Artificial Intelligence Assisted Inversion (AIAI): Quantifying the Spectral Features of $^{56}$Ni of Type Ia Supernovae

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Abstract

Following our previous study of Artificial Intelligence Assisted Inversion (AIAI) of supernova analyses, we train a set of deep neural networks based on the 1D radiative transfer code TARDIS to simulate the optical spectra of Type Ia supernovae (SNe Ia) between 10 and 40 days after the explosion. The neural networks are applied to derive the mass of $^{56}$Ni in velocity ranges above the photosphere for a sample of 124 well-observed SNe Ia in the TARDIS model context. A subset of the SNe have multi-epoch observations for which the decay of the radioactive $^{56}$Ni can be used to test the AIAI quantitatively. The $^{56}$Ni mass derived from AIAI using the observed spectra as inputs for this subset agrees with the radioactive decay rate of $^{56}$Ni. AIAI reveals that a spectral signature near 3890 Å is related to the Ni II 4067 Å line, and the $^{56}$Ni mass deduced from AIAI is found to be correlated with the light-curve shapes of SNe Ia, with SNe Ia with broader light curves showing larger $^{56}$Ni mass in the envelope above the photosphere. AIAI enables spectral data of SNe to be quantitatively analyzed under theoretical frameworks based on well-defined physical assumptions.

Unified Astronomy Thesaurus concepts: Type Ia supernovae (1728); Convolutional neural networks (1938)

1. Introduction

Type Ia supernovae (SNe Ia) are used for cosmological distance measurements based on empirical relations between their light-curve shapes and luminosities (Phillips 1993; Riess et al. 1998; Perlmutter et al. 1999; Wang et al. 2003b; Rubin et al. 2013; Aldoroty et al. 2023; Yang et al. 2022). These relations are consistent with theoretical models of the thermonuclear explosion of a white dwarf close to the Chandrasekhar mass limit (1.4 $M_{\odot}$). First-principle hydrodynamics, nucleosynthesis, and radiative transfer simulations of SNe Ia are expensive and are still far from the precision that can match those of observations, although some 3D SN Ia models can indeed provide photometric and spectroscopic fits that are comparable to those observed in SNe Ia (e.g., Bulla et al. 2016; Wilk et al. 2017; Townsley et al. 2019).

Hydrodynamic and nucleosynthesis processes are only significant in the first ∼100 s after the explosion (e.g., Röpke 2005). Thereafter, the SN ejecta expand homologously, and the observed spectra and light curves can be modeled accordingly. Modeling the radiative transfer process is essential in revealing the density profiles and elemental abundances of the SN ejecta to constrain the SN explosion mechanisms. Several codes have been developed to calculate synthetic SN spectra. One of the simplest is the SYNOW code (Parrent et al. 2010; Thomas et al. 2011), which uses line opacities as inputs to generate synthetic spectra and has been widely used for spectral line identifications. Hydra (Hoeflich et al. 1996), PHOENIX (Hauschildt & Baron 2006), and CMFGEN (Hillier & Miller 1998) are more advanced codes that allow for non–local thermodynamic equilibrium (NLTE) modeling through a finite element approach. Programs using the Monte Carlo method have also been developed for spectral simulations (e.g., SEDONA: Kasen et al. 2006; ARTIS: Kromer & Sim 2009) and have been used for spectropolarimetry modeling (Höflich 1991; Kasen et al. 2003; Bulla et al. 2015; Livneh & Katz 2022). In spectropolarimetry models, 3D effects, NLTE, and time-dependent radiative transfer effects are all important. Among these codes, TARDIS (Kerzendorf & Sim 2014) is a 1D, time-independent Monte Carlo radiative transfer program with approximate NLTE treatment of atomic processes. These radiative codes model the physical processes forwardly, starting from a given set of initial and boundary conditions. Kerzendorf et al. (2021) used a neural network (NN) to accelerate the calculation of the radiative transfer program and suggested that the method can be used for SN ejecta structure estimates, based on a nested sampling algorithm.

The Artificial Intelligence Assisted Inversion (AIAI) of SN Ia spectra (Chen et al. 2020; hereafter XLL20), on the other hand, reverses the modeling processes by training a set of NNs based on simulated spectra, using radiative transfer programs such as TARDIS (Kerzendorf & Sim 2014) to derive the ejecta structures. The NN method by XLL20 provides a new approach of deriving theoretical models using the observed data as the initial input constraints. The method has been successfully applied to study several well-observed SNe Ia around the optical maximum time (XLL20).

Among the 23 elements (from atomic number 6 to atomic number 28) that are the major products of the nucleosynthesis of SNe Ia, $^{56}$Ni stands out for two reasons. First, the decay chain of $^{56}$Ni is the primary energy source that powers the radiative process of an SN Ia. The observed light curves are dictated by the total $^{56}$Ni masses of SNe Ia (e.g., Arnett 1982; Woosley et al. 2007; Khatami & Kasen 2019). Second, the spatial distribution of $^{56}$Ni in SN Ia is directly related to the SN explosion mechanism (e.g., Piro et al. 2010; Piro &
Morozova 2016) and holds critical diagnostic power on related physical processes. The challenge in measuring the $^{56}$Ni from spectroscopic data is that unlike the Si II 6355Å and Ca II 8542Å lines, which are strong lines that are clearly distinguishable from other lines, the spectral lines of $^{56}$Ni are blended and cannot be easily measured from the observed SNe Ia spectra around the maximum. Furthermore, most $^{56}$Ni are still concealed deep inside the photosphere, and only the $^{56}$Ni above the photosphere contributes to the spectral profiles. Childress et al. (2015) use the Co III λ5893 emission line in the nebular spectra of SNe Ia to estimate the mass before the radioactive decay of $^{56}$Ni. The late-time spectra cannot constrain the radioactive Ni synthesized during the SN explosion, although other radioactive elements such as $^{44}$Ti can be constrained (Yang et al. 2018). The AIAI approach has the distinct advantage that the line measurements do not rely strongly on single spectral features. With a large enough training set, it can derive optimal estimates of the physical parameters, with the entire observed spectra contributing to the reliability of all the parameters.

