Hanxuan Kuang

Ever since I was young, scientific topics and applications always fascinate me. Not only because I enjoyed learning the materials, but also because how I perceive them as a way to understand this seemingly orderless world. My earliest knowledge of scientific research came from hearing stories of my grandfather, who went on several science expeditions to Antarctica with the Chinese Academy of Sciences as an environmental chemist. As a five-year-old, of course I did not have much idea of his work, but it did leave a long-lasting impression—it planted a seed in my mind.

When I was in fourth grade, I had a chance of visiting the flagship Chinese icebreaker for arctic expeditions, *MV Xue Long*, which brought my grandfather to and from Antarctica. The state-of-the-art technology and laboratories immediately captivated me. I was showed the new autonomous cruising technology of this ship and the world's most advanced onboard surface seawater analyzer. I also visited the onboard biological, chemical, and atmospheric laboratories. This experience encouraged my initial passion for scientific research and made me to envision conducting research.

Over the next several years, I grew interested into mathematics and physics. One of the question I have been pondering is how and why does the universe become the way it is. After reading some interesting books, such as *An Elegant Universe* by Brian Greene, *A Brief History of Time* by Stephan Hawking, and others, I have come to the realization that many things have been so coincidental. If any fundamental pieces of the universe are glued together differently, we probably will not be here today (fortunately for us, it didn't). After learning some programming knowledge and accruing some experience of using programming to solve problems, in the summer after my sophomore year, I reached out to Prof. Brett Bochner to be my research mentor. The project was a study on dark energy, which is a very popular hypothesis of the underlying reason of the cosmic expansion.

Before formally beginning my project, I had to familiarize myself with the field of cosmology and programming a Markov chain Monte Carlo (MCMC) simulation. It was certainly enriching and more intuitive to learn the topic through concrete mathematical language than pure and abstract concept. I began with reading *Dark Side of the Universe* from Iain Nicolson and continued with reading a lot of papers in the field of cosmology and computational simulation. From doing this project, I became much more familiar with using `Java`, which I used for running the MCMC simulations, and Wolfram Mathematica, which I used for data analysis and visualization.

During the first year, I worked with a student in my grade on a project, which we entered in the Siemens Competition and were nominated Semifinalist. However, in that project, a relatively hollow and unrealistic assumption was used in the computation process, which also resulted in not entirely accurate estimations. Therefore, in the summer after my junior year, I started a new project using very different forms of data and methods to trying to characterize properties of dark energy. This is the project being described in the rest of this paper. To remove any unfounded assumptions that are not necessarily true, a less popular technique known as cosmography was employed to directly extract information from the observed datasets. Because this technique directly models the data using Taylor polynomials, it avoids making assumption about the mathematical nature of dark energy. More details will be described in Methodology section.

Having done cosmology research for two years, I developed a keen interest in physics and especially cosmology. At the same time, I developed more interest regarding our role here on Earth and also in the universe. I particularly enjoyed cosmology because it helps us to understand how and where everything was formed and everything will end. I also enjoyed working on theoretical physics using statistical simulations because I enjoy expanding our knowledge through more optimized analysis of current data. As shown by recent examples such as the LHC and the James Webb telescope, developing new instruments nowadays are increasingly expensive and time-consuming. Thus, I want to make sure data we have is analyzed thoroughly instead of shifting completely to new data once it is available. My project was very rewarding to me and I look forward to doing further work in this field.

My advice to any high school students interested in doing science research is to be invested in a topic truly passionate to you. Do not choose a topic or a project because it looks more likely to win a competition. You won't make it through (OK you might, but it probably won't be a really pleasant experience). Most publications you will see are written by graduates, doctorates, professors. Many of them have spent years in that field. Sometimes, you have to learn a lot of backgrounds to even comprehend the basics of a concept. There are so many new topics so one can be very easily overwhelmed. Admittedly, this process can be get tedious, challenging, or even arduous. But if you do make it through, the final reward is also immense.

Markov Chain Monte Carlo Testing of Cosmological Constant and the Limits of Cosmography with the Union2.1 Supernova Compilation

Hanxuan Kuang
erickuang1@gmail.com

Abstract

Previous studies have shown that the cosmic expansion is accelerating despite the gravitational attraction between matter, caused by a mysterious source of energy denoted as dark energy. A cosmographic test of whether it exists in the form of a cosmological constant (Λ) or more general dark energy was performed with Markov chain Monte Carlo algorithms using the SCP Union2.1 supernova compilation. By fitting polynomials to Hubble series expansions, the Hubble Constant (H_0), the deceleration parameter (q_0), and the jerk parameter (j_0) can be estimated. Λ requires $j_0 = 1$ for all time. This study focuses on the effects of MCMC algorithms and model-building uncertainty–the dependence of results based on fitting functions used. Eight tests of different orders and distance scales were performed. Through a new program devised in Java, resulting uncertainties of all parameters are significantly smaller than those from traditional statistical techniques. Combined with cosmographic method, MCMC yields much more Gaussian distributions of cosmological parameters. Consistent with Λ, j_0 can be reliably constrained within $[-5.992, 6.693]$. We conclude that more parameters would be better to fully test Λ once more data of supernovae and other sources are incorporated.

1 Introduction

In 1927, Georges Lemaître first proposed the theory of cosmic expansion, which was later confirmed by Edwin Hubble (Hubble, 1929; Lemaître, 1927). Since stars of almost all directions are receding away from us, they must be receding away from each other as well, leading to the conclusion of an expanding universe. This prompted scientists to look for signs of cosmic deceleration since gravity tends to be attractive between matter. However, in 1998, two teams observed that the cosmic expansion is, in fact, accelerating (Riess *et al.*, 1998; Perlmutter *et al.*, 1999a). Further research into cosmic large-scale structure has also confirmed this observation (Tegmark *et al.*, 2004). The discovery of cosmic acceleration explained many phenomena that had confused astronomers for decades, one of them being the "Age Crisis", where some objects were observed to be older than the Big Bang (Turner, 2002). Yet, it also created more mystery about the root cause of acceleration. To explain this puzzling phenomenon, physicists had to develop new theories.

As of today, most explanations involve introducing a concept known as dark energy, a hypothesized form of exotic energy that dominates the cold-dark-matter-filled universe (Perlmutter, Turner, & White, 1999b). Unlike previously known baryonic matter and dark matter, dark energy possesses a negative pressure that is believed to enable dark energy to not only counteract gravity but also to push cosmic expansion to accelerate.

To understand this puzzling phenomenon, physicists had to reintroduce the concept of a cosmological constant (Λ), which was referred to by Albert Einstein as the "biggest blunder" of his career. The cosmological constant refers to the energy of vacuum space in the universe and is hypothesized to remain the same strength regardless of the amount of space it occupies. The universe filled with cold dark matter and a cosmological constant is often referred to as ΛCDM model, which is the simplest yet the most convincing dark energy model as of today (Lim, 2015).

