The Pantheon+ Analysis: Forward Modeling the Dust and Intrinsic Color Distributions of Type Ia Supernovae, and Quantifying Their Impact on Cosmological Inferences

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Abstract

Recent studies have shown that the observed color distributions of Type Ia supernovae (SNe Ia) can be well described by a combination of a dust distribution and an intrinsic color distribution. Using the Pantheon+ sample of 1701 SN Ia, we apply a new forward-modeling fitting method (Dust2Dust) to measure the parent dust and color distributions, including their dependence on host-galaxy mass. At each fit step, the SN Ia selection efficiency is determined from a large simulated sample that is reweighted to reflect the proposed distributions. We use five separate metrics to describe the goodness of fit: distribution of fitted light-curve color $c$, cosmological residual scatter with $c$, fitted color–luminosity relationship $\beta_{\text{SALT2}}$, and intrinsic scatter $\sigma_{\text{int}}$. We present the results and the uncertainty in 12-dimensional space. Furthermore, we measure that the uncertainty on this modeling propagates to an upper threshold uncertainty in the equation of state of dark energy $w$ of 0.014(1) for the Pantheon+ cosmology analysis and contributes negligible uncertainty to the Hubble constant $H_0$. The Dust2Dust code is made publicly available at https://github.com/djbrout/dustdriver.

Unified Astronomy Thesaurus concepts: Cosmology (343); Type Ia supernovae (1728); Dark energy (351)

1. Introduction

The accelerating expansion of the universe was discovered by Riess et al. (1998) and Perlmutter et al. (1999) using Type Ia supernovae (SNe Ia) to measure cosmic distances. “Dark energy,” which is commonly parameterized by an equation of state $w$, is a possible explanation for this expansion and is still an outstanding cosmological mystery today. To standardize the SN Ia brightness for accurate distance measurements, some of the early analyses attempted to separate the components of the measured color between intrinsic and Milky Way–like dust extinction (multicolor light-curve shapes; e.g., Riess et al. 1996). However, over the past decade, the majority of cosmological analyses with SNe Ia (e.g., Conley et al. 2011; Betoule et al. 2014; Jones et al. 2018a; Scolnic et al. 2018; Brout et al. 2019b) and measurements of scatter (Guy et al. 2010; G10; Chotard et al. 2011; C11) have used the SALT2 approach that is agnostic to different components of color and treats it as a single parameter (Guy et al. 2010).

While larger, more modern samples with improved calibration have led to the reduction of many systematic uncertainties in cosmological analyses with SN Ia, there remain lingering issues about how to best standardize SNe Ia. These include what has colloquially been named “the mass step,” where standardized SNe Ia are typically ~0.05 mag brighter in heavier galaxies ($>10^{10} M_\odot$) than their lighter counterparts (Kelly et al. 2010; Lampeitl et al. 2010; Sullivan et al. 2010). Furthermore, it is not understood why the empirically measured reddening law for SNe Ia differs from that measured for the Milky Way, particularly in the ultraviolet wavelength region (Betoule et al. 2014; Amanullah et al. 2015). Recently, Brout & Scolnic (2021, hereafter BS21), building off of earlier works investigating the effects of dust on SNe Ia (Folatelli et al. 2010; Chotard et al. 2011; Burns et al. 2014; Mandel et al. 2017), proposed introducing dust extinction to the SN Ia SALT2 model to include both intrinsic color variation within SNe Ia as well as dust effects tied to host-galaxy properties. This dust-based approach resulted in simulations that predict the mass step due to a difference in effective color–luminosity relationships based on host-galaxy mass (Popovic et al. 2021) and also predict the previously unexplained increase in SNe Ia Hubble scatter for redder events (Brout & Scolnic 2021).

While a simulation with the BS21 model can replicate the mass step in the optical bands, other studies on the effects of dust on SNe Ia have provided different results. One prediction of the BS21 model is that a mass step in the rest-frame near-infrared (NIR) should be significantly smaller than in the optical because the NIR is less sensitive to dust. Studies of the mass step in the NIR have been inconclusive: Ponder et al. (2021) and Uddin et al. (2020) find evidence of a poststandardization mass step in the NIR, despite the negligible effects of dust in the NIR, while Johansson et al. (2021) show a poststandardization mass step in the optical band but not the NIR. Additionally, Johansson et al. (2021) find evidence of a difference in dust distributions between high- and low-mass galaxies, though this difference is smaller than that found in BS21.

However, Brout & Scolnic (2021) left several key issues unaddressed. The original distribution of host-galaxy stellar mass assumed equal numbers of high- and low-mass galaxies, leading to biases in recovered parameters. Moreover, the model parameters for BS21 were determined via a coarse grid $\chi^2$ search, and included neither robust uncertainty measurements

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nor covariance between fitted parameters. Finally, the SALT2 and BS21 models have not been retrained to adjust the intrinsic SN Ia color law, nor the spectral energy distribution (SED) templates. While BS21 showed significant model improvements, these unaddressed issues, alongside the lack of an effective bias-correcting methodology, are significant impediments to the adoption of BS21 as a scatter model in cosmological analyses.

This paper aims to address the first two issues by describing a likelihood approach to determine model parameters, robust uncertainty calculations, and covariances between parameters. This is accomplished with the use of robust and realistic simulations of supernova surveys generated by the Supernova Analysis (SNANA) program (Kessler et al. 2009) in a novel combination with importance sampling and a Markov Chain Monte Carlo method: Dust2Dust. This method builds on approaches such as those in Scolnic & Kessler (2016) and Popovic et al. (2021) to forward-model SN Ia parameters and improves the likelihood. The ideal approach to inferring model parameters is to create new simulations with updated parameters for each iteration. This is both computationally inefficient and time-intensive. Scolnic & Kessler (2016) and later Popovic et al. (2021) eluded this computationally intensive problem by creating simulations with uniform distributions of SN Ia parameters, and creating a “migration matrix” to infer parent populations of stretch and color; here we further elaborate on this method with a fast forward-modeling methodology (Section 4.3). Model retraining of the intrinsic color law and SED templates will be developed in a later work.

Section 2 presents an overview of the SALT2 and BS21 models. In Section 3, we provide an overview of the data and simulations. The methodology of Dust2Dust is described in Section 4. Results and the impact on cosmological measurements are detailed in Section 5. Finally, we provide a discussion in Section 6 and acknowledgments.

