Koopman Dynamics

Varun Varanasi

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1 Introduction

Dynamical systems are near ubiqituous in the natural world with rich applications in biology, chemistry, physics, economics, and control theory. They are often applied in modeling real-world phenomena to predict future action, better understand how system parameters impact performance, actively control dynamic systems through interactive feedback cycles, and discover governing equations. Modeling these systems can often be difficult due to uncertainities in measurement, unknown parameters, and inexact equations of motion. They are further complicated by non-linearities which introduce added complexity and inhibit the use of well understood linear analysis techniques. With no known overarching framework for non-linear systems, they are often studied by assuming local linearity in certain phase space regimes. Koopman Operator Theory was designed to address these specific issues. The high level idea behind the operator theory is to transform the non-linear systems into a higher dimensional space where linearities can emerge. The idea is that in these high dimensional spaces we can extend the regions where linear approximations of non-linear dynamical systems are appropriate. Koopman dynamical models also provide additional physical interpretability of the system. For these reasons, Koopman dynamics have become a recent interest for the dynamical systems and control theory communities for understanding and modeling complex systems.

2 Dynamical Systems Background

Dynamical systems originate from Newtonian Mechanics and refer to the broad class of systems that are described by a function relating the position of a point over time. The state of the system is a representation of the position of the dynamical system in phase space and is given by a scalar or vector depending on the dimensions of the system. The system evolves according to an evolution rule that describes the action of the system based on its current state. In the context of this work, we refer to dynamical systems of the following form:

$$\frac{d}{dt}\boldsymbol{x}(t) = \boldsymbol{f}(\boldsymbol{x}(t), t; \beta)$$

$\boldsymbol{x}$ describes the state of the system, $\boldsymbol{f}$ is the the vector field, and β is the system parameter. In the discrete case, we represent dynamical systems as a map:

$$\boldsymbol{x}_{k+1} = \boldsymbol{F}(\boldsymbol{x}_k)$$

2.1 Dynamical System Example

Consider a 1-D system governed by the following equation:

$$\frac{d^2x}{dt^2} = -\frac{dV(x)}{dx} \qquad V(x) = \frac{x^4}{4} - \frac{x^2}{2}$$

We can equivalently state this as $\ddot{x} = -x^3 - +x$. It is clear that this is a dynamical system as our system evolves in time according to its current position. This rather unassuming governing equation produces rather complex behavior which we can visualize via a phase portrait.

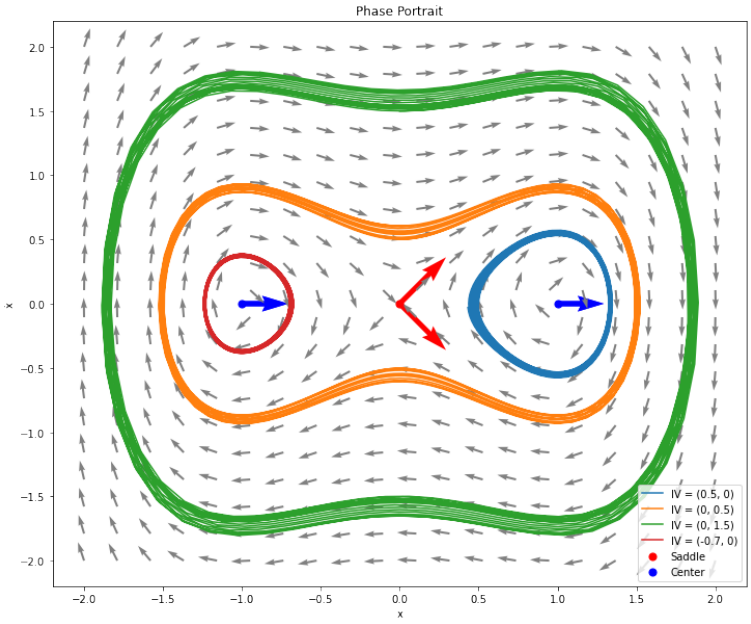

Figure 1: Phase Portrait of Example Dynamical System

It is clear that the dynamics of this system are highly dependent on the initial position and not simply characterized. The motivating question behind this work is to answer how we can predict and understand systems like this. One of such methods is via linear systems.