Despite its consistency with most observations today, Λ does have its own problem. One most apparent discrepancy is the vacuum catastrophe, where the observed value of Λ is smaller than the value suggested by Quantum Chromodynamics by 120 orders of magnitude (Weinberg, 1989). Therefore, many alternative models have been developed, such as quintessence, phantom energy, and so on (Xu & Zhang, 2016).

To understand what is the dark energy that exists in the universe today, a commonly used approach involves creating a fixed or time-varying model about the dark energy equation of state that directly characterizes the strength and consequently the type of dark energy. For instance, the CPL Parameterization uses two parameters to characterize the variation of the dark energy equation of state with respect to time (Chevallier & Polarski, 2001). However, making such assumption, namely the power of the modeling equation, about the nature of dark energy before thoroughly understanding it can lead to incorrect conclusions. Consider fitting a quadratic curve with a linear function: there are often multiple equally good ways to characterize it, which can possibly result in contradictory conclusions based on the researcher's choice of data. In addition, since these models were developed based on observational data, fitting data to them may inadvertently come across situations where trying to prove one theory using its own proof, which is recursive and inconclusive. Considering the large number of dark energy models being presented (Xu & Zhang, 2016), a direct observational examination of the cosmic expansion free from existing assumptions may be more valuable. This is where cosmography comes into play.

Cosmography refers to the underlying kinematics of the universe. This approach is independent of any models and directly measures the motion of the universe using the universe's scale factor $a(t)$ and its related time derivatives. It merely relies on the notion that the universe is homogeneous and isotropic on a large scale, which is confirmed by observations such as the Cosmic Microwave Background. In the cosmographic method, one expands observed distance functions using Taylor expansion to obtain the cosmographic parameters (Cattoën & Visser, 2007). To perform the series expansion, a cosmological redshift parameter is necessary, which describes the distance of an astronomical event, specifically supernova (SNe) emissions, in terms of $a(t)$ using $a_0 \equiv a_{SNe}(1+z)$, where a_0 is current universe's scale factor and z is the redshift parameter. The first three parameters introduced, respectively, are the Hubble constant, $H_0 \equiv \dot{a_0}/a_0$, which describes the current rate of cosmic expansion; the deceleration parameter, $q_0 \equiv -(\ddot{a_0}/a_0)H_0^{-2}$, which describes the acceleration of the cosmic expansion; and the jerk parameter, $j_0 \equiv (\dddot{a_0}/a_0)H_0^{-3}$, which describes the rate of change of the deceleration parameter. Conducting a test of cosmological constant using cosmography only demands one criteria to be satisfied: $j_0 = 1$ (Dunajski & Gibbons, 2008).

To obtain knowledge about the current scale factor a_0, celestial objects known as "standard candle" are often used to measure distances in space. The most notable standard candles are Type Ia supernovae (SNe1a), which explode at the same mass ($\approx 1.38\mathrm{M}_\odot$) and consequently produce a consistent peak luminosity, which makes them the ideal choice for distance references (Mazzali, Röpke, Benetti, & Hillebrandt, 2007). In addition, SNe1a data is the only data that directly and continuously depicts the recent cosmic expansion in the acceleration epoch (i.e. $z \sim 0.1 - 1$, which is around the last five billion years), making them more preferable than other indirect measurements (Bochner, Pappas, & Dong, 2015).

An essential difficulty in implementing the cosmographic method is that a key balance of the number of parameters used needs to be achieved. Model-building uncertainty, first observed by Cattoën & Visser (2007), refers to the phenomenon of yielding radically different results when the same data is fitted to slightly different yet equally trusted models. Too few fitting parameters lead to big model-building uncertainty due to the series truncation, just like fitting a linear line to a quadratic curve. Too many fitting parameters, on the other hand, produce large statistical uncertainties that render the results inconclusive due to the increased complexity of the parameter space and limited statistical power of SNe1a data (Cattoën & Visser, 2008). Therefore, a Markov chain Monte Carlo (MCMC) method was implemented in an attempt to reduce both statistical and model-building uncertainties. MCMC performs global searching and mapping, enabling it to effectively narrow down the optimal area in the parameter space with considerable precision, which reduces some uncertainties originated from the method (not inherent to the SNe1a data).

The purpose of this study is to test the validity of Λ in the universe and the limit of cosmography in testing hypothesis regarding dark energy. In order to obtain smaller statistical and model-building uncertainties compared to previous studies using cosmography, MCMC was implemented rather than traditional statistical techniques. MCMC using several different numbers of fitting parameters was performed to obtain a median value and an optimal range for each parameter of interest and especially j_0 to test Λ and the overall evolution of the universe.

2 Methodology

The Type Ia Supernova (SNe1a) data used in this study was from the Supernova Cosmology Project Union2.1 compilation, which includes the z-redshift and distance measurement of 580 Type Ia supernovae (Suzuki *et al.*, 2012). The measure of distance in cosmology is often inherently ambiguous due to the continuous cosmic expansion over time and the consequent cosmic redshift.

There are many different distance scale functions, and all of them can be interrelated with a factor of $(1 + z)$ using Friedmann-Lemaître-Robertson-Walker metric, which is the exact solution to Einstein's field equation (Weinberg, 2008). There are five commonly utilized distance scale functions, d_L, d_A, d_F, d_P, d_Q. Two distance scales utilized in this study were luminosity distance, $d_L \equiv a_0 r(1 + z)$, which measures distance based on luminosity and flux, and angular diameter distance, $d_A \equiv a_0 r/(1 + z) = d_L(1 + z)^{-2}$, based on supernovae's diameters and angular sizes. These two functions were chosen because they have been demonstrated to bracket the value range of resulting cosmographic parameters, making them the most efficient way to estimate the largest reasonable model-building uncertainty (Bochner *et al.*, 2015). Although all of them are perfectly fine for expressing distance between celestial objects, an issue worth noticing was the aforementioned model-building uncertainty, describing a phenomenon that radically different results can be yielded using the same data that only differs in the distance scale function model being used for fitting data (Cattoën & Visser, 2008). Therefore, it is crucial to include more than one distance scale functions in the data fitting process, so the exact error budget can be known.

Due to the inherently limited interval of convergence of fitting a polynomial to the data, the analysis focuses exclusively on y-redshift, which can be converted from z-redshift using the following equation (Cattoën & Visser, 2007):

$$y = \frac{z}{1 + z} \tag{1}$$

Compared to z-redshift that has a range of $[0, \infty)$, where $z = 0$ is the present-day universe and $z \to \infty$ represents the Big Bang, the y-redshift has a range of $[0, 1)$, where $y = 0$ is the present-day universe and $y \to 1$ is the Big Bang. By using y-redshift, the series convergence problem can be avoided.

