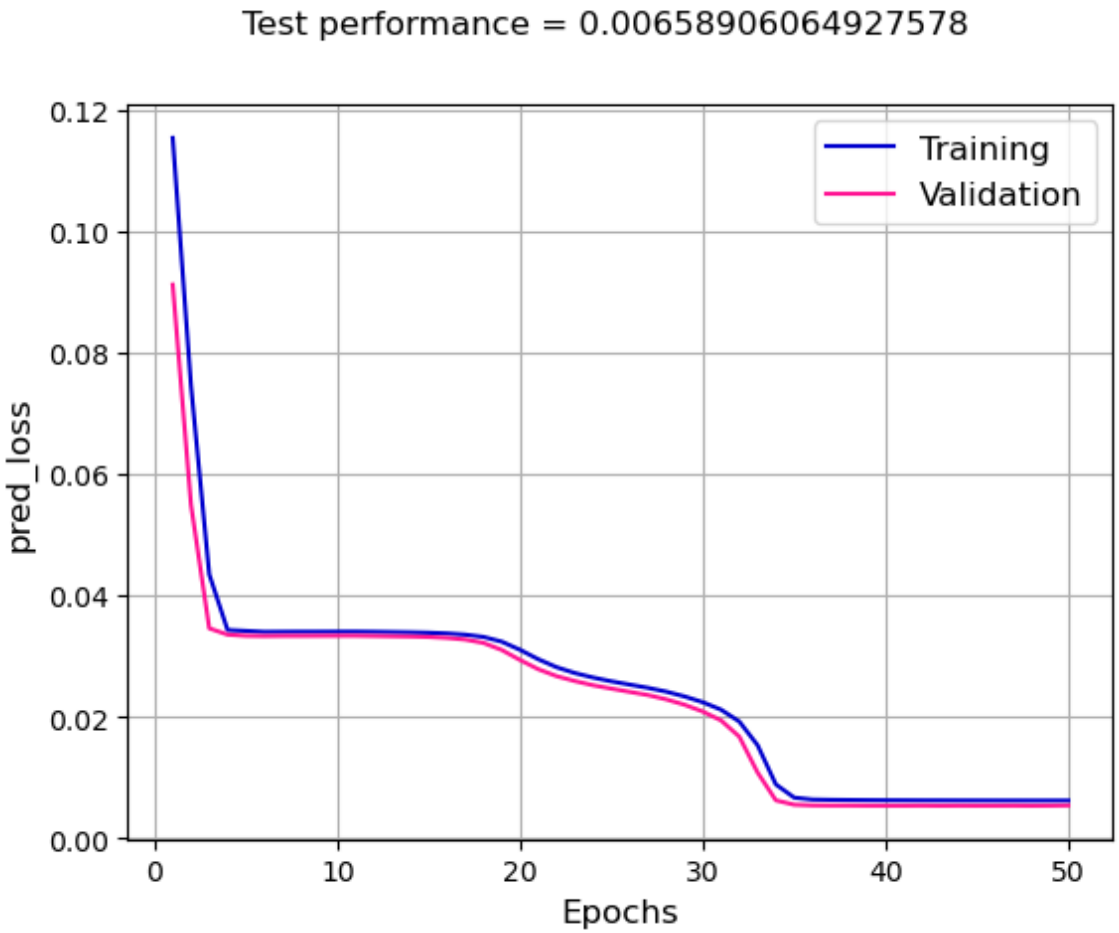
Loss seemed to reduce well, but prediction did not look correct at all, and eigenvalues were definitely not correct. This is almost certainly an implementation issue on my part.

dlkoopman

One benefit of dlkoopman is that it comes with a hyperparameter search method, wherein one can filter down what network sizes and types will best fit the data.

