A Dynamical Systems Approach to Classification in Time Domain Astronomy

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1. INTRODUCTION

SN Ia physics and cosmology is entering a new era of unprecedented discovery rate of yet-seen Type Ia supernovae (SNe Ia), but the tools that will be used to deliver scientific results are not keeping pace. Having studied supernovae cosmology systematics and developed a new SN Ia empirical model, I am well-versed in both the scientific utility time domain (TD) astronomy (or the study of objects that observationally change with time), and the nuance and challenges of using astronomical time series observations. Next generation surveys have the potential to transform our physical understanding of TD events with their orders-of-magnitude increase in observations if and only if we can accurately and efficiently classify objects algorithmically. Achieving potential scientific leaps will require an innovative classification scheme, innovation I have successfully demonstrated in my current research and propose for this 2023 NASA Hubble fellowship application: developing a novel dynamical systems model for LSST TD events and their classification.

1.1. *Past Research: Understanding Supernova Cosmology Systematics*

SN Ia are standardizable candles such that correlation between observed properties and peak brightness can be corrected for to reduce peak brightness dispersion. Exploiting these empirical relations led directly to the discovery of dark energy (Riess et al. 1998; Perlmutter et al. 1999). Ideally, correlations between SN Ia and intrinsic or extrinsic modes of spectral variation are accounted for during this standardization procedure, but established empirical relationships between host galaxy stellar mass, stellar age, and star formation rates, and peak SN Ia brightness appear after standardization in a phenomenon coined the mass step (Sullivan et al. 2010; Rigault et al. 2020). Specifically, the difference between our best-fit cosmological model's predicted peak brightness and standardized peak brightness co-varies with host properties in a step-like fashion.

My first paper presented Professor Wood-Vasey's research group's work quantifying any influence observation method (broad-band photometry or spectroscopy) or host galaxy property fitting technique on the host bias and subsequent step biases (Hand et al. 2022). Given our ignorance of the host bias and its source, considering how we observe SN Ia is an important place to start one's search. We used a PISCO SN Ia host observation subsample (Galbany et al. 2018) with SDSS and GALEX photometric coverage (Alam et al. 2015; Morrissey et al. 2007) to derive independent stellar mass and star formation rate estimates. We found no evidence that observation technique or fitting method biases, let alone produces, the SN Ia host bias and subsequent mass step, and our results were also being consistent with past comparisons of galaxy property estimators (see Conley 2013 for a review).

1.2. *Current Research: a New Supernova Model*

As a recipient of the 2019 Department of Energy Office of Science SCGSR Award, I relocated to the Lawrence Berkeley National Laboratory in August of that year to work under Dr. Alex Kim developing a new empirical SN Ia model. SN Ia theory is insufficiently developed to provide parametric models that account for observed SN Ia spectral variation, so the SN Ia researchers instead develop increasingly sophisticated empirical models trained on ever-growing photometric and spectroscopy observation sets. Such empirical models must account for intrinsic and extrinsic modes of SN Ia population variability.

Extrinsic variation is variation that is independent of the progenitor or explosion physics, largely resulting from differing attenuation by dust. This variability is phase-independent, and most SN Ia empirical models assume a single-component effective attenuation curve (Jha et al. 2007; Burns et al. 2011; Mandel et al. 2022), or group all phase-independent variation (intrinsic or extrinsic) into a single template(Guy et al. 2007; Kenworthy et al. 2021). Neither approach is satisfactory — physical consideration alone requires at least two dust attenuation curves: one quantifying optical depth and the other extracting wavelength dependence (Weingartner & Draine 2001). Effective dust attenuation models or agnostic color laws ignore per-SN variability in attenuation curve slope, an artificial constraint that may contribute to the mass step (Brout et al. 2019; Popovic et al. 2021). Cosmological parameter uncertainty derived from SN Ia distance ladders is now dominated by SN Ia model systematics (Scolnic et al. 2018), so improvements in SN Ia cosmology must come from improved empirical models that better account for these systematics.

Dr. Kim and I developed a Stan-implemented SN Ia model that simultaneously fits two physics-agnostic, phase-independent color templates and a single phase-dependent variation template (Carpenter et al. 2017). It is trained on rest frame SNfactory spectrophotometric time series (Aldering et al. 2002), and is novel in three ways:

- It is the first SN Ia model architecture to successful fit two physics-agnostic, phase-independent spectral variation templates.

- We use of bivectors to determine our best fit model, recognizing that our two color templates form the vector basis of an oriented two-dimensional structure embedded within our ten-dimensional wavelength space. A bivector represents this mathematical structure.

- We exploit our model's geometry to decompose the best-fit bivector into physically interpretable results with a first-of-its-kind application of geometric algebra to perform ten-dimensional rotations, projections, and intersections.

I developed and implemented the bivector representations technique and the geometric algebra application, both of which were fundamental to finally separating intrinsic and extrinsic modes of phase-independent spectral variation.