2.2 Linear Dynamical Systems

In general, linear dynamical systems tend to be easier to characterize. We define a linear dynamical system as one that obeys

$$\frac{d}{dt}\boldsymbol{x} = \boldsymbol{A}\boldsymbol{x}$$

In addition to being being rigorously studied, linear dynamical systems are of importance because they admit closed form solutions. For example, under certain stability conditions, the above system is solved as

$$x(t + t_0) = e^{\boldsymbol{A}t}\boldsymbol{x}(t_0)$$

Furthermore, in linear dynamical systems, the eigenvalues and eigenvectors of the matrix $\boldsymbol{A}$ fully describe the system. Assuming a sufficiently nice matrix $\boldsymbol{A}$, we can then diagonalize it by applying the spectral decomposition theorem.

$$A = Q\Lambda Q^{-1}$$

We can then plug this form into the closed form solution to yield

$$x(t + t_0) = \boldsymbol{Q}e^{\boldsymbol{\Lambda}t}\boldsymbol{Q}^{-1}\boldsymbol{x}(t_0)$$

We can think of Q^{-1} as a transformation of x such tht $z = Q^{-1}x$. Since Q is orthogonal, we see that this new space z is decoupled. Therefore, each component evolves indepedently.

$$\frac{d}{dt}z_i = \lambda_i z_i$$

Linear dynamical systems are ideal to study because we can use this eigenvalue decomposition to decouple the dynamics of the system. One of the major goals of Koopman Dynamical Theory is to construct a linear basis for non-linear systems so that we can apply this methodology to understand, predict, and control non-linear systems.

3 Koopman Operator Theory

Koopman Theory originates from Bernard O. Koopman and his work in 1931 with John von Neumann to create an operator theory for classical mechanics analagous to quantum mechanics. Their key observation was that the phase space of a system could be converted to a Hilbert space. In the language of dynamical systems, this meant that nonlinear dynamical systems can be represented as an infinite-dimensional linear operator. This linear operator, known as a Koopman operator, can be further decomposed via spectral decomposition to yield decoupled behavior as shown above in the analysis of a linear dynamic system. The challenges presented by this method then fall to representing this infinite dimensional space in as finite-dimensional matrix. In the preceeding sections we will cover the mathematical foundations and basic methodologies for determining the finite-dimensional linear representation of the Koopman operator.

3.1 Mathematical Foundation

Consider an autonomous ordinary differential equation as introduced in the discussion of linear dynamical systems. We say that our state exists in $\mathcal{X} \subseteq \mathbb{R}^n$ and is propogated forward by the flow operator $\boldsymbol{F}^t : \mathcal{X} \to \mathcal{X}$. Under this schema our system evolves according to

$$\boldsymbol{x}(t) = \boldsymbol{F}^t(x(0))$$

To introduce our Koopman operator we begin by defining a class of measurement function or observable functions $g : \mathcal{X} \to \mathbb{C}$. We refer to the set of these measurement functions as $\mathcal{G}(x)$ which is the space our Koopman operator, $\mathcal{K}$, acts on. Therefore, we have $\mathcal{K} : \mathcal{G}(x) \to \mathcal{G}(x)$ where

$$\mathcal{K}^t g(x) = g(\boldsymbol{F}^t(x))$$

We see that the koopman operator acts to propogate the observable function forward in time. We can use this interpretation to define a family of functions $g^t = \mathcal{K}g$. The choice of measurement functions is left as a design parameter, but in practice is often a Hilbert spaces or a reproducing kernel Hilber space. Note that the space of measurement functions is chosen to be much larger than the state space.

