Light a Single Candle: Studying Supernovae

Dianne P. O'Leary

Supernovae are exploding stars. For a few weeks, they can be as bright as or even brighter than their parent galaxies, as shown in Figure 1. Most types of supernovae have irregular light emissions, but for one class, Type Ia, the light curves display a very uniform and regular behavior. Because of this, a Type Ia supernova is quite useful as a **standard candle** that can be used to estimate the distance between earth and its galaxy.

Light curves from six Type Ia supernovae are shown in Figure 2. It is commonly believed that the light emissions are powered by the radioactive decay ⁵⁶Ni \rightarrow ⁵⁶Co \rightarrow ⁵⁶Fe. One obstacle for this hypothesis is that the decay rates that best fit the data are quite different from the decay rates observed on earth. Of course, the supernovae environment is also quite different, and it was observed by Rust, Leventhal and McCall (1976) that the decay rates for each supernova seem to be accelerated by a common factor.

This acceleration hypothesis is still controversial, and much more complicated models have been proposed. We investigate in this case study, following a paper by Rust, O'Leary, and Mullen (2009), how well the acceleration hypothesis fits some data accumulated in the more than 30 years since it was proposed. Some of the text and the figures in this case study are taken from that 2009 paper.

The Model: Part 1

The model can be represented schematically as follows:

$$W(t; \alpha_1, \alpha_2, \alpha_3) \longrightarrow \begin{bmatrix} 56 \text{Ni} \end{bmatrix} \xrightarrow{k_1} \begin{bmatrix} 56 \text{Co} \end{bmatrix} \xrightarrow{k_2} \begin{bmatrix} 56 \text{Fe} \end{bmatrix}$$

where $W(t; \alpha_1, \alpha_2, \alpha_3)$ is a pulse of ⁵⁶Ni deposition (created by fusion of lighter elements) and k_1 and k_2 are the nuclear decay rates of ⁵⁶Ni and ⁵⁶Co. We model



Figure 1. Supernova 205ke in optical, ultraviolet, and X-ray wavelengths. If each image is 4×4 , then it is found 2.5 units from the top of the image and 1.0 units from the left, near the bottom-left of the bright part of the galaxy. "This is the first X-ray image of a Type 1a, and it has provided observational evidence that Type Ia are the explosion of a white dwarf orbiting a red giant star. Credit: NASA/Swift/S. Immler" (See Acknowledgements pointer.)

the initial pulse by a Weibull probability density function

$$W(t;\alpha_1,\alpha_2,\alpha_3) = \frac{\alpha_2}{\alpha_3} \left(\frac{t-\alpha_1}{\alpha_3}\right)^{(\alpha_2-1)} \exp\left[-\left(\frac{t-\alpha_1}{\alpha_3}\right)^{\alpha_2}\right],\tag{1}$$

where α_1 is the starting time for the fusion pulse, α_2 is a shape parameter, and α_3 is a scale parameter. Formula (1) holds for $t \ge \alpha_1$; otherwise $W(t; \alpha_1, \alpha_2, \alpha_3) = 0$.

CHALLENGE 0.1.

(a) Plot the Weibull function for $\alpha_1 = 5.4$, $\alpha_2 = 2.4$, and $\alpha_3 = 19.3$ and for $\alpha_1 = 1$, $\alpha_2 = 1$, $\alpha_3 = 1$.

(b) Verify that it has unit area for any choice of the α parameters.

In a terrestrial setting, the decay rates k_1 and k_2 would be the inverses of the average lifetimes 8.764 days and 111.42 days, but in the high density interior of the star, the model allows these two rates to be accelerated by a common factor α_4 , so

$$k_1 = \frac{1}{8.764 \,\alpha_4} \,, \qquad k_2 = \frac{1}{111.42 \,\alpha_4} \,, \tag{2}$$

and α_4 becomes a fourth parameter for the model. If $N_1(t)$, $N_2(t)$, and $N_3(t)$ represent the abundances of ⁵⁶Ni, ⁵⁶Co, and ⁵⁶Fe, respectively, then the ordinary



Figure 2. B-magnitude light curves for six Type Ia supernovae. The label on each plot is the name assigned to the supernova, specifying the year of the explosion and the order of discovery in that year. The time unit for the measurements is Julian Days (JD), the number of days since Greenwich noon on January 1, 4713 BC. The brightness units are astronomical magnitudes measured in the B (blue) wavelength passband.

POINTER 0.1. Why use the differential equation model?