2. Model Overview

SNe Ia are analyzed with the use of a light-curve fitting program. Here we review the SALT2 framework and the dust components from BS21.

2.1. SALT2

We use the SALT2 model as presented in Guy et al. (2010) and the trained SALT2 model parameters from Taylor et al. (2021). The SN Ia flux is given by SALT2 as

$$F(SN, p, \lambda) = x_0 \times [M_0(p, \lambda) + \lambda M_1(p, \lambda) + \ldots] \times \exp[\sigma CL(\lambda)],$$

(1)

where $x_0$ is the overall amplitude of the light curve, $x_1$ is the observed light-curve stretch, and $c$ is a parameter describing the color of the SNe Ia. The $M_0$, $M_1$, and $CL(\lambda)$ parameters are global model parameters determined from a training program (Guy et al. 2010) that uses a large set of photometry and spectra. $M_0$ is the average SED at each phase, $M_1$ describes the $x_1$-dependence of SED variability, and $CL(\lambda)$ is the average color law.

We infer distances following the Tripp estimator (Tripp 1998); the distance modulus $\mu$ is found by

$$\mu = m_B + \alpha_{SALT2} x_1 - \beta_{SALT2} c - M(z),$$

(2)

where $m_B = -2.5 \log_{10}(x_0)$; $x_1$ and $c$ are defined above, and $\alpha_{SALT2}$ and $\beta_{SALT2}$ are global nuisance parameters for the stretch–luminosity and color–luminosity relationships, respectively, following Guy et al. (2010). $M(z)$ is the absolute magnitude of an SN Ia with $c = x_1 = 0$ from a Marriner et al. (2011) fit. We do not include an ad hoc step based on mass, as Popovic et al. (2021) find that a difference in $R_\mu$ distributions between high- and low-mass galaxies recreates the observed luminosity difference.

2.2. BS21

Here we present a review of the BS21 model. BS21 attributes observed SN Ia colors to two components: a color component intrinsic to SN Ia properties, $c_{int}$, and a dust component described by a distribution of reddening values drawn from the extinction ratio $R_V(E_{dust})$. The observed color, $c_{obs}$, is modeled as

$$c_{obs} = c_{int} + E_{dust} + \epsilon_{noise},$$

(3)

where $\epsilon_{noise}$ is measurement noise otherwise unaccounted for (Brout & Scolnic 2021). This approach leaves arbitrary choices for parametric modeling of distributions. Following BS21 we use the following seven parameters for SNe Ia:

1. $\tau$: the Gaussian mean of intrinsic color distribution.
2. $\sigma$: the Gaussian sigma of intrinsic color distribution.
3. $\beta_{SN}$: the Gaussian mean of distribution for intrinsic color–luminosity correlation.
4. $\sigma_{SN}$: the Gaussian sigma of distribution for intrinsic color–luminosity correlation.
5. $R_V$: the Gaussian mean of $R_V$ distribution.
6. $\sigma_R$: the Gaussian sigma of $R_V$ distribution.
7. $\tau_{E}$: the exponential distribution for $E_{dust}$.

Note that $\beta_{SN}$ and $\beta_{SALT2}$ are different parameters. $\beta_{SALT2}$, along with $\alpha_{SALT2}$, are determined from a global fit of the fitted SALT2 parameters. In the BS21 model, $\beta_{SALT2}$ is a convolution of $\beta_{SN}$ and other dust effects. Similarly, the observed color distribution, $c_{obs}$, is described by a symmetric intrinsic distribution combined with a dust model that accounts for the red tail observed in the data. The $c_{obs}$ distribution can be
phenomenologically replicated with an asymmetric Gaussian as done in Scolnic & Kessler (2016) or Popovic et al. (2021).

The dust reddening component $E_{dust}$ from Equation (3) is interpreted as $E(B - V)$ so that the $V$-band extinction is given by

$$A_V = R_V \times E_{dust},$$

where $R_V$ is selective extinction and $E_{dust} = E(B - V)$. The change in observed brightness is modeled as

$$\Delta m_B = \beta_{SN} c_{int} + (R_V + 1) E_{dust} + \epsilon_{noise}.\tag{5}$$

Following Riess et al. (1996) and Jha et al. (2007), these $E_{dust}$ values are drawn from an exponential distribution with probability

$$P(E_{dust}) = \begin{cases} \tau_{E}^{-1} e^{-E_{dust}/\tau_{E}}, & E_{dust} > 0, \\ 0, & E_{dust} \leq 0, \end{cases} \tag{6}$$

where $\tau_{E}$ is described above.

Seven unique parameters are required to describe the BS21 scatter model. To account for host-galaxy correlations, we split the $R_V$ and $E_{dust}$ distributions on host-galaxy stellar mass, specifically across galaxies with $M_{stellar} > 10^{10} M_\odot$ (high mass) and those with $M_{stellar} < 10^{10} M_\odot$ (low mass). Following BS21, the $E_{dust}$ distributions were split between low-$z$ surveys and high-$z$ surveys as well as surveys; however, the $c_{int}$ and $\beta_{SN}$ distributions are not split on host-galaxy stellar mass, as the model predicts that $c_{int}$ and $\beta_{SN}$ are intrinsic to SNe Ia and not their environments.

This splitting raises the number of fitted model parameters to 12. An accounting of the parameters and summary of the number of dimensions is shown in Table 1.

### Table 1

| BS21 Parameter | $N_{param}$ |
|----------------|-------------|
| Gaussian $c_{int}$ | 2 |
| Gaussian $\beta_{SN}$ | 2 |
| Gaussian $R_V$ (low mass) | 2 |
| Gaussian $R_V$ (high mass) | 2 |
| Exponential $E_{dust}$ (low-$z$, low mass) | 1 |
| Exponential $E_{dust}$ (low-$z$, high mass) | 1 |
| Exponential $E_{dust}$ (high-$z$, low mass) | 1 |
| Exponential $E_{dust}$ (high-$z$, high mass) | 1 |
| Total | 12 |

#### 3. Data, Simulations, and Selection

Here we provide an overview of the data, simulations, and selection requirements. While simulations are typically used for bias corrections (such as BEAMS with Bias Corrections; Kessler & Scolnic 2017) in cosmological analyses, here we leverage the ability of simulations to provide large samples with known truth values in order to forward-model the BS21 parameters in our data.