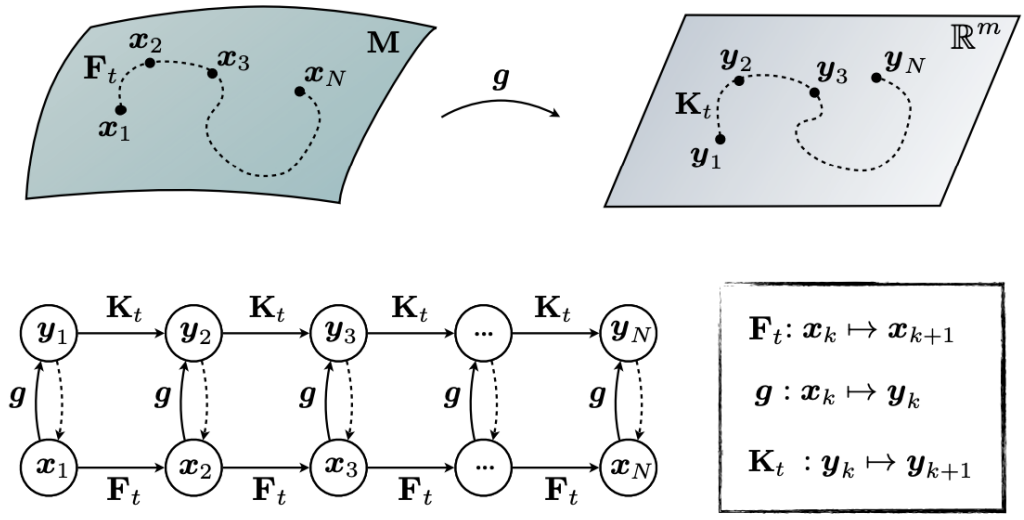

Figure 2: Schematic from "Notes on Koopman Theory"

The above digram highlights the role of Koopman Operatory theory in translating the dynamics of a system from space M to a space $\mathbb{R}^m$ via the measurement functions g. The koopman operator is then just the time propogator of the system in this new space.

An important fact of this framework is that if the space $\mathcal{G}(x)$ is a linear vector space, then the linearity extends to the Koopman operator.

$$\mathcal{K}^t(\alpha g_1(x) + \beta g_2(x)) = \alpha g_1(\boldsymbol{F}^t(x)) + \beta g_2(\boldsymbol{F}^t(x)) = \alpha \mathcal{K}^t(g_1(x)) + \beta \mathcal{K}^t(g_2(x))$$

This holds regardless of the linearity of $\boldsymbol{F}$. You can interpret this property as the koopman operator trading extra dimensionality for linearity.

3.2 Eigenfunctions

Since the Koopman operator extends the dimensionality of the system to infinity, the problem becomes increasingly complex. Instead, we attempt to exploit the additional structure provided by the Koopman operatory to identify a finite set of functions that evolve linearly with time and capture the key dynamic behavior. We can do this by finding the eigenfunctions of our Koopman operator since by definition they behave linearly.

$$\text{Continuous: } \frac{d}{dt}\psi(\boldsymbol{x}) = \mathcal{K}\psi(\boldsymbol{x}) = \lambda\psi(\boldsymbol{x}) \qquad \text{Discrete: } \psi(\boldsymbol{x}_{k+1}) = \mathcal{K}\psi(\boldsymbol{x}_k) = \lambda\psi(\boldsymbol{x}_k)$$

Notice that any conserved quantity must correspond to an eigenvalue of 0 so that its time evolution is constant. We can apply the chain rule to our eigenvalue equations to find:

$$\lambda\psi(\boldsymbol{x}) = \frac{d}{dt}\psi(\boldsymbol{x}) = \nabla\psi(\boldsymbol{x}) \cdot \dot{\boldsymbol{x}} = \nabla\psi(\boldsymbol{x}) \cdot \boldsymbol{f}(\boldsymbol{x})$$

This provides us a PDE which we can now use to computationally or analyticaly solve to find the eigenfunctions of the Koopman operator.

Another important property of eigenfunctions of the Koopman operator is that the product of two eigenfunctions is also an eigenfunction of $\mathcal{K}$. Consider the discrete case where ψ_1 and ψ_2 represent two arbitrary eigenfunctions $\mathcal{K}$.

$$\begin{aligned}\mathcal{K}_t\left(\psi_1(\boldsymbol{x})\psi_2(\boldsymbol{x})\right) &= \psi_1(\boldsymbol{F}_t(\boldsymbol{x}))\psi_2(\boldsymbol{F}_t(\boldsymbol{x})) \\ &= \lambda_1\lambda_2\psi_1(\boldsymbol{x})\psi_2(\boldsymbol{x})\end{aligned}$$

Similarly, if we consider the continuous case

$$\begin{aligned}\mathcal{K}(\psi_1, \psi_2) &= \frac{d}{dt}(\psi_1\psi_2) \\ &= \psi_1\dot{\psi_2} + \dot{\psi_1}\psi_2 \\ &= \lambda_2\psi_1\psi_2 + \lambda_1\psi_1\psi_2 \\ &= (\lambda_1 + \lambda_2)\psi_1\psi_2\end{aligned}$$

This property implies that in certain cases a subset of eigenfunctions can be used to construct all other eigenfunctions. In the context of our dynamical system problem, this means that if we can identify the subset of eigenfunctions that can generate the rest, we can readily capture the dynamics of the system.