The model (3) is simple enough that formulas for $N_i(t)$, i = 1, 2, 3, could be derived in closed form. For this case study we will leave them in ODE form, in order to get experience with computing with such models.

POINTER 0.2. Reading the Data

Three of MATLAB's input commands might be of use to you:

- The MATLAB command fopen tells MATLAB where the data file is. Example: fid = fopen('SN1990N-B.dat', 'r')
- temp = fgetl(fid) reads an entire line (useful for skipping lines).
- fscanf is a formatted read. Example: A = fscanf(fid, '%f %f %f') reads the next three data values in fid into an array A.

differential equations (ODEs) for the $^{56}\rm{Ni}$ deposition and subsequent decay processes can be written

$$\frac{dN_1}{dt} = W(t; \alpha_1, \alpha_2, \alpha_3) - \frac{1}{8.764 \, \alpha_4} N_1 , \qquad N_1(\alpha_1) = 0 , \\
\frac{dN_2}{dt} = \frac{1}{8.764 \, \alpha_4} N_1 - \frac{1}{111.42 \, \alpha_4} N_2 , \quad N_2(\alpha_1) = 0 , \qquad (3) \\
\frac{dN_3}{dt} = \frac{1}{111.42 \, \alpha_4} N_2 , \quad N_3(\alpha_1) = 0 .$$

Since the Weibull pulse has unit area, it produces a unit amount of ⁵⁶Ni, so $N_1(t)$, $N_2(t)$ and $N_3(t)$ are relative abundances that are scaled up in the fit of the model to the observed data.

In order to model well, we need to choose convenient units for the data.

CHALLENGE 0.2. In the light curves in Figure 2, astronomical magnitudes are plotted versus Julian Days.

(a) Explain why Julian Day is not the best unit for time, and why we prefer to set a zero point for time to be a few days before the first observation.

(b) The astronomical magnitude scale is logarithmic, with a difference of five magnitudes corresponding to a change by a factor of 100 in apparent brightness. The scale runs backward, with smaller magnitudes corresponding to brighter objects. Instead of fitting astronomical magnitudes, consider fitting **relative luminosities**, defined by

$$L(t) = 10^{-0.4 (B(t) - B_{ref})} , \qquad (4)$$

JD $(t=0)$	B_{ref}
2448050.0	12.0
2448350.0	11.0
2448875.0	15.0
2450900.0	12.0
2451410.0	14.5
2452725.0	13.0
	$\begin{array}{c} {\rm JD}\ (t=0)\\ 2448050.0\\ 2448350.0\\ 2448875.0\\ 2450900.0\\ 2450900.0\\ 2451410.0\\ 2452725.0 \end{array}$

Table 1. Julian Day corresponding to time 0, and values of B_{ref} , for the six supernovae.

where B_{ref} is a **reference magnitude** for the supernova. Give some advantages and disadvantages of fitting data using L(t) instead of B(t).

- (c) Solve for B(t) in terms of L(t).
- (d) Plot the SN1990N data in luminosity units.

Table 1 sets the reference magnitudes and the zero points for time.

The Derivatives

To fit our model (3) to data, we will need derivatives of N_k with respect to α_j , for k = 1, 2, j = 1, 2, 3, 4.

Notice that, for well-behaved functions,

$$\frac{d}{dt}\left(\frac{\partial N_1}{\partial \alpha_j}\right) = \frac{\partial}{\partial \alpha_j}\left(\frac{dN_1}{dt}\right).$$
(5)

Define

$$\breve{N}_{1j}(t) = \frac{\partial N_1}{\partial \alpha_j}(t).$$

Then, we can obtain the partial derivatives of \check{N}_{1j} , for j = 1, 2, 3, from (3):

$$\frac{d}{dt}\left(\breve{N}_{1j}\right) = \frac{\partial}{\partial\alpha_j}W(t;\alpha_1,\alpha_2,\alpha_3) - \frac{1}{8.764\,\alpha_4}\left(\breve{N}_{1j}\right) , \ j = 1,2,3.$$
(6)

Using the initial conditions

$$\frac{\partial N_1(\alpha_1)}{\partial \alpha_j} = 0 , \qquad (7)$$

these three equations can be integrated numerically along with the ODEs in (3). To get a valid equation for j = 4, we need to differentiate the first relation in (3) with respect to α_4 , which gives

$$\frac{d}{d\alpha_4}\frac{dN_1}{dt} = \frac{d}{d\alpha_4}W(t;\alpha_1,\alpha_2,\alpha_3) - \frac{d}{d\alpha_4}\left(\frac{1}{8.764\,\alpha_4}N_1\right) \ .$$

Use the "product rule for differentiation" on the 2nd term (since N_1 also depends on α_4) to get the final expression.