This paper presents a set of NNs and applies them to a sample of well-observed SNe Ia. The NNs are trained on the simulated spectra using TARDIS. Using the NN-predicted SN ejecta structure, we identify a correlation between the spectral feature around 3950 Å of SNe Ia spectra around the B-band maximum time and the $^{56}$Ni mass in the SN ejecta. The paper is structured as follows. Section 2 introduces the training data set, the NN architecture, the spectral sequence fitting pipeline, and the Ni element-related spectral feature measurements. Section 3 tests the NN performances and elemental abundance sensitivities. Section 4 uses SN 2011fe as an example to test the reliability of the NN-predicted elemental abundance and spectral fitting performance. Section 5 shows the results of the spectral line measurements and the Ni mass measurements. Section 6 gives the conclusions. The code for this research is available at https://github.com/GeronimoChen/DLTD and in Chen et al. (2023).

2. Method

2.1. TARDIS Spectral Calculation

In TARDIS, the SN ejecta is assumed to be spherically symmetric and expand homogeneously after the explosion. To avoid the computationally demanding time-dependent photon diffusion calculation, a simple approximation of the photosphere with a blackbody emission spectrum at the inner boundary of the SN ejecta is adopted. Given an SN ejecta structure, a target luminosity, a time after the explosion, and an inner boundary velocity, TARDIS can calculate a spectrum in $\sim$1 CPU hr.

The model spectra are calculated using the code TARDIS (version 3.0-dev3448). To set up the models, we use a dilute LTE (Lucy 1999) approximation to calculate the atomic level population, a nebular approximation (Mazzali & Lucy 1993) to calculate the ionization fraction, macroatom (Lucy 2002, 2003) to calculate the atomic level transition, and detailed to calculate the blackbody radiative rates. TARDIS uses an iterative algorithm (Lucy 2003) to calculate a self-consistent SN temperature profile. In each iteration, the plasma temperature is modified to satisfy the local energy conservation of the absorbed and emitted photons, and the inner boundary temperature is modified to satisfy the target luminosity. As in our previous work on AIAI of SNe Ia spectra (XLL20), the step of temperature iterations is set to 15, with the damping parameters being: (type:damped.damping_constant:1 threshold:0.05. fraction:0.8. hold_iterations:3. t_inner_damping_constant:1). The temperature calculation setup in our research may not return a converged temperature profile; the output spectrum may not reach the target luminosity. According to XLL20, the B-band absolute luminosity for an SN 2011fe-like model could be $\sim$0.8 Mag brighter than the observation. However, the final temperature profile is dependent on the target luminosity and the location of the inner boundary with the current iterative convergence strategy. We adopt this configuration for its flexibility in the temperature calculation, which is necessary when the observed and the simulated spectra are compared quantitatively.

2.2. Simulated Spectral Library

In this section, we parameterize the SN ejecta models based on the “Initial-Guess-Model” (IGM) in XLL20 and randomly sample the parameter space to create an SN ejecta structure library.

We treat the SN ejecta density profile as a power-law relation shown below:

$$\rho(v) = 4.712 \times 10^{-14}\left(\frac{t}{11.5741 \text{ days}}\right)^{-3} A \times 0.689^{\frac{v-12500}{1000 \text{ km s}^{-1}}} \text{g cm}^{-3},$$

where $A$ and $B$ are dimensionless parameters for the density profile, $v$ is the expansion velocity, and $t$ is the time after the explosion. When $A = 1$ and $B = 1$, the density profile is similar to the IGM in XLL20 and serves as the reference density profile in this paper. A comparison between the density profiles is shown in Figure 1. We notice the power-law density profile could approximately fit most of the theoretical SN ejecta density profiles, while a few theoretical density profiles (i.e., DEF_2014_N5DEF) require more parameters to be fitted.

We divide the SN ejecta into six discrete zones in the velocity space. The elemental abundance is assumed to be constant inside each zone. There is no layer above 24,000 km s$^{-1}$ in XLL20; we extrapolate the high-velocity component from the IGM in XLL20 to serve as the reference elemental abundance in this paper, as is shown in the left panel of Figure 1. The elemental abundance structure and the density profile of the DDT_2013_N100 model from (Röpke et al. 2012) are also shown in Figure 1 for comparison.

The parameters for generating the spectral library include:

1. The density profile parameterized by $A$ and $B$ (see Equation (1)): $A$ and $B$ are drawn from uniform distributions between [0.2, 2] and [0, 2], respectively.
2. The abundance of 23 elements in six zones of the ejecta structure: the abundance of an element in a given zone is drawn from a Gaussian distribution in the logarithmic space $N(\mu, \sigma^2)$, where $\mu$ is the log of the abundance of the reference elemental abundance structure and $\sigma$ is set to be 0.5 for all elements. Moreover, the sum of the elemental abundance in each zone is conserved to be 1.
3. The time after the explosion: the time after the explosion is drawn from a uniform distribution in [10, 40] days.
4. The SN luminosity between 6500 and 7500 Å in units of log10(L_\odot) and the location of the inner boundary: to set the parameter ranges of the SN luminosity and the location of the photosphere, we first use the reference ejecta structure (with A = B = 1 in Equation (1)) and the elemental abundance in Figure 1 to calculate a spectral sequence between 10 days and 40 days after the explosion, with varying target luminosities and inner boundary velocities. By comparing the simulated spectra with the observed SNe Ia spectral energy distributions (e.g., Hsiao et al. 2007; Hu et al. 2022), we determine the lower and upper limits of the target luminosities and the locations of the inner boundary at different epochs after the explosion; the results are shown in Table 1.

When generating spectra for the spectral library to be used for NN training, we sample the day after the SN explosion from a uniform distribution in [10, 40], then sample a target luminosity in logarithmic space from the uniform distribution between $[L_{\text{min}}, L_{\text{max}}]$, where $L_{\text{min}}$ and $L_{\text{max}}$ are taken from Table 1, with linear interpolations for days not included in the table. The inner boundary velocity is also sampled from the uniform distribution in $[V_{\text{min}}, V_{\text{max}}]$, where $V_{\text{min}}$ and $V_{\text{max}}$ are linearly interpolated from Table 1.

The wavelength range of the model spectra is between 2000 and 10000 Å, with a total of 2000 wavelength bins. Each wavelength bin is separated by a frequency difference of 5.9958 x 10^{11} Hz. A total of 108,389 ejecta models and their corresponding spectra are calculated to form the spectral training and testing set for building the NNs.