3.3 Koopman Mode Decomposition

In general, when modeling a dynamical system we observe multiple measurements of the system at each timestep. Therefore, if we generalize our above discussion of observations, we can represent our observation as a vector:

$$\boldsymbol{g}(\boldsymbol{x}) = \begin{bmatrix} g_1(\boldsymbol{x}) \\ g_2(\boldsymbol{x}) \\ \dots \\ g_p(\boldsymbol{x}) \end{bmatrix}$$

From our earlier discussion, we know that we can represent each component of the measurement as a linear combination of our eigenfunctions.

$$g_i(\boldsymbol{x}) = \sum_j^{\infty} v_{ij}\psi_j$$

Putting the two together,

$$\boldsymbol{g}(\boldsymbol{x}) = \begin{bmatrix} \sum_j^\infty v_{1j}\psi_j \\ \sum_j^\infty v_{2j}\psi_j \\ ... \\ \sum_j^\infty v_{pj}\psi_j \end{bmatrix} = \sum_j^\infty \psi_j(\boldsymbol{x})\boldsymbol{v}_j$$

We refer to v_j as the jth Koopman mode of the system.

If the system is conservative meaning that the phase space does not shrink over time, then the Koopman operator is unitary. This implies that the eignefunctions are orthonormal and that we can calculate the Koopman modes of the system via projection.

$$\boldsymbol{v_j} = \begin{bmatrix} \langle \psi_j, g_1 \rangle \\ \langle \psi_j, g_2 \rangle \\ ... \\ \langle \psi_j, g_p \rangle \end{bmatrix}$$

We can now represent the dynamics as

$$\begin{aligned} \boldsymbol{g}(x(t)) &= \mathcal{K}^t \boldsymbol{g}(\boldsymbol{x}_0) \\ &= \mathcal{K}^t \sum_j^\infty \psi_j(\boldsymbol{x}_0)\boldsymbol{v}_j \\ &= \sum_j^\infty \mathcal{K}^t \psi_j(\boldsymbol{x}_0)\boldsymbol{v}_j \\ &= \sum_j^\infty \lambda_j^t \psi_j(\boldsymbol{x}_0)\boldsymbol{v}_j \end{aligned}$$

The three values in the final equality $\{\lambda_j, \psi_j, v_j\}$ are known as the Koopman mode decomposition. In practice, the dynamics of a system can be approximated by the major terms in summation. The algorithm explored in the next section attempts to approximate these triples from data.

3.4 Invariant Subspaces

Applied Koopman dynamics is concerned with identifying a fininte subset of eigenfunctions that capture the dynamics of the system. One of the ways this is achieved is through determing a Koopman-invariant subspace.

Consider a set of functions $\{g_1, g_2, ..., g_p\}$ and their span given by an arbitrary

$$g = \sum_i^p \alpha_i g_i$$

The space is said to be Koopman-invariant if

$$\mathcal{K}g = \sum_i^p \beta_i g_i$$

Alternatively, a Koopman-invariant subspace is the span of a set of functions that remain in the space when acted upon by the Koopman operator. Any finite set of eignefunctions of the Koopman operator will span a Koopman-invariant subspace, but the challenge lies in actually determining the eigenfunctions.

3.5 Koopman Embedding Example

Consider a system governed by the following equations:

$$\dot{x}_1 = \mu x_1 \qquad \dot{x}_2 = \lambda(x_2 - x_1^2)$$

Below are a couple of candidate trajectories for given initial points, and values of μ and λ.