Expressions for each Hubble series, the SNe1a observational data fitting series, for d_L and d_A are given in Cattoën & Visser (2007). Furthermore, they are given in an alternative form, $\ln\{[d_L(y)]/y\}$ and $\ln\{[d_A(y)]/y\}$, which differ from the standard form by eliminating one varying yet cosmologically irrelevant term in the function. To describe the process of relating cosmographic parameters and Hubble series, consider the following second-order polynomial (the minimum number of terms required to estimate j_0) as an example, where c denotes the speed of light in km/s:

$$\ln\{[d_L(y)]/y\} = \ln\left(\frac{c}{H_0}\right) + \frac{1}{2}(3 - q_0)y + \frac{1}{24}(17 - 2q_0 + 9q_0^2 - 4j_0)y^2 + O[y^3] \quad (2)$$

To model the observational SNe1a data, consider the following fitting polynomial similar to a Taylor series in its generic form:

$$F(y) \equiv a_0 + a_1 y + a_2 y^2 + \cdots + a_n y^n = \sum_{i=0}^{n} a_i y^i \quad (3)$$

This fitting polynomial of order y^n possesses $N \equiv n + 1$ optimizable coefficients. The lowest-order fitting polynomial usable for estimating j_0 is the second-order polynomial $N = 3$). Though computing the cosmographic parameters of interest does not require any term in the polynomial beyond second degree, the median values of all parameters can vary significantly at different values when using different numbers of parameters for fitting. When more parameters are used, the polynomial estimations of different models are more consistent between d_L and d_A fits, thus yielding smaller model-building uncertainty but greater statistical uncertainty. When fewer parameters are used, the exact opposite behavior would happen: larger model-building uncertainty but smaller statistical uncertainty is yielded. In this study, the modeling process includes results from simulations using $N = \{3, 4, 5, 6\}$, which takes into account the inversely related statistical and model-building uncertainties.

The coefficient optimization is done by utilizing Markov chain Monte Carlo (MCMC) simulations. For an MCMC algorithm to run properly, a Markov chain that has a distribution whose equilibrium is the desired equilibrium of cosmographic parameters needs to be constructed. Though MCMC is not the only statistical method to obtain best-fit values of parameters given their distributions, it is often the preferred method because it allows for a relatively thorough search through the parameter space in a feasible amount of time. In addition, implementing MCMC for searches in complicated parameter space prevents the program from being trapped in local minima that are not the ideal global solution. Compared to traditional statistical technique, MCMC explores much more of the parameter space by taking far excursions even after finding an optimal solution, which significantly reduces the chance of mistakenly assuming a local minimum as the best global solution. Throughout this process, the program will visit the better-fit area more often and the worse-fit area less frequently. By recording the movements in each iteration, the median value for parameters and their empirical probability distributions can be obtained. In addition, the Markov property of the Markov chain allows the program to be “memoryless”, thus the movement of one iteration only depends on the last immediate movement, which further reduces the effect of being trapped in a local minimum and enhances the program’s ability to find the global best-fit value of each parameter (Berg & Billoire, 2008).

To evaluate the goodness of fit of a particular fitting polynomial to the observational data, χ^2 test statistics were used. When fitting the SNe1a dataset with N_{SN} supernovae using N terms will produce a best-fit polynomial with $(N_{SN} - N)$ as its degree of freedom ($N_{SN} = 580$ in the case of Union2.1 compilation). The χ^2 value of each fit can then be computed by

$$\chi^2 = \sum_{i=1}^{580} \frac{(d_i - F(y_i))^2}{\sigma_i^2} \tag{4}$$

where (d_i, σ_i) refers to the observed distance and the statistical uncertainty of the i^{th} supernova, respectively, and $F(y_i)$ refers to the theoretical distance of the i^{th} supernova at its specific y-redshift computed by the current fitting polynomial.

MCMC simulations were implemented using multiple programs in Java devised for this study. The starting point of the simulation is randomly located between 0.0 and 5.0 for each coefficient before the corresponding term. Since MCMC performs searches throughout the entire parameter space, the starting point does not affect the end result as much, which was also experimentally verified in the program development process. Because it takes some iterations to initialize and stabilize the MCMC algorithm, there is an inherent burn-in period that iterations during this period will be thrown away, whose length directly depends on the complexity of the parameter space (Casella & Robert, 2009). The length of each simulation’s burn-in period is determined by inspecting the movements of the simulation in terms of variability. Once the simulation is able to converge within a range of value, the burn-in period is considered completed. Only after this process finishes, the MCMC algorithm can be reliably used to simulate the distribution.

In every iteration, the value of each coefficient will make a random walk, which has a size determined by its respective proposal distribution. The choice of an appropriate proposal distribution and its density can have significant effects on the MCMC simulation. An overly high acceptance rate indicates that the proposed movements in every iteration are very close to current locations, resulting in the MCMC algorithm taking too long to reach the optimal area. On the other hand, an overly low acceptance rate suggests that many proposed movements were rejected by the program, leading to an inefficient chain design and a wastage of computational resources. In addition, the optimal proposal distribution would have a similar shape to the posterior distribution being sampled. For the Union2.1 compilation, using a symmetric normal distribution would suffice (Lim, 2015).

In the algorithm, a built-in method `nextGaussian()` from the `java.util.Random` class was used to generate a pseudo-random, Gaussian ("normally") distributed value every time it is called. The default mean and standard deviation of the distributions generated by this method are 0.0 and 1.0, respectively. In this study, the mean of step size proposal distribution was kept at 0, thus it is equally likely to make a step toward the positive or negative side. However, depending on the coefficient c_n and number of terms N of the fitting polynomial, the standard deviation of step size will be chosen differently. Because the average step size of a coefficient is directly dependent on the standard deviation of its proposal function, and the step size was observed to be directly related to its acceptance ratio in our trials, the adoption of an appropriate standard deviation for each coefficient is imperative for a reliable chain convergence. The standard deviation of each coefficient in every simulation is determined experimentally using a trial-and-error procedure, where multiple trials were conducted and the value that achieves best convergence was adopted. Overall, higher-order coefficients will have larger standard deviations because their uncertainties are naturally larger than that of lower order coefficients. Note that simulations completed using the same length of fitting polynomial have the same setting for standard deviations, regardless of the distance scale function used (either d_L or d_A). This allows for better observation of the effect of model-building uncertainty under different settings.

