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OPTIMIZING THE DISCOVERY OF UNDERLYING NONLINEAR BEAM DYNAMICS*

L. A. Pocher†, L. Dovlatyan[1], I. Haber, T. M. Antonsen Jr., P. G. O'Shea
University of Maryland, College Park, MD, USA
[1]also at Raytheon Tehcnologies, Tucson, AZ, USA

Abstract

One of the DOE-HEP Grand Challenges identified by Nagaitsev *et al.* relates to the use of virtual particle accelerators for beam prediction and optimization. Useful virtual accelerators rely on efficient and effective methodologies grounded in theory, simulation, and experiment. This paper uses an algorithm called Sparse Identification of Nonlinear Dynamical systems (SINDy), which has not previously been applied to beam physics. We believe the SINDy methodology promises to simplify the optimization of accelerator design and commissioning, particularly where space charge is important. We show how SINDy can be used to discover and identify the underlying differential equation system governing the beam moment evolution. We compare discovered differential equations to theoretical predictions and results from the PIC code WARP modeling. We then integrate the discovered differential system forward in time and compare the results to data analyzed in prior work using a Machine Learning paradigm called Reservoir Computing. Finally, we propose extending our methodology, SINDy for Virtual Accelerators (SINDyVA), to the broader community's computational and real experiments.

MOTIVATION

Nagaitsev *et al.* [1] have enumerated four Grand Challenges enabling future Department of Energy (DOE) High Energy Physics (HEP) programs. Grand Challenge #4 Beam Prediction poses the question: "How do we develop predictive 'virtual particle accelerators'"? We begin to address as aspect of this Grand Challenge in this paper. Our *aim* is to speed up commissioning and design studies of accelerators by uncovering underlying physics in virtual and real accelerators. Our *approach* is to apply an existing method from the data-driven, nonlinear dynamics community called *S*parse *I*dentification of *N*onlinear *Dy*namics (SINDy) [2, 3] to uncover physics in problems that can't be solved analytically.

This method is both *Predictive* and *Productive*. The method is predictive in the context of providing an end result model that can be used to predict beam dynamics beyond the training dataset; the method is productive such that it produce actionable results. It is slightly different than the similar adjoint method as used by our collaborators at the University of Maryland (UMD) [4]. That method can be used to accelerate the design and optimization of lattices, whereas this method is more readily applicable to predicting long-term behavior of underlying beam dynamics which can be used to intensify accelerator commissioning.

APPROACH

Our approach is to prescribe a mathematical model based upon the physics of an accelerator lattice. SINDy works by assuming one can model the evolution of some n-dimensional state vector $\mathbf{x} \in \mathbb{R}^n$ as a system of ordinary differential equations

$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x}). \tag{1}$$

The variable t is the independent variable, $\mathbf{x}$ is the n-dimensional state vector of observe able either from a simulation or experiment, and $\mathbf{f}(\mathbf{x})$ is the n-dimensional equation governing how $\mathbf{x}$ evolves.

After one obtains the number n of state variables, one can then take measurements of $\mathbf{x}$ at m equidistant times $t_j \in \{t_1, t_2, \ldots, t_m\}$ with j being and index into a matrix $\mathbf{X}$:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}^T(t_1) \\ \vdots \\ \mathbf{x}^T(t_m) \end{bmatrix} = \begin{bmatrix} x_1(t_1) & \ldots & x_n(t_1) \\ \vdots & \ddots & \vdots \\ x_1(t_m) & \ldots & x_n(t_m) \end{bmatrix}.$$

One then differentiates the matrix $d\mathbf{X}/dt = \dot{\mathbf{X}}$ which is then used in the discovery stage of SINDy. One proposes a candidate $\Theta(\mathbf{X})$ which consists of a number of intuited/desired basis functions for the underlying dynamics. The matrix $\dot{\mathbf{X}}$ is equated to $\Theta(\mathbf{X})$ times a *sparse* coefficient matrix $\mathbf{\Xi} = [\boldsymbol{\xi}_0\, \boldsymbol{\xi}_1 \ldots \boldsymbol{\xi}_{BF}]$ which is solved for the given appropriate optimization technique.