**3.1. Data**

For this analysis, we use the Pantheon+ sample (Scolnic et al. 2022), a collection of publicly available and spectroscopically classified photometric light curves of SNe Ia. The low-redshift sample is compiled from the Center for Astrophysics SN Ia data sets (CfA1-4; Jha et al. 2006; Hicken et al. 2009a, 2009b, 2012), the Carnegie Supernova Project (CSP; Stritzinger 2010; Krisciunas et al. 2017), the Swift Optical Archive (SWIFT; Brown et al. 2014), Foundation (Foley et al. 2018), the Lick Observatory Supernova Search (LOSS; Ganeshalingam et al. 2010; Stahl et al. 2019), and the Complete Nearby Low Redshift Supernova Sample (CNIa0.02; Chen et al. 2022).

The high-redshift sample is comprised of the Dark Energy Survey (DES) 3 yr sample (Brout et al. 2019a, 2019b; Smith et al. 2020), the Sloan Digital Sky Survey (SDSS; Sako et al. 2018), the Pan-STARRS survey (PS1; Rest et al. 2014; Scolnic et al. 2018), the Supernova Legacy Survey (SNLS; Betoule et al. 2014), and the Hubble Space Telescope (HST; Riess et al. 2018). Cross-calibration for all surveys is done in Brout et al. (2022a). The redshifts for the entire Pantheon+ sample have been reevaluated in Carr et al. (2022), and peculiar velocities are computed in Peterson et al. (2022).

In contrast to Brout et al. (2022b), we require $z > 0.03$ to avoid difficulties modeling Hubble scatter with significant contributions from peculiar velocities. The resulting redshift distribution of our sample is shown in Figure 1.

**3.2. Simulations**

We use the SNANA simulation software (Kessler et al. 2009, 2019) that broadly works in three steps: generation of fluxes from a source model, application of noise, and detection based on a characterization of the difference imaging pipeline and/or spectroscopic selection. The simulation generates a rest-frame SED for each SN Ia epoch and applies a combination of cosmological effects (such as dimming and redshift) and galactic effects (weak lensing, peculiar velocity, and Galactic extinction). Next, the SED is integrated for each filter to determine broadband fluxes. Poisson noise is computed from the sky noise, source flux, point-spread function, and zero-point. Next, the simulation models detection criteria and applies survey-dependent logic that requires a minimum number of detections separated in time, e.g., DES requires two detections found on different nights. Finally, a model for spectroscopic identification efficiency is applied.

We take our simulation inputs from the Pantheon+ analysis (Section 3 of Brout et al. 2022b). Table 2 presents the source of instrumental inputs to generate each survey, which includes cadence and filter information (cadence library), single-visit detection efficiency versus signal-to-noise ratio (S/N; DETEff), and spectroscopic identification efficiency (SPECEFF).

**3.3. Selection**

Each sample has survey-specific selection requirements (cuts) as detailed in their data releases and Scolnic et al. (2022). Here we implement a more restrictive range of cuts to define the sample:

1. One observation at least 5 days before peak brightness in SN rest frame, $T_{\text{rest}} < 5$.
2. S/N greater than 5 in two bands, S/N > 5.
3. Fitted stretch $-3 < x_3 < 3$.
4. Fitted color $-0.3 < c < 0.3$.
5. Fitted c uncertainty $c_{\text{err}} < 0.1$.
6. Fitted $x_3$ uncertainty $x_{3_{\text{err}}} < 1.5$.
7. Milky Way reddening $E(B - V) < 0.3$ for low-redshift surveys.
Figure 2. Plots of the metrics described in Section 4.1. The $c$ histogram, $c$ vs. $\mu_{\text{res}}$, and $c$ vs. $\sigma$ are shown from left to right. The latter two panels are split on high and low mass. Panel (a) is the observed color ($c$) distribution with purple circles as histogram data and solid gray as simulated histogram. Panel (b) is $\mu_{\text{res}}$ vs. $c$ split on high and low host-galaxy mass. Panel (c) is $\sigma$ of $\mu_{\text{res}}$ vs. $c$. Green squares are low-mass data and black triangles are high-mass data, while the blue line plots low-mass simulation and the orange dotted line plots high-mass simulation. We can see good agreement between data and simulation for our best-fit parameters.

4. Methodology

In contrast to Scolnic & Kessler (2016) and Popovic et al. (2021), which interpreted $c_{\text{obs}}$ to come from a single underlying parameter, here the nature of the BS21 model is that several intrinsic populations (e.g., c_{\text{int}}, R_V, E(B-V), and $\beta_{\text{SN}}$) inform $c_{\text{obs}}$. This added model complexity results in the need to forward-model, where simulations generated from a set of intrinsic parameters are analyzed in the same way as the data in order to compare the observed and simulated distributions.

4.1. Metric Criteria

We infer these dust-model parameters from observables that exist in conventional SN Ia cosmological analyses. Dust2Dust uses the three constraints illustrated in Figure 2, evaluated in six color bins ranging from $c = -0.2$ to $c = 0.25$ (encompassing more than 99% of our sample). Scolnic & Kessler (2016) used Figure 2(a), the histogram of observed $c$ values; following BS21 we extend our constraints to include Hubble residuals versus $c$ (Figure 2(b)) and Hubble residual scatter versus $c$ (Figure 2(c)) to better constrain models with additional complexity. A single color $\chi^2$ does not, by itself, contain enough information to separate the component pieces of the model. Broadly, the $R_V$ value dictates the slope of the Hubble residual values as a function of color (Figure 2(b)), and $\sigma_{\text{int}}$ drives both the color–luminosity relation for the very reddest SNe (Figure 2(b)), and separately, the Hubble residual scatter versus $c$ (Figure 2(c)). The distribution of $\beta_{\text{SN}}$ effects both the observed $\beta_{\text{SALT2}}$, as well as providing a scatter floor for Hubble residual scatter versus $c$ (Figure 2(c)). In addition to color-dependent constraints, Dust2Dust includes a data-simulation constraint on $\beta_{\text{SALT2}}$ and $\sigma_{\text{int}}$, though these do not have a graphical representation. The latter two constraints are determined by performing an “M11 Fit” (Marriner et al. 2011) at each Markov Chain Monte Carlo (MCMC) step. For quantities that define the constraints, uncertainties are determined from the data, with the exception of $\sigma_{\text{int}}$, which is discussed in detail later in the section.