The key configurations of the MCMC algorithms are outlined in Table 1. For convenience of discussion, μ_{a_n} was defined as the standard deviation of the step size proposal distribution of the y^n term coefficient ($n \in \{0, 1, 2, 3, 4, 5\}$), and the term "effective length" denotes the total simulation length minus the burn-in period. Once the convergence of chains is achieved, the best-fit values of the parameters of interest can be reliably estimated. The outcome of MCMC algorithms were processed in a Java program devised for this study, then the results were analyzed using Wolfram Mathematica and Microsoft Excel.

Table 1: MCMC algorithm configuration for polynomials fitting to both $\ln\{[d_L(y)/y]\}$ and $\ln\{[d_A(y)/y]\}$ at each specific N case. Some fields are marked "N/A" since polynomials fitting to case N only have N coefficients.

Fit Terms	μ_{a_0}	μ_{a_1}	μ_{a_2}	μ_{a_3}	μ_{a_4}	μ_{a_5}	Burn-in Period (Iterations)	Effective Length (Iterations)
$N = 3$	0.002	0.014	0.04	N/A	N/A	N/A	1.0×10^5	2.0×10^6
$N = 4$	0.002	0.014	0.048	0.08	N/A	N/A	4.0×10^5	8.0×10^6
$N = 5$	0.002	0.020	0.064	0.12	0.14	N/A	4.0×10^6	1.16×10^8
$N = 6$	0.002	0.020	0.064	0.12	0.15	0.18	2.0×10^7	5.0×10^8

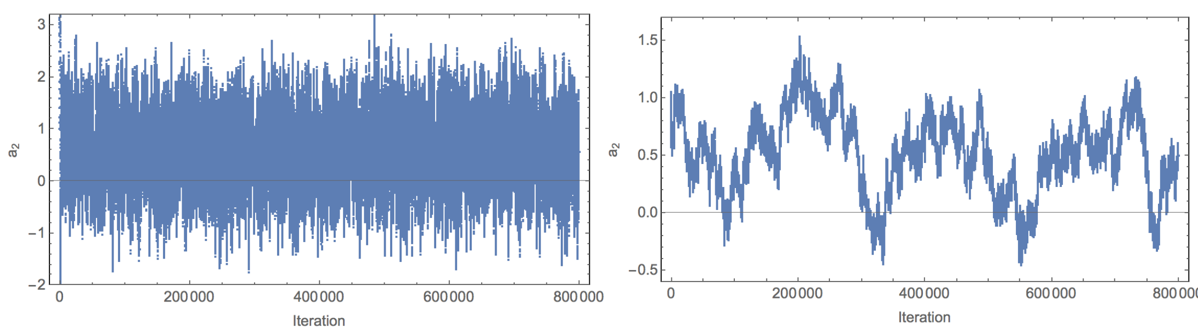
The goodness of fit after making a certain step was evaluated to determine the acceptance of that step. As mentioned before, χ^2 is computed to determine the goodness of fit of a particular fitting polynomial. A key feature of MCMC is that a better fit will always be accepted, but it a worse fit may be accepted by utilizing a probability function. In addition, a slightly worse fit to observational data will have a higher chance of being accepted than a much worse fit. This allows the program to explore the parameter space without being diverted too far away, unless it finds a better solution elsewhere. To achieve these goals, a likelihood function that evaluates the probability of acceptance based on these principles needed to be introduced. The study originally utilized a χ^2 cumulative probability distribution function as its likelihood function, but it was later observed unable to effectively converge the MCMC simulation because it is not sensitive enough for the tiny steps made in many circumstances. Simulated annealing (Khachaturyan, Semenovsovskaya, & Vainshtein, 1981) was also attempted but that method does not produce a probability distribution but only locates the best-fit value. Considering the unknown nature of the parameter being studied, it is more important to obtain a probable range and the standard deviation than prematurely conclude an absolute parameter value. Therefore, the variation of a widely used likelihood function was introduced (Berg & Billoire, 2008):

$$\mathcal{L} = e^{-\left(\chi^2_{new} - \chi^2_{old}\right)} \tag{5}$$

If $\mathcal{L} \geqslant 1$, this implies that $\chi^2_{new} - \chi^2_{old} \leqslant 0$, thus the new fit matches with the observational data better than the old fit. However, if $\mathcal{L} < 1$, a uniformly distributed random number r in the interval

$[0, 1)$ will be generated and compared to $\mathcal{L}$. If $\mathcal{L} > r$, movements made in this iteration would be accepted; otherwise, it will be rejected and the program will try to make another random step. This method of comparison ensures that a slightly worse fit, whose $\mathcal{L}$ is closer to 1, will have a higher chance of acceptance than a fit that is much worse, whose $\mathcal{L}$ is farther from 1.

Once the MCMC simulation is running, the next decision would naturally be to determine what length of MCMC is sufficient to obtain the best-fit value of the cosmographic parameters, also known as convergence diagnostics. To determine the burn-in period length and the convergence of a MCMC algorithm, a method often used is visual inspection that involves observing the chain's movement and performance in the parameter space, also known as mixing (Cowles & Carlin, 1996). To determine the overall convergence of a MCMC algorithm, every coefficient has to be individually inspected. By examining the values of a coefficient throughout the MCMC algorithm, it can be determined whether the chain is stuck in certain areas or wandering too much, indicating bad mixing, or the chain is moving around well. Examples of good and bad mixing are given below, using a_2 data from $N = 4$ simulations.



(a) Good mixing **(b)** Bad mixing

Figure 1: Illustrations of Markov chain mixing generated by MCMC using $N = 4$ coefficients in the testing stage (program configured differently from the program used to produce results discussed below).

3 Results & Discussion

3.1 Overview

In this study, Markov chain Monte Carlo (MCMC) simulations were done to fit Taylor polynomials to the SNe1a data. In order to achieve more accurate results by using more terms in the Taylor polynomials, and to test the effect on model-building uncertainties, the MCMC simulations were conducted under eight different conditions. Results discussed here are from simulations that successfully converged with good mixing discussed before. As noted before, all MCMC simulations have a burn-in period of different length for each parameter to wander around in the parameter space and find the optimal area for each of them. In order to present an accurate depiction of their probability distributions and values, the burn-in period for each simulation was excluded from all histograms and analysis presented here.