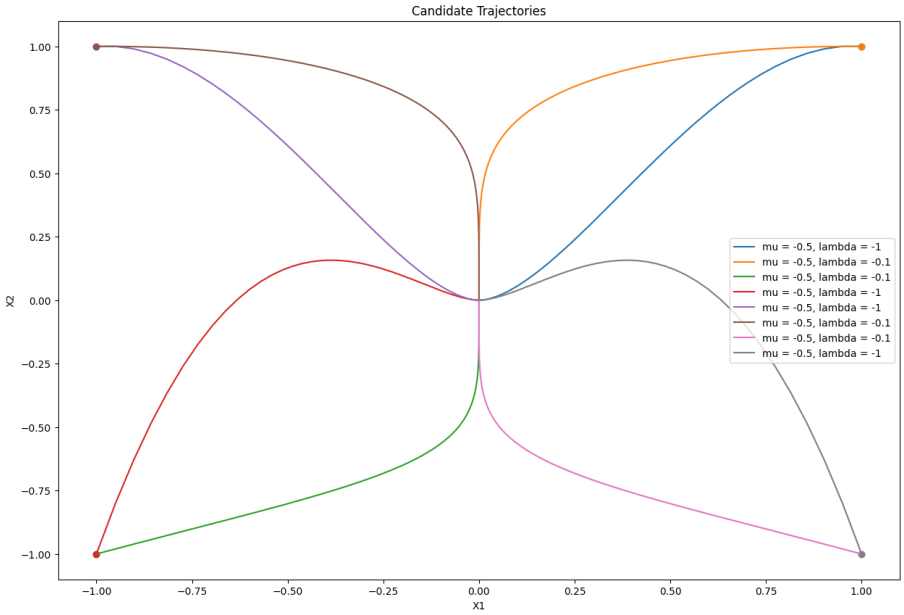

Figure 3: Example Trajectories

We can linearize this system by including an additional coordinate x_1^2. This process is analagous to the dimensional addition of measurement functions g in Koopman operator theory. We can now write the system as:

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_1^2 \end{bmatrix} = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \lambda & -\lambda \\ 0 & 0 & 2\mu \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_1^2 \end{bmatrix}$$

The corresponding eigenfunctions are

$$\psi_\mu = x_1 \qquad \psi_\lambda = x_2 - bx_1^2 \qquad b = \frac{\lambda}{\lambda - 2\mu}$$

These eigenfunctions provide us an intrinsic coordinate system tha is a koopman-invariant subspace. We can therefore use this basis to simplify our system. A deeper evaluation and explanation of this model can be found in Bruton et. al[3].

4 Dynamic Mode Decomposition

This section is focused on Dynamic Mode Decomposition (DMD), a data driven approach for approximating koopman mode decompositions. Originally invented to learn spatio-temporal relationships in high-dimensional fluid dynamic data, this method was found to be effective in estimating the Koopman operator given measurements of the state. Since Dynamic Mode Decomposition is searching for spatio-temporal relations in the data, it requires data to be collected in the pairs of $\{x(t_k), x(t'_k)\}$ where $t'_k = t_k + \delta t$. If the sampling time is uniform, we can simplify $t'_k = t_{k+1}$. This data is then translated into two data matricies $\boldsymbol{X}$ and $\boldsymbol{X'}$.

$$\boldsymbol{X} = \begin{bmatrix} x(t_1) & x(t_2) & \dots & x(t_m) \end{bmatrix} \qquad \boldsymbol{X'} = \begin{bmatrix} x(t'_1) & x(t'_2) & \dots & x(t'_m) \end{bmatrix}$$

The DMD algorithm searches for the spectral decomposition of the best-fit matrix that captures the temporal relationship between $\boldsymbol{X}$ and $\boldsymbol{X'}$.

$$\boldsymbol{X'} = \boldsymbol{A}\boldsymbol{X}$$

In the case of uniform sampling this is equivalent to finding the best fit $\boldsymbol{A}$ for $x_{k+1} = \boldsymbol{A}x_k$. This can be framed as the following optimization problem:

$$\boldsymbol{A} = \arg\min_A ||\boldsymbol{X'} - \boldsymbol{A}\boldsymbol{X}||_F = \boldsymbol{X'}\boldsymbol{X}^\dagger$$

Note that the subscript F refers to the frobenius norm and that $\boldsymbol{X}^{\dagger}$ is the pseudo-inverse. Given the large sizes of the matricies and states involved, it is often intractable to solve this problem. Instead, what the DMD algorithm does is leverage dimensionality reduction methods – particularly in singular value decompositions in the calculation of the pseudo-inverse. Since the matrix usually has more rows than columns, the $m \times n$ matrix can be reduced rank m. A is then calculated by finding its projection onto these vectors. This procedure will be explained in greater detail in the following sections.