The first Dust2Dust constraint (Figure 2(a)) is a $\chi^2$ term of fitted $c$:

$$\chi^2_c = \sum_i (N^\text{data}_{ci} - N^\text{sim}_{ci})^2 / \epsilon_{ni}^2,$$

where $N^\text{data}_{ci}$ is the number of SNe Ia in color bin $i$ in the data, $N^\text{sim}_{ci}$ is the number of SNe Ia in color bin $i$ in the simulation after scaling the integrated sum to match the data, and the

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Table 2. Source of Instrumental Inputs to SNANA Simulation

| Survey     | Cadence        | DETEFF           | SPECEFF         |
|------------|----------------|------------------|----------------|
| SDSS       | Kessler et al. (2013) | Kessler et al. (2009) | Popovic et al. (2021) |
| DES        | Smith et al. (2020)    | Kessler et al. (2019)    | Abbott et al. (2019)    |
| PS1        | Jones et al. (2018a)   | Jones et al. (2018b)    | Scolnic et al. (2018)   |
| SNLS       | Kessler et al. (2013) | N/A                | Popovic et al. (2021) |
| HST        | Scolnic et al. (2018)  | N/A                | N/A                |
| Foundation | Jones et al. (2018a)   | N/A                | Jones et al. (2018a)  |
| Low-c      | Derived from data*    | Kessler et al. (2019) | Scolnic et al. (2018) |

Note.

* See Kessler et al. (2019).

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5. Fitted peak date uncertainty PKMJ$_{\text{cutoff}}$ $< 20$ days.

6. Light-curve fit probability $P_{\text{fit}} > 0.01$ for SDSS and $P_{\text{fit}} > 0.001$ for DES and PS1. This $P_{\text{fit}}$ cut is not applied to the other surveys.

10. Chauvenet’s criterion at 3.5$\sigma$ to distance modulus residuals relative to best-fit cosmology.
uncertainty, \( e_{ni} \), is
\[
e_{ni} = \sqrt{N_i^{\text{data}}}.
\]

The second constraint (Figure 2(b)) is based on the relationship between \( c \) and the distance modulus residual \( \mu_{\text{res}} \),
\[
\mu_{\text{res}} = \mu - \mu_{\text{model}},
\]
where \( \mu \) is the measured distance modulus from Equation (2) and \( \mu_{\text{model}} \) is a reference cosmology. The Hubble residual constraint is
\[
\chi^2_{\mu_{\text{res}}} = \sum_i (\mu_{\text{res},i} - \mu_{\text{res},i}^{\text{sim}})^2 / e_{\mu_{\text{res},i}}^2
\]
where \( \mu_{\text{res},i} \) is the \( \mu_{\text{res}} \) in each \( c \) bin and the error is
\[
e_{\mu_{\text{res},i}} = \frac{\sigma_{\text{robust}}}{\sqrt{N_{\text{ei}}}},
\]
where \( \sigma_{\text{robust}} \) is the robust scatter,
\[
\sigma_{\text{robust}}(X) = 1.48 \times \text{median}(|X|),
\]
and \( N_{\text{ei}} \) is the number of SNe Ia in each \( c \) bin.

The third constraint (Figure 2(c)) is the relationship between \( c \) and the Hubble residual scatter
\[
\chi^2_{\beta_{\text{SALT2}}} = \sum_i (\beta_{\text{SALT2},i}^{\text{data}} - \beta_{\text{SALT2},i}^{\text{sim}})^2 / e_{\beta_{\text{SALT2},i}}^2
\]
where \( e_{\beta_{\text{SALT2},i}} \) is defined as
\[
e_{\beta_{\text{SALT2},i}} = \frac{\sigma_{\text{robust}}}{\sqrt{2N_{\text{ei}}}}
\]
from Particle Data Group et al. (2020, Equation (40.7)).

4.2. M11 Fit

The color–luminosity relationship, \( \beta_{\text{SALT2}} \), and the poststandardization intrinsic scatter, \( \sigma_{\text{int}} \), along with \( \alpha_{\text{SALT2}} \) and absolute luminosity \( M(z) \), are determined from a global fit of the data following Marriner et al. (2011) and Equation (3) in Kessler & Scolnic (2017). This global fit computes \( \alpha_{\text{SALT2}}, \beta_{\text{SALT2}}, \) and \( \sigma_{\text{int}} \) by minimizing Hubble scatter in bins of redshift. The M11 fit is done in reference to an arbitrary cosmological model in each \( z \) bin, where the absolute rest-frame magnitude \( M(z) \) is simultaneously determined in each \( z \) bin. Thus we can assume that the reference \( \mu_{\text{model}} \) is accurate within each \( z \) bin, but do not assume that the \( \mu_{\text{model}} \) is accurate across the entire redshift range. This M11 fit is performed at each step of the MCMC chain as part of the larger Dust2Dust method, and M11 fit results are used to evaluate the following Dust2Dust constraints:
\[
\chi^2_{\beta_{\text{SALT2}}} = (\beta_{\text{SALT2}} - \beta_{\text{SALT2}}^{\text{sim}})^2 / e_{\beta_{\text{SALT2}}}^2
\]
and
\[
\chi^2_{\sigma_{\text{int}}} = (\sigma_{\text{int}}^{\text{data}} - \sigma_{\text{int}}^{\text{sim}})^2 / e_{\sigma_{\text{int}}}^2,
\]
where \( e_{\beta_{\text{SALT2}}} \) is given by the M11 fit. M11 does not provide uncertainties for \( \sigma_{\text{int}} \); therefore, we simulate 150 independent data-sized samples and estimate the uncertainty as the observed \( \sigma_{\text{int}} \) dispersion across these samples. We find \( e_{\sigma_{\text{int}}} = 0.0036 \).