Ideally, the entire simulation should be considerably longer than the burn-in period, thus making the results more reliable and less influenced by the decision of burn-in period (Lim, 2015). In this study, the burn-in period for every simulation was verified to be less than 5% of its respective length. After obtaining the median polynomial coefficients, the optimal cosmographic parameters were computed by inverting the Hubble series. Using $\ln\{[d_L(y)/y]\}$ as an example here, the following can be obtained by comparing Equation 2 and 3 (Bochner *et al.*, 2015):

$$H_0 = ce^{-a_0} \tag{6}$$

$$q_0 = 3 - 2a_1 \tag{7}$$

$$j_0 = -6a_2 + \frac{1}{4}(17 - 2q_0 + 9q_0^2) \tag{8}$$

Moreover, combining the Friedmann Robertson-Walker acceleration equation and definition of q_0 ($q_0 \equiv -(\ddot{a_0}/a_0)H_0^{-2}$), one can obtain:

$$w_0 = \frac{1}{3}(2q_0 - 1) \tag{9}$$

where w_0 refers to the total effective equation of state of all cosmic contents.

Eight simulations shown here are categorized by the number of coefficients used in the fitting polynomial and the type of distance fitting functions. For convenience of discussion, the notation "P_X^N" is defined to denote the MCMC median values of cosmological parameter "P_0" ($P \in \{H, q, w, j\}$) using N coefficients in the Taylor polynomial fit ($N \in \{3, 4, 5, 6\}$) to distance scale function $d_{``X"}(y)$ ($d \in \{L, A\}$). For instance, $H_L^3 = 69.766$ represents the estimated median value of H_0 using luminosity distance function with $N = 3$ coefficients. Furthermore, "ΔC^N" represents the magnitude of the difference between median values of two functions using the same number of terms in the Taylor polynomials; hence, $\Delta H^3 = |H_L^3 - H_A^3| = |69.766 - 70.292| = 0.526$.

The peak and optimal range of each cosmological parameter presented in Table 2 are determined empirically through analyzing the value of each iteration sorted in ascending order. Peaks are the medians of their respective distributions. The optimal range of each parameter is defined as from -1σ to $+1\sigma$ from the median. Since the distribution is not necessarily Gaussian, the standard deviation is taken empirically by finding the values at -1σ (15.866 percentile) and $+1\sigma$ (84.134 percentile) in the sorted data and measuring their distances to the median of their distribution.

As can be seen from Table 2, the peak and the optimal range of each resulting cosmological parameter significantly depend on N. H_0 has demonstrated overall statistical consistency across all distance scale functions and numbers of fit terms. In addition, the H_0 values are also overall consistent with previous astronomical estimates done by *Hubble Space Telescope* and *WMAP* spacecraft ($H_0 = 69.32 \pm 0.80$) (Bennett *et al.*, 2014; Riess *et al.*, 2016). However, as shown in Figure 2, q_0 and j_0 have much more variability between different N and different fitting functions used. For instance, $\Delta j^3 = 6.639$, rendering it inconclusive for determining the precise value of j_0. Because of the overwhelming size of this model-building uncertainty, the value from $N = 3$ is far from consistent enough to confidently determine the existence of Λ.

Table 2: Medians and standard deviations of cosmological parameters value computed using SCP Union2.1 Supernova compilation ($N_{SNe} = 580$). Values of w_0 presented are converted from q_0 using Equation 9, since it is not an optimizable parameters in this MCMC algorithm. χ^2 values are computed by recreating fitting polynomials using median values of fitting coefficients and compare the polynomials with real SNe1a data using Equation 4. Ideal χ^2 values should be slightly smaller than the sample size (i.e. 580 supernovae).

Distance Scale	N	H_0	q_0	w_0	j_0	χ^2
d_L	3	$69.766\pm^{0.368}_{0.359}$	$-0.399\pm^{0.114}_{0.114}$	$-0.599\pm^{0.076}_{0.076}$	$-2.022\pm^{0.984}_{0.937}$	563.021
d_A	3	$70.292\pm^{0.363}_{0.367}$	$-0.799\pm^{0.105}_{0.110}$	$-0.866\pm^{0.070}_{0.073}$	$4.617\pm^{1.153}_{1.046}$	563.114
d_L	4	$70.026\pm^{0.478}_{0.476}$	$-0.615\pm^{0.262}_{0.262}$	$-0.743\pm^{0.175}_{0.175}$	$2.037\pm^{4.656}_{4.366}$	562.471
d_A	4	$69.906\pm^{0.474}_{0.469}$	$-0.483\pm^{0.255}_{0.259}$	$-0.655\pm^{0.170}_{0.173}$	$-1.480\pm^{4.439}_{4.112}$	561.980
d_L	5	$69.382\pm^{0.650}_{0.640}$	$0.106\pm^{0.556}_{0.557}$	$-0.263\pm^{0.371}_{0.371}$	$-17.611\pm^{13.749}_{12.423}$	561.304
d_A	5	$69.408\pm^{0.649}_{0.638}$	$0.073\pm^{0.548}_{0.564}$	$-0.285\pm^{0.365}_{0.376}$	$-16.403\pm^{14.054}_{12.333}$	561.339
d_L	6	$69.087\pm^{0.855}_{0.857}$	$0.518\pm^{1.011}_{0.978}$	$0.012\pm^{0.674}_{0.652}$	$-32.263\pm^{33.077}_{30.487}$	561.238
d_A	6	$69.081\pm^{0.894}_{0.891}$	$0.537\pm^{1.045}_{1.021}$	$0.025\pm^{0.697}_{0.681}$	$-33.223\pm^{34.099}_{30.732}$	561.259

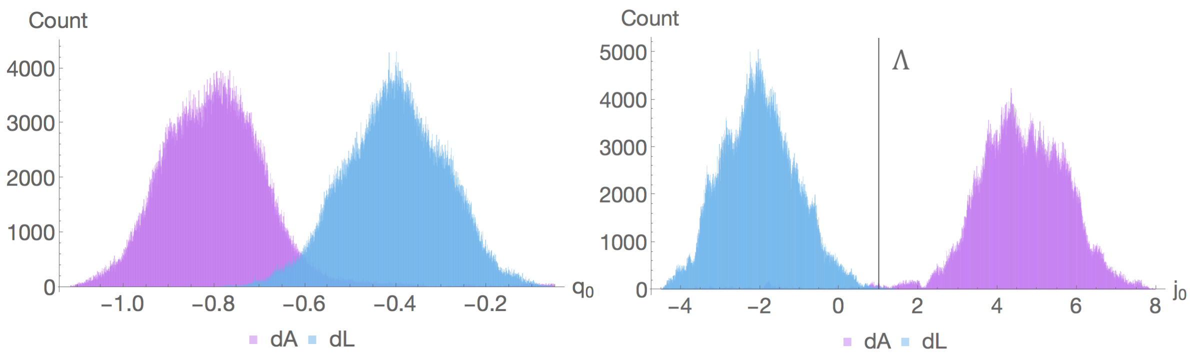
At the same time, $N = 6$ cases produce a much more stable result of $\Delta j^6 = 0.960$, which is much more reliable than $N = 3$ cases. However, a problem with using more fitting parameters is the significant increase of statistical uncertainties in each resulting cosmographic parameters. Nonetheless, MCMC algorithms can yield results with much smaller model-building uncertainties and statistical uncertainties (up to 36%) across all parameters compared a to previous cosmographic study using Union2.1 compilation (Bochner *et al.*, 2015).