4.1 Step 1: Singular Value Decomposition

The first step is to compute the singular value decomposition of $\boldsymbol{X}$. The SVD of $\boldsymbol{X}$ can be written as

$$\boldsymbol{X} \approx \tilde{\boldsymbol{U}}\tilde{\boldsymbol{\Sigma}}\tilde{\boldsymbol{V}}^{*}$$

where $\tilde{\boldsymbol{U}} \in \mathbb{C}^{n\times r}$, $\tilde{\boldsymbol{\Sigma}} \in \mathbb{C}^{r\times r}$, and $\tilde{\boldsymbol{V}} \in \mathbb{C}^{m\times r}$. The dimension r is our approximate rank of the matrix $\boldsymbol{X}$.

4.2 Step 2: Psuedo-Inverse

We can obtain A by computing the psuedo-inverse of $\boldsymbol{X}$ according to the following expression:

$$\boldsymbol{A} = \boldsymbol{X'}\tilde{\boldsymbol{V}}\tilde{\boldsymbol{\Sigma}}^{-1}\tilde{\boldsymbol{U}}^{*}$$

However, since we are only concerned with the most significant eigenvalues and vectors of A, we can project A into the space defined by $\tilde{\boldsymbol{U}}$.

$$\tilde{\boldsymbol{A}} = \tilde{\boldsymbol{U}}^{*}\boldsymbol{A}\tilde{\boldsymbol{U}} = \tilde{\boldsymbol{U}}^{*}\boldsymbol{X'}\tilde{\boldsymbol{V}}\tilde{\boldsymbol{\Sigma}}^{-1}$$

This matrix has the same non-zero eigenvalues as A! It further provides a linear model for the associated vectors.

4.3 Step 3: Spectral Decomposition

We finally compute the eigenvalues of our projected matrix $\tilde{\boldsymbol{A}}$ via spectral decomposition.

$$\tilde{\boldsymbol{A}} = \boldsymbol{W}\boldsymbol{\Lambda}\boldsymbol{W}^{-1}$$

4.4 Step 4: Reconstructing DMD Modes

Now, we can reconstruct the desired modes using our eigenvectors $\boldsymbol{W}$ and the time-shifted matrix $\boldsymbol{X'}$.

$$\Phi = \boldsymbol{X'}\tilde{\boldsymbol{V}}\tilde{\boldsymbol{\Sigma}}^{-1}\boldsymbol{W}$$

These vectors are eigenvectors of the unreduced matrix $\boldsymbol{A}$. Note that there exists methodology to recover information about eigenvectors with eigenvalues equal to 0, but their explanation is beyond the scope of this text.

4.5 Step 5: Recovering System State

The final step in the process is to recover our system state from the calculated quantities.

$$x_k = \sum_{j=1}^{r} \phi_j \lambda_j^{k-1} b_j = \boldsymbol{\Phi}\boldsymbol{\Lambda}^{\boldsymbol{k-1}}\boldsymbol{b}$$

The only thing left to compute is the mode amplitude vector $\boldsymbol{b} = \Phi^{\dagger}x_1$. Modes are computational expensive to compute so often times they are calcualted using projected data via $b = (\boldsymbol{W}\boldsymbol{\lambda})^{-1}\tilde{x}_1$

5 Recent Advances

Representing Koopman eigenfunctions for general dynamic systems still remains an open problem with many breakthroughs only occuring within the last 20 years. Recent emphasis has been placed on developing data driven approximations for koopman eigenfunctions. Interest in koopman dynamics is driven by the interpretability and explanatory power it provides into traditionally black-box systems. Recent work has even found connections between level sets of Koopman eigenfunctions and invariant parititions of the dynamical system state space. There are also fundamental connections between Koopman theory and ergodic systems which are also being investigated. Other research areas include the intersection between Koopman dynamics and control theory – particularly in regard to data based system identification. Other recent areas of interest have been in applying deep learning methods to koopman eignfunction estimation.

6 References

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