The M11 fit is implemented by the Beams with Bias Corrections (BBC) code from Kessler & Scolnic (2017); however, in our case, explicit bias corrections are not necessary because constraints (Equations (7), (10), and (13)) are based on data and sims that are processed with the same M11 fit. Thus Dust2Dust accounts for selection effects from analyzing simulated samples, not from BBC bias corrections.

4.3. Dust2Dust Model Fitting

Here, we improve on the BS21 fitting of parameters by developing an MCMC program, named Dust2Dust, to both provide robust error modeling and the simultaneous fitting of the model parameters. The forward-modeling process contains two steps: an M11 fit is performed on the data and simulated supernova, and the results of this fit are used in the Dust2Dust likelihood to propose new steps in the MCMC chain.

A brief overview of the Dust2Dust process is provided in Figure 3 and summarized here:

1. Before running Dust2Dust, a reference simulation is created for Dust2Dust to quickly sample the parameter space.
2. Dust2Dust proposes a specific set of model parameters from the BS21 model.
3. Dust2Dust importance-samples from the reference simulation to create a weighted simulation characterized by the proposed set of model parameters.
4. The M11 fit is run on both the data and Dust2Dust-created weighted simulation.
5. A data-sim \( \chi^2 \) is computed for the proposed model parameters and is used to inform the next proposed model parameters.
Details of the Dust2Dust process are as follows. Dust2Dust begins with generating reference simulations (as described in Section 3.2) containing bounding distributions of our model parameters, both SN Ia and host-galaxy properties. Of note, the simulated \( x_1 \) distribution is excluded from the Dust2Dust process, as the BS21 model does not propose a relationship between \( x_1 \) and host-galaxy mass. Instead, the simulations are generated with stretch distributions taken from Popovic et al. (2021), which include correlations with host-galaxy mass. These reference simulations are fitted with the SALT2 model and are used in the MCMC process.

At each MCMC step, a new simulation is extracted by randomly selecting a subset of SNe from the reference simulation as follows. For SN Ia parameters \( \Theta = \theta_i, i = 1, 2, 3, 4 \), we define for each event

\[
p_{\text{ref}} = \prod_{i=1}^{4} P_{\text{ref}, i} \quad (\text{Ref Sim Params})
\]

\[
p = \prod_{i=1}^{4} P_i \quad (\text{MCMC Params}),
\]

where \( P_{\text{ref}, i} \) is the bounding function probability for the \( i_{th} \) parameter used to generate the reference/bounding simulation, and \( P_i \) is the probability of the SNe in the weighted simulation for the current MCMC step. The weight function for each event in the ref sim is

\[
P(X) = \begin{cases} 
\frac{P}{P_{\text{ref}}} & \text{if } \frac{P}{P_{\text{ref}}} < U((0,1)) \quad 0 \\
\frac{P}{P_{\text{ref}}} & \text{if } \frac{P}{P_{\text{ref}}} \geq U((0,1)) \quad 1
\end{cases}
\]

where \( U((0,1)) \) is a random number in the range \([0, 1]\).

For \( \tau_{\text{E}} \), the bounding function is \( \frac{1}{\tau_{\text{E}}} e^{-\tau_{\text{E}}/\Delta_{\text{Dust2Dust}}} \). For Gaussian distributions, our bounding function is chosen to be a “flat top” asymmetric Gaussian that is uniform between two boundaries, \( \mu_1 \) and \( \mu_2 \) (where \( \mu_1 < \mu_2 \)), with standard deviations \( \sigma_1 \) and \( \sigma_2 \):

\[
P(X) = \begin{cases} 
e^{-\frac{(X-\mu_1)^2}{2\sigma_1^2}} & \text{if } X \leq \mu_1 \\
1 & \text{if } \mu_1 < X < \mu_2 \\
e^{-\frac{(X-\mu_2)^2}{2\sigma_2^2}} & \text{if } X \geq \mu_2
\end{cases}
\]

An example of this bounding function, along with the reweighting from Equation (18), is shown in Figure 4. Both the resulting distribution and the bounding function are normalized to have a peak probability of 1, though the bounding function does not integrate to unity by design.

This bounding function approach saves time by simulating fewer SNe Ia in parameter spaces that are unlikely to be used. The increase in efficiency can be approximated as the quotient of the areas covered by the bounding function and a uniform distribution, raised to the number of dimensions. In the case that all four of our reference distributions are bounded similarly to Figure 4, the quotient is \( \sim 1.3 \), and the computational efficiency is approximately 1.3 \( \sim 4 \) times more efficient than uniform distributions. The combination of reference simulation, bounding functions, M11 fits, and the emcee package (Foreman-Mackey et al. 2013) is the basis for our MCMC named Dust2Dust.

In the case that \( p/P_{\text{ref}} > 1 \), the proposed distribution is considered to be out of range and flagged. The reference simulation can be iteratively regenerated with new centers and widths to cover the appropriate regions of parameter space. The number of such cases in our fit was on the order of \( 10^{-4} \), and therefore negligible.

Dust2Dust initially keeps all simulated SNe Ia with a weight of 1. The resulting simulation size is heavily dependent on the proposed parameters—a tighter sigma beta cut will naturally
have fewer SNe than a wider one. In order to avoid statistical fluctuations, the simulation is downsized to a uniform selected size, in this case 5000 SNe. In the case that Dust2Dust is not able to downsize the sample, the results are flagged as being a bad fit and a log-likelihood of −infinity is returned. For example, with the given fiducial results of the paper, both \( \sigma_{\text{SN}} \) values can be as low as 0.3 without triggering the 5000 SNe threshold. \( \sigma_{\text{SN}} \) can be as low as 0.05 without triggering the 5000 SNe threshold. The number 5000 was chosen to minimize statistical fluctuations. Neither this downsizing nor the selection of model parameters significantly affect nonmodel distributions such as redshift or stretch.

The design of Dust2Dust is to use the simulation frameworks developed in Kessler et al. (2009, 2019), Kessler & Scolnic (2017), and other works, while significantly reducing the simulation time compared to the naive approach of generating a new sample for each MCMC step. Minimizing the time spent simulating is achieved via the use of the reweighting algorithm, which generates an arbitrary desired distribution of SN Ia properties after a single simulation. Table 3 shows the boundaries for the walkers generated by Dust2Dust. These bounds were determined after a number of iterations using Dust2Dust to ensure that our choice of prior does not impact the results.