3.2 $N = 3$ Results

The overall estimations of the Hubble constant are very consistent with previous measurements from the *Hubble Space Telescope* and *WMAP* spacecraft (Bennett *et al.*, 2013; Riess *et al.*, 2016), regardless of the distance scale function or the number of terms used in the fitting polynomial. The value of H_0, however, only tells the current rate of expansion but not any trend. Therefore, it is not related to any other cosmological parameters and it does not determine any property of dark energy. Nevertheless, determining H_0 can be used as an indicator of one MCMC's performance, since its value are very well determined. Observing a very consistent H_0 in this study allowed for concluding values of other parameters of interest with greater validity and confidence.

The deceleration parameter q_0 of $N = 3$ cases shows the biggest model-building uncertainty of all q_0 results with the net difference Δq^3 equals to 0.400. As demonstrated in Figure 2a, both distributions are roughly symmetrical. However, their values are radically different with hardly any overlap in the middle. The results of q_0 determination are inconclusive since two equally trusted models produced drastically different results. This model-building uncertainty renders citing an appropriate q_0 value from $N = 3$ simulation impossible.

The results of the jerk parameter j_0 under $N = 3$, as in Figure 2b, is also inconclusive. Though standard deviations of j_0 is small, the results are internally inconsistent. Recall that in order to for Λ be valid, $j_0 = 1$ must be true for all times. However, the median values are on two sides of $j_0 = 1$ and are almost equally far from Λ. Since $j_0 \equiv \dddot{a}_0/a_0$, this means the result from d_L is suggesting cosmic acceleration is slowing down while that of d_A suggests it is speeding up. In both distributions, Λ is more than 3σ away from the median. Furthermore, though the distributions of j_0 are somewhat symmetrical, j_L^3 and j_A^3 have almost no overlap, making it almost impossible to determine the true optimal value of j_0. Overall, though $N = 3$ case can estimate values of H_0 well, the model-building uncertainty renders it worthless to determine q_0, j_0, and the exact nature of the current state of cosmic expansion.



(a) q_L^3 and q_A^3 **(b)** j_L^3 and j_A^3

Figure 2: Histograms of q^3 and j^3 distribution generated by MCMC using $N = 3$ coefficients. The vertical line in j_0 histograms show the value of Λ.

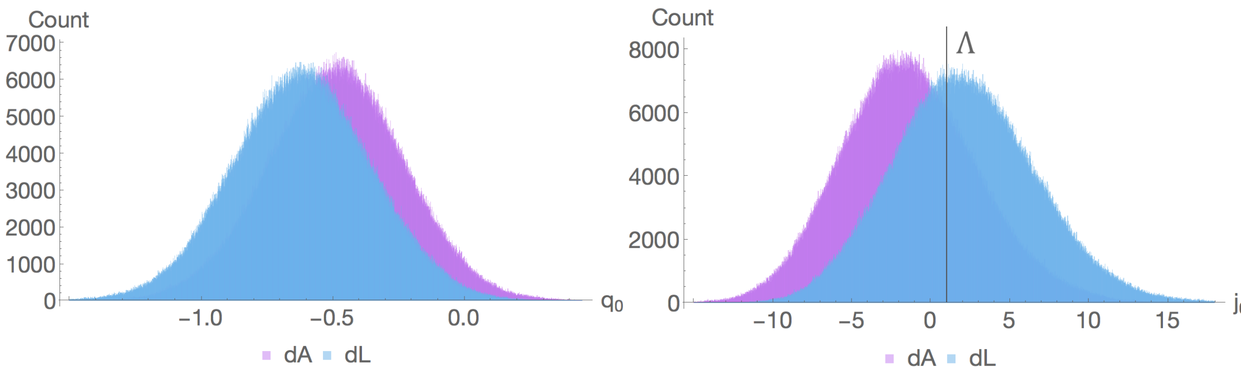
3.3 $N = 4$ Results

The results from $N = 3$ cases perfectly reveal the dilemma of attempting to estimate the jerk parameter j_0 with relative accuracy. If only $N = 3$ cases are studied, both $j_0 = -2.022\pm^{0.984}_{0.937}$ from $\ln\{[d_L(y)/y]\}$ and $j_0 = 4.617\pm^{1.153}_{1.046}$ from $\ln\{[d_A(y)/y]\}$ can be quoted to support two directly opposite theories. The model-building uncertainty of $N = 3$ cases is so large that it is inconclusive. By adding another fitting parameter to the fitting polynomial, though it is not used in calculating any of the cosmographic parameters, the model-building uncertainty is significantly reduced. In $N = 4$ simulations, the distributions of H_0 overlap more with each other due to the reduced model-building uncertainty ($\Delta H^4 = 0.120$ compared to $\Delta H^3 = 0.526$). By adding fitting parameter to higher N, the standard deviations increased while the model-building uncertainty decreased. Nonetheless, the results of H_0 stay consistent with prior measurements.

The deceleration parameter q_0 from $N = 4$ cases shows an indication of converging from results in $N = 3$ cases toward $q_0 \approx -0.5$, as shown by comparing Figure 2a with Figure 3a. The model-building uncertainty is greatly reduced from $\Delta q^3 = 0.400$ to $\Delta q^4 = 0.132$, while the statistical standard deviations increased as expected. The distributions of q_0, as can be seen in Figure 3a, are much smoother but still somewhat bimodal. Since w_0 value is computed by performing operations directly on q_0 value, it would possess similar statistical characteristics. Both q_0 and w_0 from $N = 4$ confirms that the universe is accelerating expanding ($q < 0$) and if dark energy exists as Λ, it should contribute to around 70% of total mass-energy, which is consistent with results from the

Planck spacecraft and *WMAP* nine-year mission ($\Omega_\Lambda = 0.7135\pm^{0.0095}_{0.0096}$) (Bennett *et al.*, 2013; Planck Collaboration *et al.*, 2014).

The jerk parameter j_0 of $N = 4$ simulations show similar patterns as expected. The net difference of model-building uncertainty Δj^4 halved compared to Δj^3. At the same time, as shown in Figure 3b, the distributions of j_0 is a lot smoother and wider compared to those in Figure 2b. Though the values are still on two sides of $j_0 = 1$, they are considerably closer to each other. Although the overall pattern is still somewhat bimodal, but at least the model-building uncertainty is much smaller than each distribution's statistical uncertainty.