$$\dot{\mathbf{X}} = \begin{bmatrix} \dot{\mathbf{x}}^T(t_1) \\ \vdots \\ \dot{\mathbf{x}}^T(t_m) \end{bmatrix} = \begin{bmatrix} \dot{x}_1(t_1) & \ldots & \dot{x}_n(t_1) \\ \vdots & \ddots & \vdots \\ \dot{x}_1(t_m) & \ldots & \dot{x}_n(t_m) \end{bmatrix} = \Theta(\mathbf{X})\mathbf{\Xi}$$

Our intuited dynamics consist of simple harmonic motion (SHM), Fig. 1(b), a Fourier series based on a Fourier transform of the lattice, Figs. 2(a) and 2(b), and a nonlinear interaction (NL) motivated by the power law observed in Fig. 2(b) and the oscillating amplitudes of the lowest order wavenumbers in the $x_c(z)$ spectrogram in Fig. 3:

$$\mathbf{f}(\mathbf{x}) \approx \underbrace{\boldsymbol{\xi}_0\mathbf{x_0} + \boldsymbol{\xi}_1\mathbf{x}}_{\text{SHM}} + \sum_{i=1}^{3}[\underbrace{\boldsymbol{\xi}_c\cos(k_i z) + \boldsymbol{\xi}_s\sin(k_i z)}_{\text{Fourier}} + \underbrace{\boldsymbol{\xi}_{nc}\,\mathbf{x}\cos(k_i z) + \boldsymbol{\xi}_{ns}\,\mathbf{x}\sin(k_i z)}_{\text{NL}}]\,. \tag{2}$$

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* Work supported by US DOE-HEP grants: DE-SC0010301 and DE-SC0022009.
† lpocher@umd.edu

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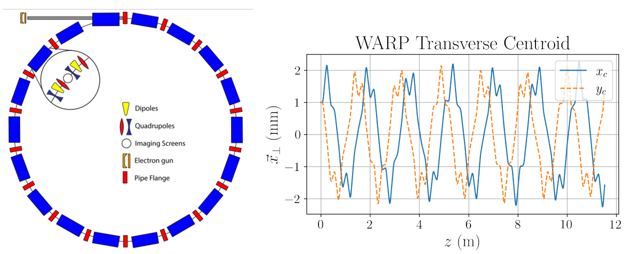
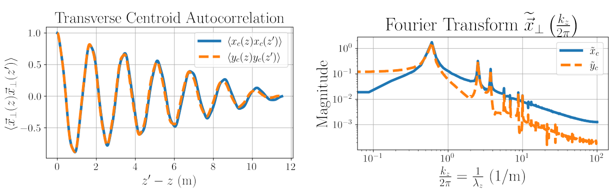
Our proposed candidate library takes the following form $\Theta(\mathbf{X}) = [\mathbf{1}, \mathbf{X}, \cos(k_i z), \sin(k_i z), \mathbf{X}\cos(k_i z), \mathbf{X}\sin(k_i z)]$. The learned sparse coefficient matrix is $\mathbf{\Xi} = [\xi_0, \xi_1, \xi_c, \xi_s, \xi_{nc}, \xi_{ns}]$ which has dimensions of $n \times n_{BF}$.

The example problem we are applying SINDy to is analyzing the transverse centroid $\vec{x}_\perp = (x_c \equiv \langle x \rangle, y_c \equiv \langle y \rangle)$ dynamics Fig. 1(b) of a electron beam from a WARP [5] simulation of the University of Maryland Electron Ring (UMER) Fig. 1(a) over one turn. Turns 2 and 3 were used for prediction.



(a) (b)

Figure 1: (a) Graphic showing the UMER lattice. (b) Beam centroid measurements with respect to pipe center as a function of z for one turn.