To fit our model, we minimize a modified version of Equation (8) in BS21:

\[
\chi^2_{\text{Tot}} = \chi^2_c + \chi^2_{\sigma_{\text{SN}}, \text{low}} + \chi^2_{\sigma_{\text{SN}}, \text{high}} + \chi^2_{\mu_{\text{res}}, \text{low}} + \chi^2_{\mu_{\text{res}}, \text{high}} + \chi^2_{\chi_{\text{SALT2}}} + \chi^2_{\chi_{\text{int}}},
\]

(20)

where \( \chi^2_c \) is Equation (7), \( \chi^2_{\sigma_{\text{SN}}, \text{low}} \) and \( \chi^2_{\sigma_{\text{SN}}, \text{high}} \) are Equation (13) split on \( M_{\text{stellar}} \), \( \chi^2_{\mu_{\text{res}}, \text{high}} \) and \( \chi^2_{\mu_{\text{res}}, \text{low}} \) are Equation (10) split on \( M_{\text{stellar}} \), and \( \chi^2_{\chi_{\text{SALT2}}} \) and \( \chi^2_{\chi_{\text{int}}} \) are Equations (15) and (16), respectively. A summary of these criteria is presented in Table 4.

The updated simulation is compared to the data and a log-likelihood is computed to determine the goodness of fit. The log-likelihood is defined as

\[
\mathcal{L} = -\frac{1}{2} \times \chi^2_{\text{Tot}},
\]

(21)

where emcee maximizes, equivalent to minimizing \( \chi^2_{\text{Tot}} \).

For the purposes of this paper, we choose to split the BS21 model on host-galaxy \( M_{\text{stellar}} \); however, any arbitrary external property can be used.

### 5. Results

Here we evaluate and present the results from Dust2Dust run on the sample described in Section 3. Section 5.1 discusses the constraints on model parameters and how well they describe the data, including uncertainties and MCMC efficiency. Section 5.2 presents a comparison to the original BS21 model parameters. Section 5.3 reviews the impact of statistical and systematic model uncertainties on \( w \).

#### 5.1. Fit of Model Parameters

The results for our best-fit parameters are given in Table 5, and these results are discussed in this section. Figure 5 shows the posterior likelihoods for our model parameters after discarding 100 steps for burn-in. After this burn-in, our chains comprised 18,900 steps with 24 walkers. The acceptance fraction is 15%, and the autocorrelation time is 100. While this autocorrelation time could be improved by running Dust2Dust longer, we are already near the computation limits of our setup. In general, the posteriors are unimodal, though not well approximated by a Gaussian. We give the mean values from the chains as our fiducial result.

As described in Section 4.1, Figure 2 shows three of the five criteria used to constrain the BS21 model parameters. A more specific breakdown of the \( \chi^2 \) values is shown in Table 6. Dust2Dust returns a \( \chi^2 \) that is 2× smaller than the original BS21 (BS21-Original) and nearly 5× smaller than two commonly used scatter models: Guy et al. (2010, hereafter G10) and Chotard et al. (2011, hereafter C11). Both G10 and C11 follow SALT2 in not including an explicit dust-based color law; G10 ascribe approximately 75% of observed scatter to achromatic effects and the remaining 25% to chromatic effects. C11, in contrast, attribute 75% of scatter to chromatic variations and the remaining 25% gray. The equivalent criteria of Figure 2 for the G10 and C11 scatter models are shown in Figures 6 and 7, respectively. For both the G10 and C11 models, the Hubble residual and \( \sigma_r \) distributions are poorly recreated by simulations.

Dust2Dust finds model parameters such that simulations predict the observed \( c \) distribution and \( \mu_{\text{res}} \) behavior, as well as

| Model          | Sample                  | \( \epsilon \)   | \( \sigma_{\epsilon} \) | \( \bar{\chi}^2_{\text{SN}} \) | \( \sigma_{\chi_{\text{SN}}} \) | \( R_V \)    | \( \sigma_{R_V} \) | \( \tau_E \)    |
|----------------|-------------------------|-------------------|---------------------------|-------------------------------|-------------------------------|---------------|-------------------|---------------|
| Mean:          | High-mass               | CFA, CSP, Foundation DES, PS1, SNLS, SDSS | -0.077 ± 0.006 | 0.058 ± 0.005 | 2.064 ± 0.174 | 0.308 ± 0.08 | 2.138 ± 0.25 | 1.061 ± 0.429 | 0.107 ± 0.018 | 0.114 ± 0.015 |
| Original:      | High-mass               | CFA, CSP, Foundation DES, PS1, SNLS, SDSS | -0.084 ± 0.004 | 0.042 ± 0.002 | 1.98 ± 0.180 | 0.35 ± 0.200 | 1.50 ± 0.250 | 1.300 ± 0.200 | 0.190 ± 0.080 | 0.150 ± 0.020 |
| Low-mass       | CFA, CSP, Foundation DES, PS1, SNLS, SDSS | 2.75 ± 0.350 | 1.300 ± 0.200 | 0.010 ± 0.010 | 0.012 ± 0.020 |
$\beta_{\text{SALT2}}$ and $\sigma_{\text{int}}$. The Hubble residual rms term ($\chi^2_{\sigma}$) is the largest contributor to the overall $\chi^2$.

We test the robustness of Dust2Dust by analyzing 16 data-sized simulations using parameters taken from the means in Table 5 and compare the aggregate results. The resulting $\chi^2_{\text{tot}}$ ranges from 42 to 105, with an average of 70. These $\chi^2_{\text{tot}}$ are significantly smaller than for the data ($\chi^2_{\text{data}} = 129$), which suggests that improvements to the model, notably $\sigma_{r}$, are likely needed.