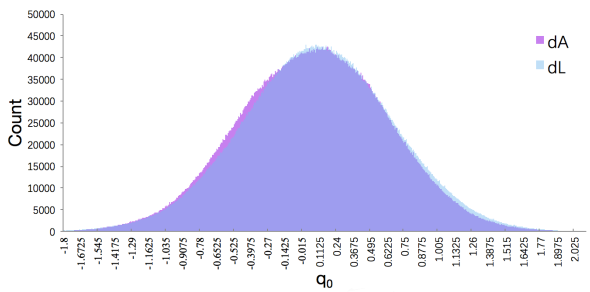
(a) q^4_L and q^4_A **(b)** j^4_L and j^4_A

Figure 3: Histograms of q^4 and j^4 distribution generated by MCMC using $N = 4$ coefficients.

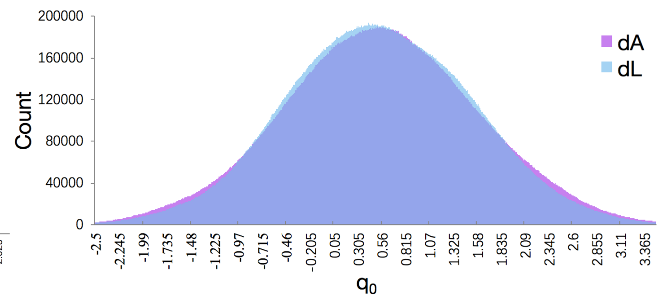
3.4 Large-N Cosmographic Results

Motivated by the observed trend of decreasing model-building uncertainty, we then moved on to perform MCMC using as many optimizable parameters as possible. However, once the MCMC was run for $N = 5$ and higher cases, an interesting feature was noticed. Typically, every time a new optimizable coefficient was added into the fitting polynomial, the MCMC algorithm runtime in terms of iterations will grow by a factor of 4-5 times (as can be seen in Table 1, from $N = 3$ to $N = 4$ and from $N = 5$ to $N = 6$). However, in the case of $N = 4$ to $N = 5$, the runtime necessary for MCMC to yield useful results grew 15 times. In addition, though the median values of H_0 still remained consistent with previous studies, values of q_0 and j_0 make little physical sense in the current universe. This raises the question of how many coefficients can be reliably optimized.

As can be seen in Figure 4a and 4b below, for $N = \{5, 6\}$, peak q_0 values are greater than 0 and consequently peak w_0 values are greater than $-1/3$. Recall the definition of $q_0 \equiv -(\ddot{a}_0/a_0)H_0^{-2}$, these peak values imply that the cosmic expansion is not even accelerating anymore. In addition, one extreme case of w_0, $w_A^6 = 0.025\pm^{0.697}_{0.681}$, presents a value that is even greater than $w_0 = 0$, which, according to Friedmann Robertson-Walker acceleration equation, indicates a universe dominated by matter. When median values of q_0 and j_0 distributions are examined together, the positive q_0 and very negative j_0 seem to suggest an alternative theory that current dark energy was rather weak, but because of the very negative j_0 value, the dark energy has recently become more powerful (i.e. asserts greater repulsive force) and rapidly accelerates the cosmic expansion.

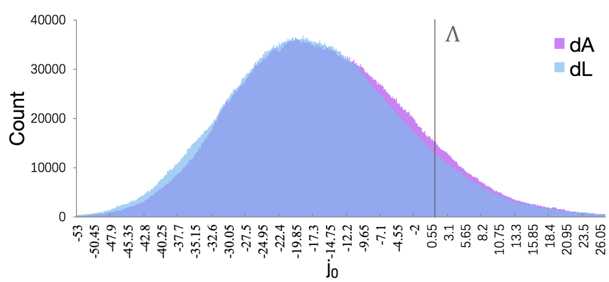


(a) q_0 in $N = 5$ cases

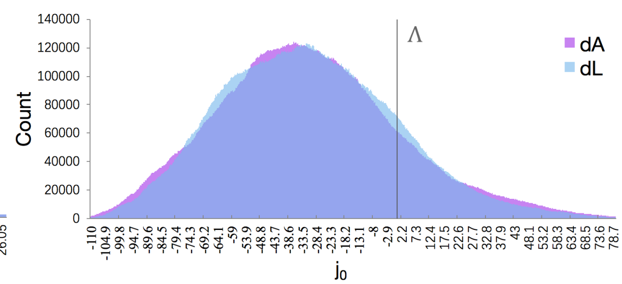


(b) q_0 in $N = 6$ cases

Figure 4: Distributions of q_0 in large-N cases generated by MCMC using $N = 5$ and $N = 6$ coefficients.



(a) j_0 in $N = 5$ cases



(b) j_0 in $N = 6$ cases

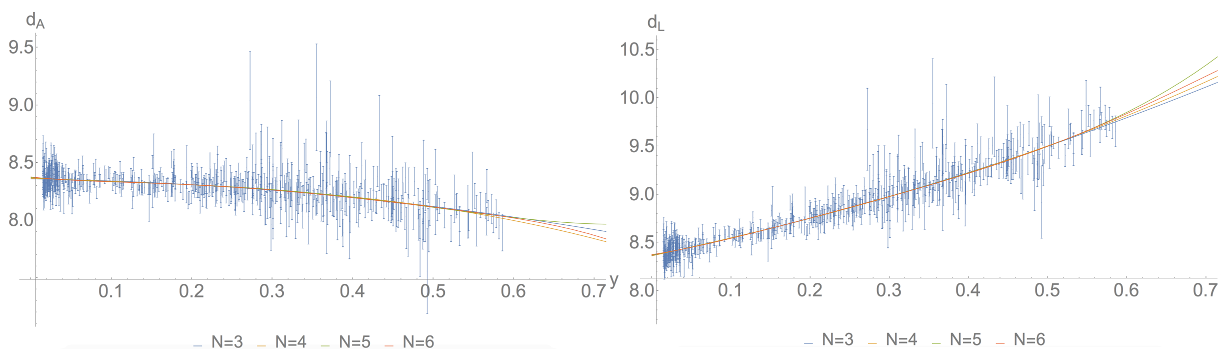
Figure 5: Distributions of j_0 in large-N cases generated by MCMC using $N = 5$ and $N = 6$ coefficients.

An important note to take away from $N = 5$ and $N = 6$ simulations is that even though they present rather odd peak values, they are actually not statistically inconsistent with values from other studies or ΛCDM model. More specifically, their distributions have very large statistical standard deviations due to the inherent limitation of original SNe1a data's statistical power. All results here are only around 1σ away from the requirement of Λ, $j_0 = 1$. Nonetheless, despite the overall statistical consistency of $N = \{5, 6\}$ with Λ and its relative immunity to model-building uncertainty, the constraint on the range of q_0 and especially j_0 is robust but weak.