(a) (b)

Figure 2: FOMs for SINDy to reproduce. (a) Autocorrelation of the centroid data. (b) Fourier transform

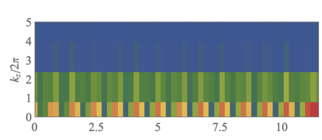
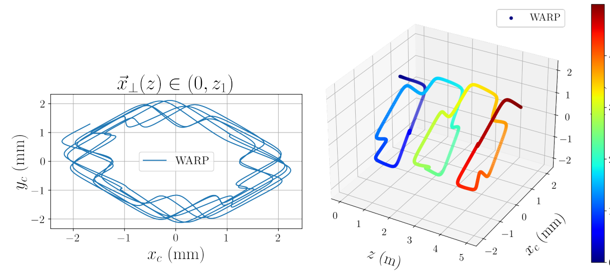


Figure 3: $x_c(z)$ spectrogram. Note the periodic amplitudes of the lowest order modes with blue, low amplitude and red, high amplitude.

Examining the Centroid Data

Our choice of basis functions is predicated upon both the physics of the lattice and the dynamics present within the data. We motivate the form of Eq. (2) with SHM, Fourier, and NL terms in this section.

SHM motion is readily observable from a phase space plot Fig. 4(a), while an examination of the Fourier transform of the data and a spectrogram, Figs. 2(b) and 3, both motivate the inclusion of Fourier modes and the NL terms. The physics and dynamics captured with these terms is readily



(a) (b)

Figure 4: (a) Stroboscopic plot of the beam centroid Fig. 1(b) over one turn. (b) Phase space plot of $\mathbf{x} = [z, x_c, y_c]^T$.

interperateable, however there may also be other physics present within the data that has not been included with just these basis functions.

Since SINDy works by assuming the dynamics present within the data may be modeled as a ODE, we must ensure that the input data models an ODE. Figure 4(a) is a self-intersecting line which means that every point in phase space is *not* unique which is a requirement for a well behaved ODE. To ensure uniqueness in phase space, we use the independent variable z to unwind the 2D phase space.[1]

In addition to motivating basis functions we have chosen the autocorrelation Fig. 2(a) of the centroid data with itself and the Fourier transform Fig. 2(b) of the data as Figures of Merit (FOM) for the data. FOMs are metrics which we seek to reproduce as exactly as possible, and give indication as to whether the proposed dynamics match the underlying physics. Table 1 details the three lowest order lattice modes of the data which are injected into our $\Theta(\mathbf{X})$.

Table 1: Three lowest order Fourier modes of $\widetilde{x}_c(k_z/2\pi)$ from Fig. 1(b). The parenthetical superscript refers to the index i.

i	$\mathbf{\frac{k_z^{(i)}}{2\pi}}$ **(1/m)**	$\mathbf{L_z^{(i)}}$ **(m)**
1	0.61	10.34
2	2.52	2.50
3	3.62	1.68

The final addition to our proposed basis function is based on a spectrogram of the data Fig. 3. The periodic amplitude of the lowest order modes may be replicated with a NL interaction between the oscillatory centroid data and the lattice Fourier modes.

RESULTS

The results using the SINDy algorithm are described in this section. Three distinct tries were detailed in our presentation. Only the last and best try is detailed here for brevity.

[1] Using the paraxial approximation, we transform the independent variable from $t \to z$.

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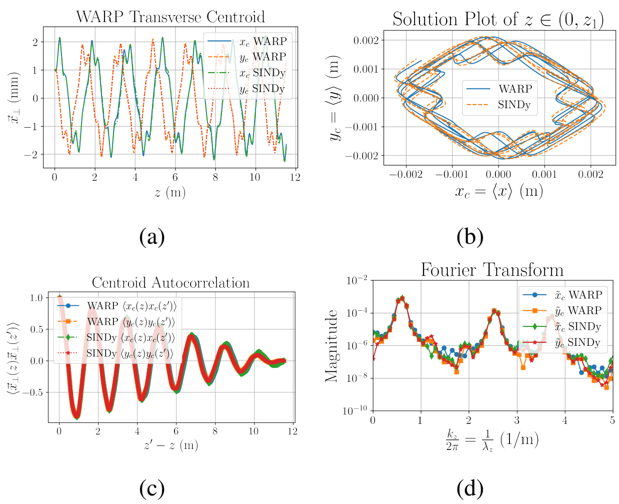
Try 3: Fourier + SHM + NL

Our highest fidelity try on learning the dynamics in the data included all of the terms in Eq. (2): Fourier, SHM, and NL interaction. The dynamics are captured almost exactly between the WARP simulation and the SINDy model Figs. 5(a) and 5(b). The FOMs are also captured very well Figs. 5(c) and 5(d). The WARP simulation dataset and the SINDy model result are compared directly in phase space and show excellent agreement Fig. 6.