### Table 1

| Time (days) | Luminosity (log10(L_\odot)) | Velocity (km s^{-1}) |
|-------------|-----------------------------|-----------------------|
| 10          | 8.2–8.35                    | 10,500–13,000         |
| 12          | 8.3–8.4                    | 10,000–13,000        |
| 14          | 8.4–8.5                    | 9000–12,000         |
| 16          | 8.5–8.6                    | 7800–10,000        |
| 18          | 8.5–8.7                    | 7000–8200         |
| 20          | 8.55–8.7                   | 6400–7500         |
| 22          | 8.55–8.65                  | 5700–6700        |
| 24          | 8.5–8.65                   | 5200–6200        |
| 26          | 8.47–8.62                  | 4500–5800        |
| 28          | 8.42–8.6                   | 4300–5100        |
| 30          | 8.38–8.52                  | 4000–4900        |
| 32          | 8.3–8.5                    | 3750–4700        |
| 34          | 8.15–8.45                  | 3500–4700        |
| 36          | 8.1–8.35                   | 3500–4700        |
| 38          | 8.0–8.3                    | 3500–4700        |
| 40          | 7.8–8.2                    | 3500–4700        |

### 2.3. NN

A typical NN consists of an input, an output, and multiple hidden layers. The input layer receives data as input tensors, and the hidden layers process the tensors and send the results to the output layer. Different types of layers, representing different mathematical calculations, can be used in the hidden layers. For example, the convolution layer convolves the data tensor with a convolution core, the activation layer applies a nonlinear function onto the data tensor, the pooling layer reduces the size of the data tensor by binning the adjacent data with the maximum values or the average values, and the fully connected layer multiplies a matrix to the input tensor for a review, see Lecun et al. 2015.

The goal of the NN is to provide predictions (y_{\text{pred}}) over a variable of our interest that is close to the truth (y_{\text{true}}) from the given information (X). Initially, the values of the trainable parameters (i.e., the convolution core in the convolution layers and the matrix in the fully connected layers, all denoted as w) are randomly assigned. The NN then calculates the output (y_{\text{pred}}) using the known information X as input, and a loss function (i.e., mean squared error, or MSE: Loss = Mean(y_{\text{true}} - y_{\text{pred}})^2) is calculated to evaluate the performance of the prediction. The trainable parameters are updated with respect to the gradient \partial L/\partial w and a predefined learning rate to minimize the loss function. The training data set is separated into batches for computational efficiency, and the trainable parameters are updated at each batch. The NN browses the data set multiple times; one browse is defined as one epoch.
We adopt the deep ensemble NNs (Lakshminarayanan et al. 2016), which can make predictions and uncertainties simultaneously. Compared to typical NNs, such as AlexNet (Krizhevsky et al. 2012) and VGG16 (Simonyan & Zisserman 2014), the output of deep ensemble NNs is not just the prediction value, but also the prediction mean $\mu$, together with the prediction error $\sigma$, assuming a Gaussian noise distribution. The loss function is:

$$\text{Loss} = \text{Mean} \left( \ln(\sigma(x)) + \frac{(y_{true} - \mu(x))^2}{\sigma(x)^2} \right),$$ (2)

where $x$ is the input information of the NN, including the spectrum, the time after the explosion, and the density parameters; $\mu$ and $\sigma$ are written in function forms to represent the NN.

We use the multiresidual NNs (Abdi & Nahavandi 2016; XLL20) for the NN architecture. In brief, we introduce a block structure with two convolution layers, a batch normalization layer and an activation layer, and repeat the block structure seven times. The input of the block structure is the sum of the output of all the previous block structures and the input of the first block structure. Moreover, the NN has two inputs, the 2000-element array input_1 that receives the input spectra with 2000 pixels from 2000 to 10000 Å, and the 3-element array input_2 that receives the density parameters $A$ and $B$ shown in Equation (1) and the time after the explosion. We use the Scaled Exponential Linear Unit function as the activation function for all the hidden layers:

$$\text{selu}(x) = \begin{cases} \text{scale} \times x, & (x > 0) \\ \text{scale} \times \alpha \times (e^x - 1), & (x \leq 0), \end{cases}$$ (3)

where $\text{scale} = 1.05070098$ and $\alpha = 1.67326324$. The detailed architecture is shown in a figure in our GitHub repository at https://geronimochen.github.io/images/Model_1_0.h5.pdf.

Among all 108,389 spectra, 80% are assigned to the training set, and the remaining 20% are in the testing set. The training data set updates the trainable parameters, while the testing data set only monitors the loss function after every epoch. Note that not all the observed spectral data cover the entire UV–optical–IR wavelength from 2000 to 10000 Å. Data augmentation is applied to the data set to cope with the problem. In this augmentation method, we duplicate the training and the testing data sets by making five copies of them. The spectra in the first copies of the training and testing data sets remain the same as those in the original spectral library. For each spectrum in the other four copies, we randomly select an observational facility (telescope and instrument) that was used to acquire the spectral observations of SNe in the WISEREP database, then apply the wavelength coverage of that facility onto the spectrum. Furthermore, each spectrum is normalized by dividing the spectrum by the average pixel value to avoid overflow in the NNs.

We used the adam algorithm (Kingma & Ba 2014) to update the trainable parameters with a batch size 200. The training process consists of two phases with different learning rates. In the first phase, the learning rate is 0.00003 and decays $10^{-6}$ per batch. The loss in Equation (2) is calculated on the training and testing data sets, respectively, after every epoch. When the loss on the testing data set does not decrease in the 10 most recent epochs, we cease the first phase and keep the model with the smallest loss for the second phase. In the second phase, the learning rate is 0.0000003 and decays $10^{-6}$ per batch. We also monitor the losses on the training and testing data sets at every epoch. When the loss on the testing data set does not decrease for 10 consecutive epochs, we cease the training and keep the NN model with the smallest loss on the testing data set.

We trained seven sets of NNs in total; the first six NNs are designed to predict 30 elemental abundances (from H to Zn) in Zones 0–5, and the seventh NN is designed to predict the inner boundary velocity and the luminosity. The seventh NN outputs a two-element vector, while the other six NNs output 30-element vectors. The losses on the testing data set are shown in Figure 2 and Figure 3.