More importantly, even though the large-N simulations produced rather large standard deviations, at the same time they are able to mostly eliminate model-building uncertainty in the distributions. In Figure 4 and 5, the d_L and d_A distributions almost completely overlap each other. This observation allows us to conclude the probable range of cosmological parameters with much greater confidence. However, considering the purpose of eliminating model-building uncertainty, it is not necessary to increase the fitting parameter N from 5 to 6. Although $N = 3$ and $N = 6$ simulations have little benefit, both $N = 4$ and $N = 5$ simulations have their own merits: $N = 4$ analysis produces rather tight constraint with some model-building uncertainty, while $N = 5$ has almost no model-building uncertainty and somewhat larger statistical uncertainty. Though $N = 4$ can be used to yield usable values of cosmological parameters, it is much more preferable to utilize at least $N = 5$ if good enough data is available to reduce statistical uncertainty.

3.5 Overall Cosmographic Fit

Graphical demonstrations of polynomial fits in Figure 6 are done to examine the overall quality of fits with peak parameter values. Overall, all fits performed are closely fitted to real SNe1a data based on their small χ^2 value, as shown in Table 2. The χ^2 values indicate that as N increases, χ^2 does slightly decrease, meaning a better fit was obtained, but this fit is not yet able to tightly constrain the exact value due to the limited statistical power of the SNe1a data. The variations in χ^2 values also confirm that hardly any benefit is gained from performing $N = 6$ instead of $N = 5$ fits, since the χ^2 values only decreased very slightly.



(a) Fitted using $\ln\{d_A(y)/y\}$. **(b)** Fitted using $\ln\{d_L(y)/y\}$.

Figure 6: All polynomial fits ($N = 3$ to $N = 6$) to SCP Union2.1 data in terms of both distance scale functions. Plots are generated using median values of each simulation's polynomial fitting coefficients (i.e. a_0, a_1, a_2, $\ldots$). Both plots are solely used to verify the overall fits to SNe1a data are good (Illustration by author).

Although the polynomial fitting is still plagued by the dilemma between model-building uncertainty in small-N cases and statistical uncertainty in large-N cases, this study demonstrates that large-N simulations can effectively eliminate model-building uncertainty while yielding results statistically consistent with Λ and other cosmographic studies. At the same time, compared to a previous study done using the same data under traditional statistical techniques, results of cosmological parameters presented here have slightly smaller model-building uncertainty and around 24% to 36% smaller statistical uncertainty (Bochner *et al.*, 2015), which is due to the implementation of MCMC in this study. Unlike the previous study, $N = 5$ simulations can be somewhat trusted due to the significantly reduced statistical uncertainties. The $N = 6$ fits, however, have too large statistical uncertainty to be reliable. The $N = 3$ fits are also inappropriate to produce constraint due to the model-building uncertainty, despite the production of the tighter constraint. The $N = 4$ fits are the most reliable options to generate constraint under these compromises. The constraint of j_0 using $N = 4$ takes into account its model-building and statistical uncertainty, which can be best expressed as $[(j^4_A - \sigma_{j_0,A}), (j^4_L + \sigma_{j_0,L})] = [(-1.480 - 4.112), (2.037 + 4.656)] = [-5.992, 6.693]$. This new range, obtained by MCMC algorithm, is roughly 21% smaller than range determined previously (Bochner *et al.*, 2015). Though the data is not precise enough yet to strongly test Λ, the consistency of $N = 4$ and $N = 5$ fits with $j_0 = 1$ does highlight the overall consistency of current dark energy with cosmological constant.

4 Conclusions and Future Research

In this study, a test of Λ was performed by looking for signs of deviation from $j_0 = 1$ based on the most useful data set that continuously traces the recent cosmic expansion—SCP Union2.1 compilation. The cosmographic approach allowed for studying the universe in a kinematic approach. Polynomial fitting was performed to observational data based on Taylor expansion and derived estimates of H_0, q_0, w_0, and j_0 from the fitting coefficients.

A key difficulty in fitting polynomials using a particular model is that it will be depended on the model due to series truncation. Too few parameters result in large model-building uncertainties, while too many parameters result in very large statistical uncertainties. Fittings were done using the two most different distance scales and four different numbers of optimizable coefficients to fully test the effects of uncertainties and to find a balance between them. Both $N = 4$ and $N = 5$ have their merits: one has smaller statistical uncertainty but larger model-building uncertainty, and the other one has exact opposite statistical characteristics. The most reliable constraint of j_0 yielded is $j_0 \sim [-5.992, 6.693]$, which is a tighter constraint than previous studies, though still not precise enough to completely confirm or disprove Λ. Nonetheless, this study demonstrated that even though limited by the statistical power of observational data, an improved methodology such as MCMC can significantly improve the estimation. The results presented here do certainly highlight the overall consistency with Λ.

This paper confirmed the model-dependence of cosmographic study and created suspicions about all cosmological studies in general when done in low-order data fitting (i.e. small number of fitting parameters). Therefore, it is imperative to include more than one model to verify the internal consistency of results yielded. However, as examined from our results, the adoption of MCMC in our coefficient optimization has essentially eliminated model-building uncertainty in $N = 5$ and above cases. In addition, the MCMC algorithms produced results across all cosmological parameters with significantly smaller statistical uncertainties and model-building uncertainties than previous study done with analytical best fits (Bochner *et al.*, 2015).

Furthermore, very smooth and Gaussian distributions were generated in most cosmological parameters distributions. Our results demonstrated the ability and value of the MCMC algorithm applied to the cosmographic method to produce much more reliable results than parameterizing dark energy using some not fully tested parameterization formula, such as the CPL Parameterization (Chevallier & Polarski, 2001). Through the cosmographic approach, no assumptions at all need to be made about the nature of dark energy, which thus reflects its behavior more objectively.

In the future, more Type Ia supernova data can be incorporated once they become available through upcoming NASA missions such as the *WFIRST*. Though Figure 6 shows high-redshift data is more necessary, all additional SNe1a data can potentially improve the precision of the results. Data from other sources can also be potentially integrated into the MCMC optimization. Although Cosmic Microwave Background is too distant to directly map the more recent cosmic acceleration, the Baryon Acoustic Oscillation and Gamma Ray Bursts can be used to study dark energy and cosmic expansion. Even gravitational wave events can possibly be used for this purpose, especially the most recent neutron star merger (GW170817) that are observed through electromagnetic waves in addition to gravitational wave (Abbott *et al.*, 2017). Some other mathematical functions such as logarithmic functions, potentially more suitable for fitting these data, may also be tested and implemented instead of polynomials.

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