(a) (b) (c) (d)

Figure 5: (a) SINDy axial solution comparison. (b) Phase space. (c) Autocorrelation Comparison. (d) Fourier transform of SINDy model.

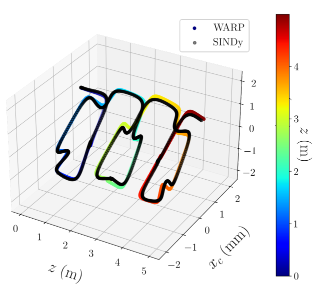
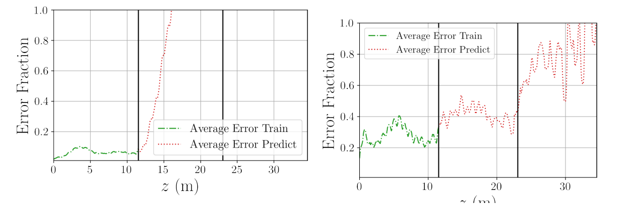


Figure 6: Comparison of the WARP simulatoin $\mathbf{x} = [z, x_c(z), y_c(z)]$ and the trained SINDy model using Eq. (2).

Comparison to Machine Learning

The SINDy method for capturing beam centroid dynamics may be compared to the machine learning method reservoir computing as performed by our colleagues Komkov *et al.* [6]. Figures 7(a) and 7(b) show the training (green) and prediction results (red) of the third try SINDy model integrated forward in the lattice over turns 2 and 3 and compared to the actual data. The vertical black lines mark turns in meters: $z_1 = 11.52$, and $z_2 = 23.04$. The predicted error quickly goes beyond the order of the data in Fig. 7(a). However, if we use a slightly different set of basis functions for the Fourier terms we trade off error in the training for better



(a) (b)

Figure 7: Error fraction for SINDy training (green, turn1) and prediction (red, turn2 and turn3) for the third try (a), and a slightly modified third try (b).

results reproducing the "climate" of the phase space dynamics in turns 2 and 3. This goes to show that discovering underlying nonlinear dynamics has room for improvement.

If we compare the data to machine learning results produced by Komkov *et al.* we note the prediction error is much less than our method Fig. 8. This is a result of the higher dimensionality of the utilized reservoir computing method. A drawback of reservoir computing, and all machine learning methods, is a lack of interpretability in the resultant model. One cannot point to a specific term/node in the architecture and declare "this is the physics going on". An advantage of the SINDy technique is the built in interpretability of the underlying physics based model. If our SINDy results can be improved we believe that the interpretability of the model will enable a more predictive framework for virtual and real accelerators.

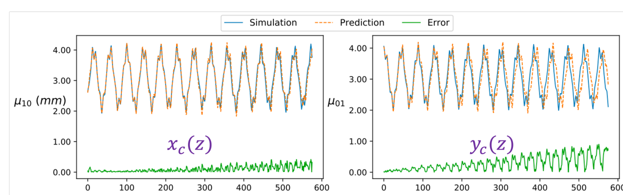


Figure 8: Machine Learning results from Komkov *et al.* [6] over turns 2 and 3 in the lattice. (Left) $x_c(z)$ prediction. (Right) $y_c(z)$ prediction.

CONCLUSION

We believe SINDy is a promising method that enables the intensification of accelerator commissioning by uncovering the underlying physics of beam dynamics. We have shown both recoverable beam dynamics Fig. 6 and FOMs Figs. 5(c) and 5(d). With this methodology we aim to develop a *Predictive* and *Productive* framework for beam dynamics with high fidelity. We desire to apply SINDy in areas of interest to the broader community.

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