### 2.4. Density Structure

We propose two density estimation methods in this research. In the first method, we assume the density profile of an SN Ia follows Equation (1), with $A$ and $B$ parameters independent of velocity and time after the explosions, then we design a grid-search method to find the simulated spectral time sequence that best matches the observed spectral time sequence in the parameter space $0.2 \leq A \leq 2$ and $0 \leq B \leq 2$; the spacing is 0.1 for $A$ and $B$, as introduced in the Appendix. This method assumes that Equation (1) is universally correct and is
Figure 4. A comparison of the observed spectra (red lines) and simulated spectra of SN 2011fe with fixed (gray lines; \(A = 1.0, B = 1.1\)) and epoch-dependent (green lines) \(A\) and \(B\). The epochs after the explosion and the density parameters are shown above their corresponding spectra. The symbols on the right mark the different epochs, different ejecta layers are exposed, and the density parameters \(A\) and \(B\) vary (\(\diamond\): William Herschel Telescope (WHT) 4.2m / ISIS; \(\dagger\): HST / STIS; \(\ddagger\): P200 / DBSP; \(\circ\): Gemini-N / GMOS). The observed spectra are deredshifted and corrected for Milky Way and host galaxy dust reddening, as in kaepora (Siebert et al. 2019).

apparently an oversimplification. Indeed, we found the simulated spectra from this method failed to model the entire time sequence of some well-observed SNe Ia, especially in the UV, where the spectra are most sensitive to the density profiles. An example is shown in Figure 4 for SN 2011fe. While the majority of the data are well fitted, the model UV spectra (Figure 4; gray lines) on days 16.59 and 19.61 show significant deviations from the observations (red lines). In reality, at different epochs, different ejecta layers are exposed, and the density profiles may deviate from Equation (1).

We therefore introduce the second method that allows the density parameters \(A\) and \(B\) to change with time and their values to be derived using only the spectra taken at the corresponding epochs; the same \(A\) and \(B\) grid defined for the first method is used to search for the values of \(A\) and \(B\) that lead to optimal spectral fits. To assess the goodness of the spectral fit, we use the NNS to predict the chemical structure of the ejecta for each spectrum and each pair of \(A\) and \(B\) in the grid. A TARDIS model spectrum is calculated using the predicted ejecta structure as input. An MSE is derived using the following equation to estimate the best-match chemical structures and density profile parameters \(A\) and \(B\):

\[
MSE = \sum_{\lambda} (F_{\text{obs}}(\lambda) - F_{\text{sim}}(\lambda))^2 / n,
\]

where \(F_{\text{obs}}(\lambda)\) and \(F_{\text{sim}}(\lambda)\) are the observed and simulated spectra normalized by their corresponding means, respectively, and \(n\) is the number of wavelength bins. Here, the wavelength grid is resampled according to the simulated spectrum, and the regions with missing observations are set to have zero weights.

The simulated spectra with varying \(A\) and \(B\) parameters show noticeable improvements in reproducing the observed spectra over the models with fixed \(A\) and \(B\), as shown in Figure 4 for SN 2011fe as an example; the fits to days 16.59 and 19.61 are significantly better. However, we note that the difference in density structure is typically small for the two different treatments of \(A\) and \(B\) and does not lead to significant discrepancies in the abundance estimates, as can be seen in Section 5 and the Appendix.

Overall, the quality of the spectral fits is worse in the UV than in the visible wavelength. This may be due to several reasons. First, the density profile used in this simulation is a simple exponential function throughout the ejecta, which can be an oversimplification and the primary source of the mismatch in the UV spectral region; the UV flux is extremely sensitive to the ejecta moving at all velocities. Second, the NLTE effect becomes more significant at the late-time SNe Ia spectra, while TARDIS only uses the nebula approximation to account for this effect. Third, the assumption that all photons initiate from a sharp inner boundary is only approximately correct, which could lead to systematic flux errors, especially in the UV (see Blondin et al. 2022 for a comparative study of TARDIS and other radiative transfer models). Fourth, the high dimensionality of the model parameter space means that the library of theoretical models may not be extensive enough to cover completely all the subtypes of SNe Ia and could be improved with a more comprehensive spectral library. Nonetheless, the AIAI approach, as adopted in this study, makes it possible to derive model-based quantities that are sensitive to the chemical structures of the ejecta, although these derived quantities are dependent on the adopted models and the radiative transfer program.

2.5. \(^{56}\text{Ni}\) Line Identification

To identify the spectral lines from Ni, we apply our algorithm to the Hubble Space Telescope (HST) spectrum of SN 2011fe at 19.61 days after the explosion to derive the chemical structure of the SN ejecta. Based on this ejecta structure, we artificially modify the elemental abundance in the velocity range between 13,000 and 17,000 km s\(^{-1}\) (denoted as Zone 3) and the velocity range 10,000–13,000 km s\(^{-1}\) (denoted as Zone 2), by changing the Ni fraction while rescaling the abundances of the rest of the elements to keep the density profile conserved. Figure 5 shows the simulated spectra with Ni abundance in Zones 2 and 3 varying from \(10^{-4}\) to \(10^{-0.7}\) and \(10^{-4}\) to \(10^{-0.35}\), respectively. We notice that Ni strongly affects the spectral features at 3750–3950A, which can be attributed to the blueshifted absorption of the Ni II 4067 A transition lines. This is the only line in the optical in which the strength of Ni II absorption can be directly measured. This line is especially
prominent when the Ni fraction is above $10^{-2}$ in these velocity regions. Note also that the pseudo-equivalent width (pEW) of the Si II absorption line at $\sim 4000$ Å is affected by the Ni II transition lines. It has been shown in previous studies (Silverman et al. 2012; Walker et al. 2011) that the pEW of the Si II absorption line at $\sim 4000$ Å is correlated with the light-curve stretch parameter and the absolute magnitude of SNe Ia. In reality, the measurement of the pEW of the 4000 Å feature captures the combined effect of the Ni II, Ca II, Fe II, and Si II lines in this wavelength region. Figure 5 demonstrates that the origin of the correlation between the pEW of the 4000 Å feature and the light-curve shape and the absolute magnitude of the SNe Ia is more likely to be directly associated with the strength of the Ni II 4067 Å line.