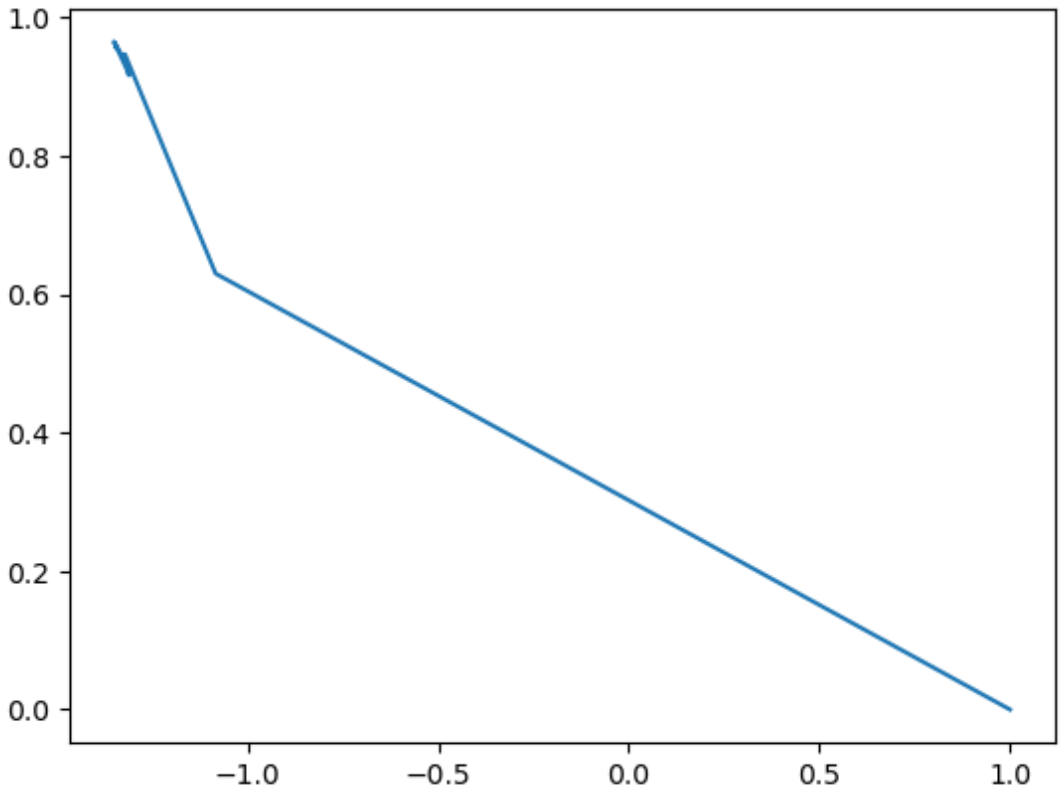
dlkoopman

$\alpha = -1, \beta = 1, \delta = \gamma = 0$



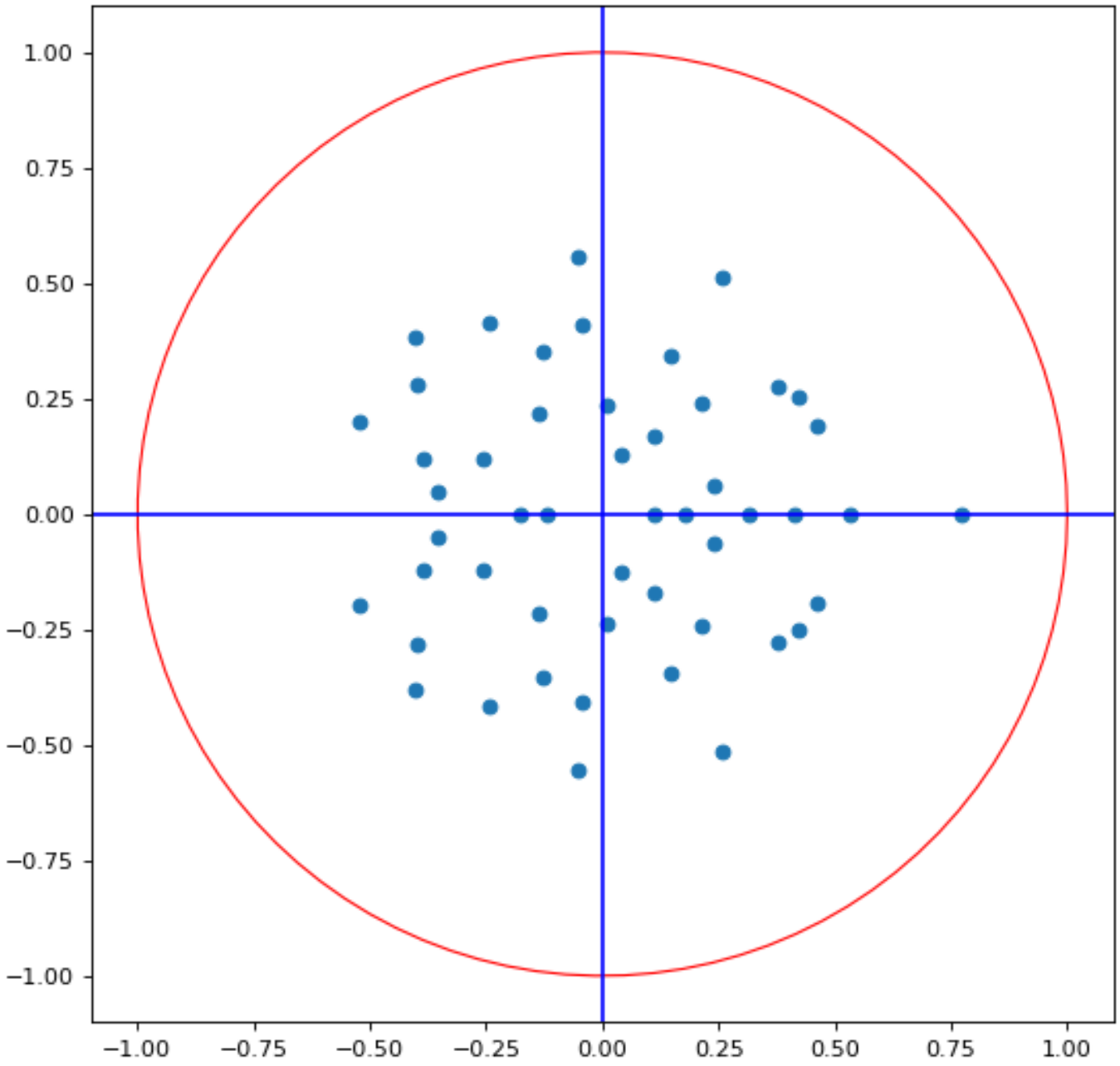
dlkoopman

$\alpha = -1, \beta = 1, \delta = \gamma = 0$



dlkoopman

$\alpha = -1, \beta = 1, \delta = \gamma = 0$



In conclusion, deep Koopman neural net can weakly identify Hamiltonian systems, but struggles with higher cycle and chaotic behavior.