A similar derivation gives a way to calculate

$$\breve{N}_{2j}(t) = \frac{\partial N_2}{\partial \alpha_j}(t). \tag{8}$$

To use the ODE-solver this way, it is necessary to find expressions for the three partial derivatives of $W(t; \alpha_1, \alpha_2, \alpha_3)$ defined by (1). You can use MATLAB's Symbolic Math Toolbox with the program

```
syms a1 a2 a3 t
w = a2/a3*(t-a1)^(a2-1)/a3^(a2-1) * exp(-((t-a1)/a3)^a2)
dw_da1 = diff(w,a1)
dw_da2 = diff(w,a2)
dw_da3 = diff(w,a3)
```

to generate these derivatives.

CHALLENGE 0.3. Apply one of MATLAB'S ODE solvers to our model, (3), (6), (8). with $\boldsymbol{\alpha} = [14, 2, 15, .6]$. Plot N_1 , N_2 , and N_3 for 300 days. On two separate figures (k = 1, 2), plot $\partial N_k(t)/\partial \alpha_j$, j = 1, 2, 3, 4.

The Model: Part 2: Fitting the Luminosity Data

We now convert our model to luminosities. Define

$$\Phi_1(t; \boldsymbol{\alpha}) = \frac{1}{8.764 \,\alpha_4} N_1(t) , \qquad \Phi_2(t; \boldsymbol{\alpha}) = \frac{1}{111.42 \,\alpha_4} N_2(t) , \qquad (9)$$

where Φ_1 and Φ_2 are the relative contributions to the total luminosity by the decays of ⁵⁶Ni and ⁵⁶Co, respectively. The total observed luminosity can then be written

$$L(t, \boldsymbol{\alpha}, \boldsymbol{c}) = c_1 \Phi_1(t; \boldsymbol{\alpha}) + c_2 \Phi_2(t; \boldsymbol{\alpha}) , \qquad (10)$$

where c_1 and c_2 are linear adjustable parameters that convert the relative luminosities to observed luminosities. So our model has 6 free parameters: 4 nonlinear parameters α_1 , α_2 , α_3 , and α_4 that specify the properties of the central engine generating the gamma rays that power the luminosity, and 2 linear parameters c_1

and c_2 that specify how the gamma rays interact with the expanding atmosphere and/or the surrounding planetary nebula to generate the observed luminosity.

We now have the set up to do a (nonlinear) least squares fit of the luminosity data for each supernova to the model (10) to determine the 6 parameters:

$$\min_{\boldsymbol{\alpha},\boldsymbol{c}} \sum_{\ell=1}^m \omega_\ell |L_\ell^{meas} - (c_1 \Phi_1(t_\ell;\boldsymbol{\alpha}) + c_2 \Phi_2(t_\ell;\boldsymbol{\alpha}))|^2,$$

where ω_{ℓ} are given weights. We have several computational options:

- Use lsqnonlin to find the 6 parameters, without a Jacobian matrix.
- Use lsqnonlin to find the 6 parameters, providing a finite-difference approximation to the Jacobian matrix. The fact that noisy derivatives cause difficulty in optimization settings has been previously documented.
- Use lsqnonlin to find the 6 parameters, providing the closed-form formulas for the Jacobian matrix.
- Use lsqnonlin to find the nonlinear parameters, determining the optimal linear parameters in the function evaluation for each iteration of lsqnonlin.
- Use varpro, which has now been programmed in MATLAB and is available on the website.

CHALLENGE 0.4. Use your code from the previous challenge and lsqnonlin and varpro, with Jacobian matrices, to find values of α and c for each of the 6 datasets on the website so that the 2-norm (Euclidean norm) of the difference between the predicted luminosities and the measured luminosities is minimized. Use the weights $\omega_{\ell} = (1/L_{\ell}^{meas})^2$.

Make a table of parameter values α that you found and the times (tic/toc) that the two algorithms used.

Plot the data points and the model predictions (B-magnitude) for each supernova.

Validating the Model

How can we decide whether we have a good fit to the data?

• First, we want to be sure that the model fits the data well, so we should plot the data points and the model predictions in a single figure and check that the predictions are within the error bars for the data.