We focus on the flux ratio of the emission around 3950 Å and the absorption feature around 4000 Å; the two spectral features can be measured in most of the observed SNe Ia spectra. The wavelength range is small, so the flux ratio is less affected by dust reddening. First, we measure the flux of the local minimum close to 4000 Å and define it as $F_{\lambda 4000}$. Then we measure the nearest local maximum flux to the blue side of the local minimum and define it as $F_{\lambda 3950}$. We define the flux ratio $\text{FRNi} = F_{\lambda 3950}/F_{\lambda 4000}$ and use it as a spectral indicator of Ni abundances. The following equation is used to calculate the local signal-to-noise ratio ($S/N$) of the spectra:

$$S/N = \frac{F(\lambda)}{\text{STD}(\lambda - 30, \lambda + 30)}.$$  \hspace{1cm} (5)

where $\lambda$ is the wavelength of interest, $F(\lambda)$ is the flux at the wavelength of interest, and $\text{STD}(\lambda - 30, \lambda + 30)$ is the standard deviation of the flux at the pixels between the $\lambda - 30$ and $\lambda + 30$ Åwavelengths. The $S/N$ of the local minimum $F_{\lambda 4000}$ and local maximum $F_{\lambda 3950}$ are denoted as $S/N_{\text{min}}$ and $S/N_{\text{max}}$, respectively. The uncertainty of FRNi is calculated as

$$\sigma_{\text{FRNi}} = \frac{F_{\lambda 3950}}{F_{\lambda 4000}} \sqrt{\frac{1}{S/N_{\text{min}}} + \frac{1}{S/N_{\text{max}}}}.$$  \hspace{1cm} (6)

3. Tests of the NNs

3.1. Error Estimate

We use two methods to estimate the elemental abundance uncertainty from the NN predictions.

The first method uses the NN-predicted error. In Figure 6, we use the NN to predict the Ni abundance in Zone 3 using the testing data set and its associated predictive error ($\sigma$). When the predictive error is small, we notice that the predicted value is consistent with the true value. With increased predictive error values, the predicted values systematically move away from the truth values. When the predictive errors are larger than 0.4 dex, the predicted values become insensitive to the truth values and take values between $-2.0$ and $-1.5$. Therefore, we use $\sigma < 0.4$ dex as a criterion to measure the goodness of prediction on the observed spectra.

In the second method, we use the NN-predicted SN ejecta parameters to run a TARDIS model, then compare the model spectrum with the observed spectrum using the MSE value defined in Equation (4). Most of the spectroscopically normal SNe are well fit with MSE $\leq 0.06$; on the other hand, fits to peculiar SN 1991bg-like SNe, SNe Iax, and some of the SN 1991T- or SN 1999aa-like SNe show larger MSEs. This is most likely due to the construction of the model spectral data set used for training the NN, which is built based on spectroscopically normal SNe Ia (see Section 5 for more discussions). In this study, we focus on spectroscopically normal SNe and will focus on models and data with MSE $\leq 0.06$. 

![Figure 5](image-url) - An illustration of measuring the spectral line flux ratio FRNi. The red lines are the spectra of SN 2011fe at 19.61 days after the explosion. The lines with different colors are the simulated spectra using TARDIS. The simulated spectra on the left and right are computed with varying Ni mass fractions in the velocity ranges 13000–17000 km s$^{-1}$ (Zone 3) and 10000–13000 km s$^{-1}$ (Zone 2), respectively. The Ni mass fractions are shown in the legends of the two figures. All the spectra are normalized to the local minimum flux near 4000 Å. The black arrows indicate the local minimum and maximum that are used to measure the spectral line flux ratio FRNi = $F_{\lambda 3950}/F_{\lambda 4000}$.
3.2. Ni Abundance Sensitivity

In this section, we use the SN ejecta structure predicted from the HST spectra of SN 2011fe at 12.6 days, 19.61 days, 22.89 days, and 28.84 days to simulate four spectral sequences with different Ni abundances in 13 000–17 000 km s\(^{-1}\) (Zone 3). In these ejecta models, we allow the mass fraction of Ni in Zone 3 to vary from \(10^{-4}\) to \(10^{3}\), while keeping the relative ratio of other elements in Zone 3 unchanged. Other model parameters, such as the density structures, are kept the same. We employ the NNs to predict the elemental abundances using these simulated spectral sequences. This can test the capability of the NN in recovering the assumed model abundances in the context of ejecta models similar to a real SN Ia. Figure 7 shows the predicted and the true Ni abundance in Zone 3 of the spectral sequences. The typical prediction errors are \(\sim 0.2\) dex, and the predicted values are generally consistent with the truth when Ni abundance is larger than \(10^{-2.5}\) for the spectra in all four phases. The linear relation is lost when the abundance drops below \(\sim 10^{-2.5}\), indicating the sensitivity limit of the models. We surmise the low Ni abundances cannot produce spectral features stronger than the Monte Carlo noise in the simulations and that there may be hidden degeneracies in the model that are still not fully understood.

Moreover, a bias of \(\sim 0.3\) dex is observed on the SN 2011fe spectra 12.6 days after the explosion. A possible reason is that electron scattering is still important in Zone 3 at the early epochs, reducing the sensitivity to Ni abundances in the spectral formation. To correct this bias, we use each best-fit simulated spectrum as the input to the NNs and its associated best-fit parameters \(A\) and \(B\) to repredict the elemental abundances. In the left panel of Figure 8, we compare the repredicted Ni mass fractions in Zone 3 with those predicted by the observed spectra.

The repredicted Ni mass fractions are systematically lower than those predicted directly from the observed spectra. The difference is phase-dependent and is shown in three bins of the time after the explosion in Figure 8 (left). The spectra are split into six groups according to the phase after the explosion to correct this bias. The time intervals for these five groups are [9, 14], [14, 19], [19, 24], [24, 29], [29, 34], and [34, 40] days. An average bias is calculated for each group. The Ni mass fraction is corrected using the average bias in their corresponding time bin.

We further iterate by calculating simulated spectra using TARDIS with the bias-corrected ejecta structure. The bias-corrected ejecta structure shows insignificant improvements over the MSEs for the fits, as shown in Figure 8 (right), which compares the MSE differences between the observed and simulated spectra with and without the bias corrections in Zone 3. The absence of a significant difference in the MSE suggests that bias is not the dominant source of our model uncertainties. We emphasize that our spectral library is still far too small to cover the entire parameter space of SNe Ia. The TARDIS code also has its own limitations when applied to model SN observations. A much larger simulation data set with more complete coverage of all spectral types of SNe Ia and a fine-tuned NN structure are necessary for future studies. For these reasons, we did not adopt this bias correction in the subsequent studies of this paper.