The 12 fitted parameters are consistent with simulated inputs to within their uncertainties. Similar to our fiducial result, we use the mean values from the chains as the results for the 16 fits to data-sized simulations. From these fits, we compute the standard deviation of parameter values to compare to our estimated uncertainties. We find the medians of the 16 posterior widths agree to within 15% of the scatter ($\sigma$) of the 16 posterior means: the errors reported for the parameter fits are accurate to within 15% of the standard deviation of the 16 best fits, though they are underestimated. We then check how consistent the posterior means are to the true value of each parameter. We find of the 12 parameters, only one shows a 2.9$\sigma$ bias—this is the low-mass $\sigma_{Rv}$ parameter. The median value of the

Figure 5. Triangle plot for fitted Dust2Dust parameters. Parameters were fit simultaneously and include covariances. $\tau$, $\sigma_{c}$, $\beta$, and $\sigma_{\beta}$ are fit for the entire sample. $R_{v}$ and $\sigma_{Rv}$ are fit separately for low-mass and high-mass galaxies. $\sigma_{x}$ is fit four times across $z$ and $M_{\text{stellar}}$. 

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distribution of recovered low-mass \( \sigma_{R_0} \) values is within 2\( \sigma \) of the input value when using the medians of the posterior widths. To verify this, we ran on a single large simulated sample of 50,000 SNe to check for parameter recovery biases. Three of our recovered parameters are more than 1\( \sigma \) from the input values; none are greater than 2\( \sigma \).

Under the assumption of our model, we find evidence of different \( R_V \) distributions as a function of host-galaxy mass. The mean \( \bar{R}_V \) values in Table 5 differ between high- and low-mass galaxies by 2.8\( \sigma \), and the \( \sigma_{R_0} \) values are within 1\( \sigma \).

We find evidence that the \( \beta_{SN} \) distribution is not a delta function: \( \sigma_{\beta_{SN}} \geq 0 \) with >3\( \sigma \) confidence for the mean Dust2Dust results. G10 and C11 both assume a delta function for \( \beta_{SALT2} \), which is not consistent with our Dust2Dust results.

### 5.2. Comparison with Original BS21 Parameters

For \( \sigma \) (Table 5), we find peak probability (−0.077 ± 0.006) comparable to that of BS21-Original (0.084 ± 0.004), though the standard deviation (0.058 ± 0.005) is higher than that of BS21-Original: 0.042 ± 0.002.

Our \( \beta_{SN} \) and \( \sigma_{\beta_{SN}} \) values are consistent with BS21-Original, and our values are higher. Our \( \sigma_{\beta_{SN}} \) uncertainty is ∼4× smaller. Our \( \beta_{SN} \) is 2.064 ± 0.174, compared to 1.98 ± 0.18.

In contrast to BS21-Original, who found a low-mass \( \bar{R}_V \) value at 1.5 ± 0.25, we find low-mass \( \bar{R}_V \) to be ∼2.0 ± 0.25.

Our high-mass \( \bar{R}_V \) (∼3.0 ± 0.4) is consistent with BS21-Original.

The Dust2Dust-recovered \( \sigma_{R_0} \) results are lower or consistent with those in BS21-Original. While the low-mass \( \sigma_{R_0} \) are consistent, our high-mass \( \sigma_{R_0} \) is smaller compared to BS21-Original.

Brout & Scolnic (2021) found that \( \tau_E \) has little impact on the overall \( L \), particularly for the low-\( z \) subsample (BS21, Figure 9). Using Dust2Dust and a larger data sample, we find that all four \( \tau_E \) values are similar (0.08–0.11), but the low- and high-mass components are more self-similar than the original BS21.

### 5.3. Systematic Uncertainties on Cosmological Parameters

For the SN Ia cosmology analysis (Brout et al. 2022a, hereafter B22), the fitted Dust2Dust parameters are used in simulations for bias corrections, and here we evaluate the associated systematic uncertainty on the dark energy equation-of-state \( w \), matter density \( \Omega_M \), and the Hubble constant \( H_0 \). We compare two systematic evaluation methods: (1) a forward-modeling approach using hundreds of simulations, each analyzed with a fast cosmology \( \chi^2 \) minimizer, and (2) a covariance matrix approach with wifi.

We perform a cosmology analysis that includes

1. SALT2 light-curve fitting to standardize the brightness (Section 2.1).
2. Generating a large simulated sample for bias corrections to account for selection effects.
3. Using BBC (Kessler & Scolnic 2017; Popovic et al. 2021) to produce a Hubble diagram corrected for biases in four dimensions: \( \{c, z, X_1, M_{\text{stellar}}\} \).
4. A cosmology fit.

The first three steps are performed in the same manner as in B22. For our blinded cosmology fitting, we use a simple and fast minimization program in SNANA (wifi) that uses a Planck-like cosmic microwave background (CMB) prior based on the \( R \)-shift parameter (see \( \sigma_R \) tuning discussion at the end of Section 3 in Sánchez et al. 2022).

To model the systematic uncertainty in \( w \) from BS21 parameter uncertainties, we generate 400 statistically independent data-sized simulations with BS21 model parameters drawn randomly from Dust2Dust chains, thus accounting for the
uncertainty and covariance between model parameters. To account for the statistical uncertainty, we additionally generated 400 statistically independent data-sized simulations with best-fit BS21 model parameters. Each data-sized simulation is analyzed using the four steps above.

We define the systematic uncertainty from population parameters to be

$$\sigma_{w_{\text{sys}}} = \sqrt{\text{STDEV}(w_{\text{syst+stat}})^2 - \text{STDEV}(w_{\text{stat}})^2},$$  \hspace{1cm} (22)

where $\text{STDEV}(w_{\text{syst+stat}})$ is the standard deviation of $w$ values from 400 simulations including the randomly drawn parameters, and $\text{STDEV}(w_{\text{stat}})$ is the standard deviation of $w$ values from 400 simulations using the best-fit parameters. We find $\sigma_{w_{\text{sys}}} = 0.014 \pm 0.001$.

While this simulation approach is effective for evaluating a single systematic, it is impractical for the commonly used covariance matrix method that is used in the Pantheon+ cosmology analysis. Instead, we attempt to model the systematic uncertainty in the covariance matrix method using four bias-correction perturbations that mimic the 400 simulations approach.

For this covariance matrix approach, we generate the nominal bias-correction simulation using the maximum likelihood set of parameters. Next, we generate three bias-correction simulations with model parameters that are $\Delta \chi^2 \sim 10$ (approximately $1\sigma$ away from the mean) away from our best-fit results. The resulting Hubble diagram and statistical + systematic covariance matrix is processed through wfit to determine cosmological parameters using a CMB prior from Planck Collaboration et al. (2016). A summary of this process is given in Section 2.2 of B22. While our forward-modeling method only evaluated the $w$ systematic, here we evaluate the systematic uncertainty on both $w$ and $H_0$.