POINTER 0.3. Acknowledgements

The light curves were found using two very helpful websites:

Jet Propulsion Laboratory NASA/IPAC Extragalactic Database (NED) http://nedwww.ipac.caltech.edu/.

Nickolay Pavlyuk and the SAI Supernovae Research Group, "SAI Supernova Light Curve Online," http://virtual.sai.msu.ru/~pavlyuk/snlcurve/.

Figure 1 is taken from http://www.nasa.gov/centers/goddard/news/topstory/2006/supernova_mugshot.html

This case study would not have been possible without the help of Bert Rust.

- Second, we should check the residuals, the differences between the values predicted by the model and the data points. If we believe, for example, that the error in the data is uncorrelated from data point to data point and normally distributed with mean 0 and constant standard deviation (a reasonable assumption for this problem), then
 - A plot of the residuals should zig-zag rather evenly.
 - A histogram of the residuals should look like a bell curve.
 - The periodogram of the residuals should look like a well-mown lawn. The periodogram fr of a vector r is formed using the following statements:

```
n = length(r);
fr = fft(r);
fr = fr .* conj(fr)*2/n;
m = ceil((n-1)/2);
fr = fr(1:m);
```

- The cumulative periodogram of the residuals should look like a straight line. The cumulative periodogram is the sequence formed from 0, then the 1st component of fr, then the sum of the 1st two components, then the sum of the 1st three components, etc. We could quantify agreement with the straight line by computing the length of the cumulative periodogram, or 95% confidence intervals for it, but we will not do that in this case study.

We have a rather small number of data points, but let's check how well our model fits the data.

POINTER 0.4. Some Tips

- Define the Weibull function to be zero when t is less than α_1 .
- Use symbolic arithmetic once, to get the formulas used in the program that the ODE solver calls. Don't use it every time the ODE solver needs a function value; that is too slow.
- Graphs are only useful if they convey information. They are useless if they don't have labels on the axes, or don't indicate the units, or are printed so small that the information is not clear, or have several gray-colored curves that can't be distinguished. Use xlabel, ylabel, title, and legend when appropriate. Use different line styles (solid, dashed, dotted, etc.) even if you use color plots, because an estimated 10% of the population is color blind.
- Use an ODE solver appropriate for stiff systems unless you are sure that the system is not stiff.
- Real data files are messy. When you have a set of them, they very often have small differences in formatting. It is a bad idea to retype data (too much chance for error). Instead, write a program that handles format variations.
- Some of the datafiles have multiple observations at a given time. It is important to use this data properly:
 - It is not OK to average the values. This changes the standard deviation of the error for those observations, so the weighting is bad.
 - It is not OK to shift the times by a small number (although I admit that this works). This changes the data, and, scientifically, it is wrong.
 - It is not OK to delete data. Each of the data values should produce an entry in the "observed - model" vector.
- Studying residuals with histograms and periodograms is a good check, but it relies on having enough data points. 52 is a rather low number, so I wouldn't expect ideal-looking results.

CHALLENGE 0.5. For the SN1998aq supernova, plot the residual (in luminosity units), the histogram of the residual, the periodogram, and the cumulative periodogram. Discuss the four plots and your conclusion.

POINTER 0.5. Further Reading

This case study is closely related to Chapter 13. The paper we build upon is:

B. W. Rust, M. Leventhal, S. L. McCall is "Evidence for a radioactive decay hypothesis for supernova luminosity," *Nature* 262 (July 1976), pp. 118–120.

The more recent paper, from which much of the material in this case study is extracted verbatim, is:

"Modelling Type Ia supernova light curves," Bert W. Rust, Dianne P. O'Leary, and Katharine M. Mullen, in *Exponential Data Fitting and Its Applications*, V. Pereyra and G. Scherer, eds., Bentham Science Publishers Ltd. 2010, pp. 169-186. http://www.bentham.org/ebooks/9781608050482/

As an example of the difficulties in using numeric derivatives in optimization, see:

Ralf Leidenberger and Karsten Urban, "Automatic differentiation for the optimization of a ship propulsion and steering system," University of Ulm, Germany, 2008. http://www.mathematik.uni-ulm.de/numerik/ staff/urban/html/veroeff.html

An example of a model for supernovae that involves spatial dependence is:

W. Schmidt, J. C. Niemeyer, W. Hillebrandt, and F. K. Röpke, "A localised subgrid scale model for fluid dynamical simulations in astrophysics II. Application to type Ia supernovae," *Astronomy and Astrophysics* 450 (2006), pp. 283-294. DOI: 10.1051/0004-6361:20053618