3.3. Ni Abundances and Data Noise

Most of the observed spectral data have no published errors. This paper quantifies the S/N using data between 3900 and 4100 Å, following the method defined in the DER_S/N algorithm (Stoehr et al. 2008). This wavelength range is covered by most of the SNe Ia spectra. The noise is calculated using the following:

\[
\sigma = \frac{1.482602}{\sqrt{N}} \med([2F(i) - F(i - 2) - F(i + 2)]) \tag{7}
\]

where \(F(i)\) is the spectral flux at the \(i\)th pixel and \(N\) calculates the median value over all pixels. The signal is taken as the median flux value.

We use the HST spectrum of ASASSN-14lp at day 14.49, which has an S/N of 81, as an example to discuss the effect of the observational noise on the elemental abundance estimations. The predicted Ni mass fraction at Zone 3 is around \(10^{-1.5}\), which is much higher than the \(10^{-2.5}\) sensitivity limit according to Section 3.2. Gaussian noises are applied to the observed spectrum, and the NN is used to estimate the elemental abundances and predictive errors of the Ni element in Zone 3. As shown in Figure 9, for data with S/N \(\geq 20\), the predicted Ni element mass ratio is stable around \(10^{-1.5}\) and the predictive error is around 0.3 dex. This shows an error floor of the abundance estimates and the limitation of the current NNs. The predicted Ni element mass ratio becomes unstable with the decreased spectral S/N, and the predictive error increases to \(\sim 0.45\) dex. There is no significant bias in the Ni mass due to observational noise.

4. SN 2011fe as an Example

This section uses SN 2011fe to show the deep-learning-based pipeline’s spectral fitting performance and elemental abundance accuracy, using the well-observed SN 2011fe as an example.
in the velocity range 13,000 km s$^{-1}$ of each ejecta structure derived for SN 2011fe, but vary the Ni mass fraction in the velocity range 13,000–17,000 km s$^{-1}$ (Zone 3). The spectra used for these predictions are generated from TARDIS based on the abundance of $^{56}$Ni in Zone 3 as the only varying parameter. The horizontal and vertical axes show the truths and predictions, respectively, of the logarithmic Ni mass fraction $\log_{10}(\text{Ni})$ in the velocity range 13,000–17,000 km s$^{-1}$ (I. E. S. A. 962:125 (14pp), 2024 February 20 Chen et al.).

The times after the explosion of the simulated spectra are labeled in the upper left corner. The predicted value compared to the truth value of the NN with the MSEs between the observed and the TARDIS simulated spectrum are split into three groups based on the time after the explosion: 9–15 days (red), 15–30 days (green), and 30–40 days (blue). Right: the $x$-axis shows the MSEs between the observed and the TARDIS simulated spectra after applying the Ni mass fraction correction in Zone 3, and the $y$-axis shows the same without this correction. The different colors on the data points indicate the time after the explosion. Purple means early and yellow means late.

Figure 10 shows the elemental abundances derived from the observed spectra of SN 2011fe on days 9.47 and 22.89. Only the chemical structure above the photosphere can be characterized with the spectra at the photospheric phase. The elemental abundances derived from these two spectra are highly consistent at zones above 10,000 km s$^{-1}$, despite the rapid evolution of the spectral features during the two epochs (Figure 4). The abundance structure of SN 2011fe we derived can be compared with the $\rho=11$fe model (Mazzali et al. 2014; Heringer et al. 2017) emanated from spectral modeling and the DDT_2013_N100 model (Röpke et al. 2012) calculated from hydrodynamic and nucleosynthesis simulations, as shown in Figure 11. The elemental abundances derived using data 22.89 days after the explosion are used for these comparisons because the observed spectrum covers a broad wavelength range of 2000–10000 Å, and the observed spectrum is well fitted by the TARDIS simulated spectrum (see Figure 4). For the DDT_2013_N100 model (downloadable at HESMA), specific isotopes are available, while for the $\rho=11$fe model, we assume all the Ni to be $^{56}$Ni initially and calculate the elemental abundances at day 22.89 by propagating the nuclear decay processes of radioactive elements.

The three ejecta structures are remarkably consistent in the Fe, Co, and Ni distribution (Figure 11, bottom panels). A sharp dropoff is seen at velocities above 20,000 km s$^{-1}$. Our model is also broadly consistent with DDT_2013_N100 in other elements, such as C, O, Mg, and Ca, but significant discrepancies are found for Si and S where our NN predicts much less Si and S at velocities above 15,000 km s$^{-1}$ than DDT_2013_N100. The Ca abundance from this study is much higher than the other two models at velocities below 13,000 km s$^{-1}$, but note that the Ca features are strongly affected by the NLTE effect. The C and O abundance is consistent above Zone 3 among the three models, confirming the presence of unburned materials at the outermost layers of the ejecta. Overall, the agreement between the NN-derived chemical structure and DDT_2013_N100 is remarkable, supporting the notion that SN 2011fe is the result of the explosion of a Chandrasekhar mass white dwarf.

5. Applications of the Method and the Results

We searched all the available SN Ia spectra from WISEREP (Yaron & Gal-Yam 2012) and kaepora (Siebert et al. 2019) and

https://hesma.h-its.org/
found 1087 spectra from 124 SNe Ia, which were observed between −10 days and 20 days relative to the B-band maximum time with the rest-frame wavelength covering 3800–7000 Å and the spectral S/N (as defined in Section 3.3) larger than 20. This forms the data set for our analysis to apply the NNs to a sample of well-observed SNe. We also collected the Δm15 parameters of these SNe from kaepora (Siebert et al. 2019) or calculated the Δm15 parameters using the light curves from kaepora (Siebert et al. 2019) or the Open Supernova Catalog. All the spectra are converted to rest frame and corrected for dust extinction effects using the data from the relations between the Ni abundances in Zone 3 and the spectral line ratio FRNi are shown in Figure 13 for the three epochs, as in Figure 12. The FRNi shows a linear correlation to the logarithmic Ni abundance in Zone 3 log56Ni, especially for the spectra between 12 and 15 days after the explosion. Such a linear correlation is weaker for the spectra between 15 and 18 days after the explosion, probably because the Ni abundances have decreased below the detection limit for most of the SNe. The Ia-99aa and Ia-91T subtypes of SNe show higher Ni abundances and lower FRNi parameters than spectroscopically normal SNe Ia. The Ia-91bg subtype SNe show lower Ni abundances and larger FRNi.