Figure 7. The $c$ histogram, $c$ vs. $\mu_{\text{sys}}$, and $c$ vs. $\text{rms}(\mu_{\text{sys}})$ are shown here from left to right. The latter two panels are split on high and low mass. Purple circles are histogram data and solid gray is a simulated histogram. Green squares are low-mass data and black triangles are high-mass data, while the blue line plots low-mass simulations and the orange dotted line plots high-mass simulation. The C11 model significantly overestimates the rms and does not accurately replicate the $\mu_{\text{sys}}$ split.

### Table 7

| Model          | $\sigma_{H_0}$ | $\sigma_{w_{\text{sys}}}$ |
|----------------|----------------|---------------------------|
| Forward        | $\ldots$       | 0.014(1)                  |
| Covariance     | 0.145 km s$^{-1}$ Mpc$^{-1}$ | 0.011                  |

We define the systematic uncertainties from population parameters to be

$$\sigma_{w_{\text{sys}}} = \sqrt{\sigma_{w_{\text{syst+stat}}}^2 - \sigma_{w_{\text{stat}}}^2},$$  \hspace{1cm} (23)

$$\sigma_{H_{\text{sys}}} = \sqrt{\sigma(H_{\text{sys+stat}})^2 - \sigma(H_{\text{stat}})^2},$$  \hspace{1cm} (24)

where $\sigma_{w_{\text{syst+stat}}}$ is the $w$-uncertainty from wfit using a systematic+statistic covariance matrix, and $\sigma_{w_{\text{stat}}}$ is the statistical-only $w$-uncertainty. Analogous definitions apply to $\sigma_{H_{\text{sys+stat}}}$ and $\sigma(H_{\text{stat}})$. We find $\sigma_{w_{\text{sys}}} = 0.011$, and $\sigma_{H_{\text{sys}}} = 0.145$ km s$^{-1}$ Mpc$^{-1}$. A summary of the cosmological results is given in Table 7.

The results from the forward-modeling and covariance matrix methods, while not within error, are similar in their impact on $w$. With only three different biasCor simulations, our covariance matrix approach may be affected by noise. Adding more biasCor simulations represents a significant computational challenge. To maintain consistency with the forward-modeling approach, we binned the Hubble residuals for the covariance matrix approach. Implementing an unbinned approach from Brout et al. (2021) allows the data to “self-correct” for certain systematics, and may decrease this systematic uncertainty from population modeling. The forward modeling is therefore an upper bound on the associated systematic uncertainty.

### 6. Discussion, Future Work, and Conclusion

Although we have used Dust2Dust to fit model parameters based on $M_{\text{stellar}}$, any external host property can, in principle, be used. Future works can fit for parameters based on other properties such as galaxy morphology or specific star formation rate ($sSFR$). Meldorf et al. (2023) show that fitting on $sSFR$ may prove promising for determining total extinction and reddening in SN Ia samples.

Our SN Ia model assumes a single intrinsic color–luminosity relationship ($\beta_{\text{SN}}$) and differing $R_V$ distributions ($\Delta R_V = 1$) to explain the mass step. González-Gaitán et al. (2021) take an alternative approach, assuming no dust contribution and instead investigating differing $\beta_{\text{SN}}$, though they do not find this assumption sufficient to explain the mass step. While we find evidence of differing $R_V$ distributions across low- and high-mass galaxies ($2.8\sigma$), studies such as Thorp et al. (2021) find no
significant $R_V$ difference. We have chosen to assume a single intrinsic color distribution for all SNe Ia with differing underlying $E(B - V)$ distributions as a function of host properties, in line with the theory provided by BS21. However, future analyses using Dust2Dust may wish to further investigate this claim by allowing the intrinsic color to vary with host-galaxy $M_{stellar}$.

With regards to the mass step, Johansson et al. (2021) find that a $\Delta R_V = 0.5$ difference is sufficient to explain the mass step in optical bands, and furthermore, do not find a mass step in the NIR. It is worth noting that Johansson et al. (2021) were not able to replicate the observed NIR mass step presented in Uddin et al. (2020), nor that of Ponder et al. (2021), though NIR data analyzed by Jones et al. (2022) observe consistent findings to Ponder et al. (2021) and Uddin et al. (2020).

Our forward-modeling approach was chosen over other potential Bayesian frameworks due to difficulties in modeling systematic errors that inhere in traditional Bayesian approaches. The choice to use simulations allows us to account for selection effects and parameter covariances that are difficult to analytically model in a Bayesian approach. Preserving these selection effects and covariances makes for more accurate parameter modeling and the ability to estimate systematic uncertainties.

We find a set of valid BS21 model parameters and that our choice in model parameters has a small ($w_{sys} < 0.01$) impact on $w$ and a negligible impact on $H_0$. This $w$-impact is smaller than previous estimates for intrinsic populations and choice of scatter model (Brout et al. 2019c). While continued work is needed to further constrain $R_V$ and $E(B - V)$ distributions, these results are promising for further research into the effects of host-galaxy properties on SN Ia samples, and other avenues of research could further inform our priors.

Future photometric samples, while not statistically limited with the implementation presented in this approach, present issues for more complex modeling of parameters and subsamples. The most notable of these issues is the potential of core-collapse supernova contamination in the Ia sample, biasing recovered model parameters; concerns with properly identifying host galaxies and redshifts will also present problems. We expect the increased statistics for future surveys such as LSST-SN and the Nancy Grace Roman Supernova Survey to allow improved models to account for changing parameters across the chosen external parameter. Nonetheless, the change from spectroscopic to photometric identification will present its own issues.

Dust2Dust will also be a crucial tool in future cosmological analyses. Recalibration and the retraining of light-curve fitting tools, such as SALT2 (Taylor et al. 2021) and SALT3 (Kenworthy et al. 2021), can significantly affect scatter model parameters. This shift in calibration and light-curve fitting will necessitate inferring new scatter model parameters for use in generating bias-correcting simulations. As such, these new surveys will require implementing Dust2Dust into their cosmological pipelines to significantly reduce unnecessary overhead.

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