Instead of extracting two dust-sourced color templates, we recover one dust-like component and another component that is a nontrivial mixture of extrinsic and intrinsic features. This phase-independent intrinsic variability is most notable around the Ca H&K spectral feature, a feature that exhibits relatively little time-dependence during the photospheric phase of SN Ia explosions (Branch et al. 1993; Riess et al. 1996). More importantly, in recovering effectively both intrinsic and extrinsic phase-independent variation, our results largely negates the narrative that unmodeled SN Ia systematics results primarily from incomplete extrinsic variation modeling (Brout et al. 2019).

These two extracted color templates provide us with unprecedented capacity to explore dust variation between SNe Ia, which we study further with hierarchical Bayesian dust model also implemented with Stan. We find that SN Ia with phase-independent variation dominated by intrinsic modes (SNe Ia with little to no dust attenuation) systematically fit for steeper attenuation curves than their extrinsic-dominated counterparts. Nominally quantified with the total-to-selective ratio R_V, past estimates of SN Ia effective attenuation curves have consistently been steeper than the Milky Way sight line average of $R_V = 3.1$. Our results find having intrinsic-dominated SN Ia in one's sample biases your effective R_V estimate lower than it otherwise should be, although this does not entirely account for suspiciously low SN Ia R_V values.

A paper summarizing this new model currently undergoing internal review within the Nearby Supernova Factory group. Meanwhile, Dr. Kim and I are increasing our model's wavelength resolution and integrating a two-component dust attenuation recipe directly into its architecture. Higher resolution will enable quantification of spectral feature properties and a built-in attenuation model will help separate intrinsic phase-independent variation from its extrinsic counterpart. This newer model will directly extract per-SN R_V values and provide a first-ever comparison of SN-derived R_V values with local environment R_V estimates. Any discrepancies between

these R_V estimations would be evidence of SN Ia variability bleeding into recovered effective attenuation curves, furthering our understanding as to why SN Ia 'prefer' systematically low R_V values.

2. MODELING TIME-DEPENDENT OBJECTS AS DYNAMICAL SYSTEMS

SN Ia science is one part of the much larger field of time domain (TD) astronomy, a field to be revolutionized by the Vera C. Rubin Observatory Legacy Survey of Space and Time (LSST) and its expected ≈ 20 TB/night of raw observation data *per night* (Narayan et al. 2018; Ivezić et al. 2019). TD phenomena inform many physical processes, such as variable stars and core collapse SNe (Type Ib/c or II) constraining stellar interior and end-of-life stellar evolution models, respectively (See Section 4.3 of Ivezić et al. (2019) for more examples). TD events are characterized into two broad categories: variable objects that whose brightness continuously varies, and transient objects that undergo one phase of changing brightness. Variable and transient events are further classified into physical subtypes (Mira variables versus Cepheids, supernovae versus tidal disruption events, etc.). LSST TD research groups are developing cloud-based alert-broker pipelines to flag TD events in the LSST data stream. Alerts will then be efficiently and accurately characterized and classified followed by prompt distribution to interested research groups via the broker (Narayan et al. 2018). Current surveys rely on spectroscopic followup or the human eye for classification, approached made untenable by LSST's $\approx 10^7$ TD observations each night. This leaves any LSST alert-broker dependent on an algorithm-based classifier.

Programmatic classifiers, including machine learning (ML) algorithms, cannot easily account LSST data products' particular structures, such as observation uncertainty heteroskedasticity (more distant objects are more difficult to detect than) and missed observations (such as weather-related delays). Proposed photometric classifiers circumvent this by representing photometric time series via a template model or wavelet decomposition dimensionality reduction (Malz et al. 2019). The reduced representation features then serve as inputs for a classifier algorithm (see Lochner 2016 for SN-specific transient classification details). There is ample room for improvement over current representations and subsequent classification, with an example being stripped envelope core-collapse SNe classification false negative rates of $\approx 10\%$ (Malz et al. 2019). This will then lead to LSST SN Ia cosmology sample contamination by core-collapse SN, reducing per-SN statistical weight in deriving cosmology parameters.

Current TD representations fail to properly model TD observations, which are capturing snapshots of fundamentally dynamical processes. Furthermore, photometric TD classification relies heavily on how an object's flux changes with time, so representation features should be derived from a dynamical systems approach. Such an improved TD event representation better capturing dynamical properties may not only improve classification performance, but be a powerful tool to study individual

events themselves, especially yet-seen phenomena that LSST surely will discover. It is such improvements I believe can be reached with data-driven, dynamical systems approach called dynamics discovery.