In Figure 14, we show the relation between the spectral line ratio (FRNi) measured from the observed spectra and the Δm15 values. A linear relation exists between the FRNi values and the Δm15 values for most of the subtypes of SNe Ia at different phases between 9 and 18 days after the explosion. The Ia-91bg subtype shows higher FRNi and Δm15 values than normal SNe Ia. The Ia-91T and Ia-99aa subtypes show the lowest Δm15 and FRNi compared to other subtypes of SNe Ia. The lax subtype shows low FRNi and a high Δm15 value, which is slightly off from the correlation defined by the other SN Ia subtypes.

Figure 15 shows the time evolution of the Ni abundance in Zone 3 for a few best-observed SNe: SN 2011fe, SN 2005cf, SN 2013dy, ASASSN-14lp, SN 2014J, and SN 2015F. The decay rates, as shown in Figure 15, deserve further remarks. While the values of the Ni mass fractions of SN 2013dy, ASASSN-14lp, and SN 2014J appear to be consistent with the half-life time of 56Ni, that of SN 2011fe is considerably flatter and that of SN 2005cf is much steeper than given by the radioactive decay rate. One possibility is that this is intrinsic to the approximations adopted in the code TARDIS, which only utilizes approximated NLTE processes. On the other hand, taking the numbers literally may indicate the inadequacy of the spherical geometry we have adopted. During these observations, even for the fixed velocity zones, the lines are formed in different regions, as the photosphere recedes considerably to deeper layers at later times. Chemical inhomogeneities are found to be common in literally all SNe Ia ejecta from polarimetry observations (Wang et al. 2003a; Wang & Wheeler 2008; Cikota et al. 2019; Yang et al. 2020, 2022b). Theoretical models suggest that the chemical structure of SNe Ia may be considerably off-centered, although the expected level of continuum polarization in such cases is low and challenging to detect through polarimetry (Hoeflich et al. 2023). A recent study shows that the signatures of chemical asymmetry may have imprints on the shapes of the color–magnitude diagrams of SNe Ia (Aldoroty et al. 2023), where a “picket fence” structure is proposed to explain the “bump morphology” of the CMAGIC diagram of SNe Ia. Such a “picket fence” structure would introduce varying amounts of 56Ni above the photosphere at different times after explosion, leading to variations of the 56Ni mass responsible for the 56Ni absorption features at different epochs. In the nebular phase, the blueshift of the centroid of the [Ni II] 7378 Å line was found to be correlated to the evolution of the velocity of the P Cygni absorption of the [Si II] 6355 Å line, and it was proposed that global asymmetry may be expected in all SNe Ia, despite the lack of significant continuum polarization (Maeda et al. 2010).
Multidimensional NLTE radiative transfer models may be needed for further progress.

6. Conclusion

We employed the radiative transfer program TARDIS to build a set of NNs to calculate the Ni elemental abundance in SNe Ia ejecta. We measured the Ni abundances and their time evolution in the 13,000–17,000 km s$^{-1}$ regions of 153 SNe Ia and correlated the Ni abundance to the spectral feature around 3950 Å and the SN light-curve parameter $\Delta m_{15}$. The NN prediction on the Ni in the 13,000–17,000 km s$^{-1}$ region can reach 0.2 dex accuracy on the simulated SN 2011fe spectra and the sensitivity can reach $10^{-2.5}$ of the Ni mass fraction. The predicted Ni abundance is correlated to the spectral line feature FRNi, which may allow us to measure the amount of Ni in SN ejecta directly. The predicted Ni abundance is also correlated with the light-curve parameter $\Delta m_{15}$, especially in the early-phase spectra, probably due to more $^{56}$Ni being present in the early-phase SNe Ia ejecta. The Ni spectral line feature FRNi and the ejecta structures predicted by the NNs may be further used in cosmological studies requiring more accurate distance measurements with well-controlled systematic errors.

The simulated spectra based on the NN predictions represent a significant improvement in the quality of the spectral modeling of SNe compared to similar models in the literature. This is obviously because of the optimization procedure involved in the AIAI modeling, which searches for and interpolates the best
solution from a large set of theoretical models. However, there are many approximations involved in our models; most noticeably, they include the approximate NLTE calculation in the radiative transfer simulation program TARDIS, the limitations on constructing a comprehensive training data set, and the oversimplification of the theoretical SN ejecta geometry and density profiles. Note that the deviation of the TARDIS model from Sedona and CMFGEN is found to be the largest in the UV wavelength range (see Figure 12 in Blondin et al. 2022). The TARDIS code generates all its photons from an inner boundary, and the other part of the ejecta only reprocesses photons from the inner boundary. Sedona made the improvement of more realistically generating photons in the Monte Carlo simulation, but Sedona models are much more costly to compute.

AI makes it possible to “calibrate” codes with simplified approximations to make them agree with results from codes
with a more complete treatment of physical processes. The physical-model-based parameterization of the observational data of SNe Ia as developed in this study can be extended to other radiative transfer codes (e.g., Hoeflith et al. 1996; Baron & Hauschildt 1998; Hillier & Miller 1998; Kasen et al. 2006). The physical parameters in the AI models can also be used for refining SNe Ia as distance indicators. The large quantity of these allows for a comprehensive search for the dominant effects on the SN luminosities. This approach is different from what has been done so far based on empirical models of SN Ia luminosity–distance relations (e.g., Phillips 1993; Tripp 1998; Wang et al. 2003b, 2006, 2009; Guy et al. 2005; Jha et al. 2007). For future projects of SN cosmology, such theoretical-model-based parameterization has a different sensitivity to the systematic errors of SN evolution—AIAI may prove to be helpful in constraining the systematic evolution of the age and metallicity of SN Ia progenitors, especially when very-high-redshift (z ∼ 3–6) SNe Ia are involved (Lu et al. 2022).