2.1. *A Dynamics Discovery Approach to TD Classification and Dimensionality Reduction*

LSST will observe the night sky with six photometric filters *ugrizy* each centered at different effective wavelengths. Consider a single set of flux values for some TD event as a six-component vector $\mathbf{F}$, each corresponding to one of the mentioned photometric filters. For TD events, this vector's components each vary with time, so $\dot{\mathbf{F}} \neq 0$. In this application, dynamics discovery promotes this flux derivative to a differential equation $\dot{\mathbf{F}} = g(\mathbf{F}, t|\mathbf{\Theta})$ and discovers from data the functional form of the unknown function $g(\mathbf{F}, t|\mathbf{\Theta})$ that describes the evolution of the $\mathbf{F}$. Here, $\theta \in \mathbf{\Theta}$ parameterize the discovered dynamics. LSST TD observations will provide the noisy 'snapshots' from which the dynamics are determined via machine learning. Each event can be characterized as variable or transient based directly on the discovered dynamics, while extracted dynamics parameters and subsequently derived properties can be the features for an improved TD classifier. Dynamics discover also exploits the timescales from observations like wavelet decomposition, but it also directly exploits the data's estimated derivatives in its dimensionality reduction procedure. Unlike template model classifiers, this technique is physics-agnostic and will not be sensitive to template-related systematics.

Dynamics discovery models an implicit representation $\mathcal{F}$ of each TD event such that $\mathcal{F}(t_i) \approx \mathbf{F}^*(t_i)$ for observation time t_i of observation $\mathbf{F}^*(t_i)$. The dynamics $g(\mathbf{F}, t|\mathbf{\Theta})$ of the TD event is simultaneously modeled with a representation $\mathcal{G}$. $\mathcal{F}$ is found by minimizing the loss between observations and their implicit representation, while $\mathcal{G}$ is found by minimizing loss between $\mathcal{F}$ derivatives and the modeled dynamics. $\mathcal{F}$ and $\mathcal{F}$ are further coupled with an additional loss component that compares predicted time-integrated evolution to the implicit representation expected value. Section 3 of Goyal & Benner (2022) summarizes this workflow with a purely NN implementation. The simultaneous training of representations $\mathcal{F}$ and $\mathcal{G}$ is also not tied to a particular machine learning technique (see Raissi & Karniadakis (2018) for a purely Gaussian process (GP) alternative.)

Data-driven dynamics discovery and modeling is well-developed field of study, but has never been applied to astronomical observations directly. This proposed TD classification proposal is not only innovative, but will be relatively straightforward to implement. Indeed, I am in contact with Dr. Mattia Cenedese at ETH Zürich to discuss how to extend their nonlinear spectral submanifold learning techniques to LSST TD data (Cenedese et al. 2022).

2.2. *LSST Dynamics Discovery Project Sequence*

There are two specific deliverables expected by this project: a dynamics discovery representation of TD events, and a subsequent classifier using said representation's features as inputs. Year one will focus first on developing the architecture for the implicit and dynamics representations $\mathcal{F}$ and $\mathcal{G}$, respectively. Implementing $\mathcal{F}$ with GPs has the particular advantage of simplifying error propagation. The derivative of an GP is, by definition, another GP, which would again simplifies flux derivative estimation. GP scalability is hindered by potentially costly matrix inversion calculations, though, so selecting a GP and NN architecture for $\mathcal{F}$ after comparison of results will be an important milestone to be reached that first year. The first year will see $\mathcal{G}$'s architecture developed and then testing the full dynamics discovery model on simulated LSST data (Malz et al. 2019).

By the beginning of the second year, a dynamics discovery feature classifier should be selected using accuracy and efficiency metrics summarized in Malz et al. (2019). Assuming a dynamics discovery representation improves characterization and TD feature classification, the second year will initially focus on integrating the proposed methodology into LSST alert-brokers. Integrating the dynamics discovery methodology into LSST's LINCC Framework as an end-user software deliverable will be another important objective for the second year.

If time permits, year three can be spent developing a generative dynamics discovery mixture model for characterized TD events. Such a model would simultaneously fit numerous generative models, each corresponding to the dynamics of the sample's subpopulations. This ambitious model would be made feasible from the massive amount of data expected from LSST. Indeed, tens of thousands of TD events will be observed by LSST, each which can be used to develop this model.

2.3. *Why Carnegie Mellon University?*

Carnegie Mellon University (CMU) is home to the McWilliams Center for Cosmology with professors holding leadership positions in LSST's Dark Energy Science Collaboration. CMU is a hub and founding member of the LINCC framework, a program developing the software and data management infrastructure needed to address the unprecedented scale and complexity LSST's data products. LINCC will be a collaboration between software engineers, data scientists collaborate, and research scientists to develop scalable and deployable software tools within a cloud-based framework for widespread scientific use. CMU's Statistics and Data Science department is actively involved in LINCC, helping develop and implement the machine learning algorithms necessary for LSST's delivery of usable products. A dynamics discovery methodology would be a tool to be implemented into the LINCC Framework, and my presence at CMU will facilitate its integration. University of Pittsburgh faculty also hold important LSST-DESC leadership positions and is closely connected with CMU's LINCC initiatives, being particularly focused on LSST's TD science pipeline development. Furthermore, Professor Wood-Vasey's research group at the University of Pittsburgh

is developing a candidate LSST alert-broker in collaboration with Google, and my being at CMU provides the proximity to more effectively integrate a dynamics discovery classifier into their pipeline.

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