It is also essential to have a fast code to generate surrogate models of 3D radiative transfer to account for the asymmetric geometry of the ejecta as found from spectropolarimetry observations (Wang et al. 1996; Wang & Wheeler 2008; Cikota et al. 2019; Yang et al. 2022b) and theoretical models (e.g., Neopane et al. 2022). These works will be reported in a forthcoming study (X. Chen et al. 2023, in preparation).

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Appendix

Caveats on the Density Structure

In this section, we design a grid-search method, aiming to find a density profile that could fit an SN Ia spectral time sequence. For an observed spectral time sequence of an SN Ia, we first use the NNs to predict the time sequences of the elemental abundances, the luminosities, and the velocities of the inner boundary for a given grid of density parameters and the phase of each spectrum. We use TARDIS to recalculate the simulated spectral sequences for this density parameter grid. The simulated spectral sequences are compared with the observed spectral sequence using the squared error (SE) as the merit function:

$$\text{SE}(A, B) = \sum_{i} \sum_{\lambda} (F_{i, \text{obs}}(\lambda) - F_{i, \text{sim}}(\lambda, A, B))^2,$$

where \(i\) is the index of the spectrum in the spectral sequence, \(F_{i, \text{obs}}(\lambda)\) is the \(i\)th observed spectrum, and \(F_{i, \text{sim}}(\lambda, A, B)\) is the \(i\)th spectrum in the simulated spectral sequence using the density parameters \(A\) and \(B\). The simulated spectra are masked according to their wavelength coverage of the observed spectra, with the missing wavelength regions being set to have zero weights and normalized by dividing the spectra by the average pixel value. The observed spectra are resampled with the wavelength grid of the simulated spectra and are normalized by their average pixel values.

The density profile Equation (1) has only two free parameters, \(A\) and \(B\), to be determined. However, finding the best \(A\) and \(B\) parameters that minimize Equation (A1) in a typical 19 × 21 grid space still involves a large number of spectral model computations. We have applied the following method for further improvement. The method has five iterations; each iteration calculates the spectral sequence in a different subgrid. In the first iteration, the subgrid is set to be \(A = [0.5, 1.1, 1.7], B = [0.5, 1.1, 1.7]\). In the second iteration, the subgrid is specified as \(A = [a - 0.2, a, a + 0.2], B = [b - 0.2, b, b + 0.2]\), where \(a\) and \(b\) are parameters set with the smallest SE from the first iteration. In the third iteration, the subgrid is replaced by \(A = [a - 0.2, a, a + 0.2], B = [b - 0.2, b, b + 0.2]\) with \(a\) and \(b\) being the values that give the smallest SE from the second iteration. In the fourth iteration, the subgrid is refined to \(A = [a - 0.1, a, a + 0.1], B = [b - 0.1, b, b + 0.1]\), where \(a\) and \(b\) are the parameters set with the smallest SE from the third iteration. In the fifth iteration, the subgrid is refined to \(A = [a - 0.1, a, a + 0.1], B = [b - 0.1, b, b + 0.1]\), where \(a\) and \(b\) are the parameters set with the smallest SE from the fourth iteration. Finally, the parameter set with the smallest SE among all the subgrids will be adopted to be the density parameter of the SN.

For a well-observed SN with ∼30 spectra (e.g., SN 2005cf), the total computation time could still exceed 1000 CPU hours using this grid-search method. Therefore, we limit the number of observed spectra used in the grid search to about 10, based on the quality of the spectral data. For well-observed SNe, we only select the spectra from ground-based telescopes with apertures larger than 3 m in diameter and the HST. The spectra
are visually inspected to eliminate data with obvious abnormal flux calibrations.

We use 11 spectra of SN 2011fe between 9 days and 40 days after the explosion to explore the best-fit density parameters, observation time, and instruments, as shown in Figure 4. The left panel of Figure 16 shows the SE values (Equation (A1)) of several selected grid points in the density parameter space. The number of TARDIS models to be calculated is \((9 + 8 + 0 + 8 + 5) \times N_{\text{obs}}\), where 9, 8, 0, 8, and 5 are the number of grid points in the five iterations described above and \(N_{\text{obs}}\) is the number of observed spectra. The grid points that are calculated in the previous iterations will not be calculated again, therefore the second, fourth, and fifth iterations have numbers of grid points smaller than 9. Because the best point after the second iteration is \(A = 1.1, \ B = 1.1\), the subgrid in the third iteration overlaps with the searched grid points, and no calculation is executed in the third iteration. Finally, the best-fit density parameters \(A\) and \(B\) are found to be 1.0 and 1.1 for SN 2011fe.

The simulated spectral time sequence using this fixed density structure is shown as the gray lines in Figure 4.

In order to test the stability of this density estimate method, we use SN 2011fe as an example and apply the bootstrap resampling method. In each of the iterations, we randomly delete half of the observed spectra, then use the remaining spectra to estimate the density parameters. We run 1000 iterations, then draw a histogram of the estimated density parameter distributions, as shown in Figure 16. The result for SN 2011fe shows that about 45% of the estimated density parameters are the same as the estimated density parameters using all of the observed spectra. Moreover, the density distribution in the SN 2011fe result shows roughly two clusters. In Figure 17 and Figure 18, we compare the estimated Ni element mass ratio in Zone 3 with the light-curve parameter \(\Delta m_{15}\) and the spectral feature FRNi value again. The density parameters are fixed for an SN Ia at a different observation time to obtain the minimal SE value between the simulated spectral time sequence and the observed spectral time sequence. We notice the correlations between the Ni mass ratio and \(\Delta m_{15}\), and between the Ni mass ratio and FRNi, are retained with the change of density parameters. Moreover, we observe many

![Figure 16](image1.png)

![Figure 17](image2.png)
spectral fitting results provide an MSE larger than the 0.06 criterion, resulting in more transparent data points in the figures.

To conclude, using a two-parameter density model in Equation (1) could be an oversimplification of the actual SN Ia density structures, especially for SNe Ia with multi-epoch observations, such as SN 2011fe. A density profile with more parameters or a 3D density structure could be used in future SNe Ia structure modeling research, in order to provide a more self-consistent ejecta structure.

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Figure 18. The same as Figure 13, but the density parameters are fixed for an SN Ia at different observation time.

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