Abstract. Many schemes have been proposed to perform a model-independent constraint on cosmological dynamics, such as nonparametric dark energy equation of state (EoS) $\omega(z)$ or the deceleration parameter $q(z)$. These methods usually contain derivative processes with respect to observational data with noise. However, it still remains remarkably uncertain when one estimates the numerical differentiation, especially the corresponding truncation errors. In this work, we introduce a global numerical differentiation method, first formulated by Reinsch(1967), which is smoothed by cubic spline functions. The optimal solution is obtained by minimizing the functional $\Phi(f)$. To investigate the potential of the algorithm further, we apply it to the estimation of the transition redshift $z_t$ with simulated expansion rate $E(z)$ based on observational Hubble parameter data (OHD). An effective method to determine the free parameter $S$ appearing in Reinsch Splines is provided.

Keywords: dark energy theory, cosmological phase transitions
1 Introduction

The central task of modern cosmology is to uncover the dynamic evolution and the geometric structure of the universe. According to plenty of cosmological observations, such as distant Ia supernovae (SNe Ia), cosmic microwave background (CMB) and so forth, the recent universe, dominated by the so-called dark energy, is undergoing accelerated expansion. The Lambda CDM model (ΛCDM) based on general relativity can provide consistent explanation with the observational data. Whereas, the nature of the dark energy still remains mysterious. In order to study the characteristics of the accelerated universe, many different methods have been proposed to free the limitation of the concrete cosmological models, e.g. the direct reconstruction of the equation of state (EoS) of dark energy $\omega(z)$ [1, 2] or the expansion rate and deceleration parameter $E(z), q(z)$ [3].

How to treat the numerical differentiation correctly is one common problem appearing in the above works. The accuracy of numerical differentiation of noisy observational data is difficult to control. It encompasses many subtleties and pitfalls that may cause large error in the actual computation. From the mathematical point of view [4], the derivative of a given function is obtained by infinitesimal calculus, it’s, however, impractical for real experimental data due to the discrete property. Additionally, for most cases, we must take the measured error or noise into consideration. An effective estimation of the derivative of noisy sample $y(x_i)$ with respect to the variable $x_i$ has to cope with these two restrictions.

To compute the numerical differentiation of a given sample without knowing the underlying function, typically one needs to obtain the approximation with some basic functions. Then one can hope that the derivative of the approximation is good enough to represent the actual situation. *Finite differences* is the general, but very crude method which works by fitting or interpolating on some sub-interval of the sample domain. If the boundary points of the sub-interval are very close, the subtraction of the two numbers will be ill-conditioned. It may render the final result meaningless. In addition, the optimal function obtained by such method is not smooth. As a result, it’s hard to represent the real world. Therefore, *finite differences* method may be a bad choice in many cases. Reinsch [5] developed another optimal algorithm to perform numerical differentiation with spline functions, here referred as Reinsch Splines. The method can overcome some difficulties arising from the *Finite differences*. The main task of the work is to analysis the Reinsch Splines and its practical potential on observational data. More detailed descriptions will be presented in the following sections.

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This paper is organized as follows: The fundamental algorithm of Reinsch Splines and the corresponding errors are furnished in Sec. 2. In order to investigate the potential of the algorithm, we apply the algorithm in Sec. 3 to estimate the transition redshift $z_t$ with simulated cosmological expansion rate $E(z)$ based on OHD. Finally, the brief summary and discussion will be given in Sec. 4.

2 Reinsch Splines Method

Reinsch Splines is first proposed by Reinsch [5] to replace strict interpolation by some kind of smoothing. The appropriate trial functions to estimate the experimental data is spline functions.

Given a sample $(x_i, y_i)$ ($i = 1, ..., n$) which satisfies that

$$x_1 < x_2 < ... < x_n,$$

then the problem can be stated as a special instance of Tikhonov regularization method, which is just to look for the minimum of the functional

$$\Phi(f) = \alpha \sum_{i=1}^{n} \left( \frac{y_i - f(x_i)}{\sigma_i} \right)^2 - S + \|f''(x)\|^2,$$

(2.1)

where $\sigma_i$ is the noise, $f(x)$ is the optimal square integrable function over the domain. $\|f''(x)\|$ denotes the $L^2$-norm

$$\|f''(x)\| = \left( \int_{x_1}^{x_n} f''(x)^2 \, dx \right)^{1/2}.$$

$S > 0$ is a given constant, allowing for an implicit rescaling of the quantities $\sigma_i$, which controls the extent of smoothing. If $\sigma_i$ is the estimate of the standard deviation of $y_i$, the value will lie within

$$n - \sqrt{2n} \leq S \leq n + \sqrt{2n}.$$  

(2.2)

It should be noted that $S$ is very sensitive to the experimental noise $\sigma_i$, sometimes the limitation must be relaxed, especially when the noise is crude, although the confidence interval of $S$ is accurate enough for small deviations. $\alpha$ is the Lagrangian parameter satisfying $d\Phi(f)/d\alpha = 0$ and $\alpha \neq 0$.

Hanke & Scherzer [6] provides a rigorously proof that the minimizer of equation (2.1) is a natural cubic spline. Following the notation of Reinsch [5], we express $f(x)$ as

$$f(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3,$$

(2.3)

where

$$x_i \leq x \leq x_{i+1}, i = 1, ..., n - 1.$$  

The spline functions satisfy specified smoothing and boundary conditions. But there is no need to agree exactly with the experimental data $y_i$ on the node $x_i$. Once we obtain the coefficients $a_i, b_i, c_i$ and $d_i$, the spline functions will be determined uniquely. A constructive
algorithm for calculating the splines has been given by Reinsch [5]. In the remaining part of
this section, we will focus on the error analysis of the Reinsch Splines.

Three sources of errors will impact the final evaluation of the numerical differentiation:
experimental errors resulting from individual data point, truncation errors between the optimal
$f'(x)$ and the true derivatives, and the rounding errors due to the narrow length of
sub-interval. It is precisely because of the existence of the rounding errors attributed to the
loss of significance of digits, finite differences fails to estimate the differentiation effectively.
Reinsch Splines, however, can overcome the embarrassment to some extent. The truncation
errors greatly dependent on the choice of the algorithm and the fitting accuracy. Hanke &
Scherzer [6] provides a formula of the truncation errors, and the rigorous proof can also be
found. Note that some slight adjustments should be done to match the Reinsch Splines,
though the correction is straightforward. As for the experimental errors, the propagation of
them is dealt with the conventional expression

$$
\sigma_m^2 = \sum_{i=1}^{N} \sigma_i^2 \left( \frac{\partial m}{\partial y_i} \right)^2,
$$

where $m$ denotes the coefficients of the spline functions, and $N$ is the number of the points
of sub-interval.

3 Estimation of the Transition Redshift

Observations show that the universe has undergone a dynamic phase transition from
deceleration to acceleration expansion which leads to the change of the sign of deceleration
rate $q(z)$. The transition redshift $z_t$ has profound impact on the evolution of the universe.
Different groups have measured $z_t$ with SN Ia, BAO and CMB observations [7, 8]. In or-
der to constrain $z_t$ model-independently, various parametric expressions of $q(z)$ have been
presented. Such parametric expressions e.g. $\omega(z)$ and $q(z)$, are extremely convenient
and effective for cosmological research. But the situation will remarkably change if one introduces
the nonparametric forms of them. Just as we have mentioned, derivative calculations often
appear in these expressions. Therefore the first difficulty must to be solved is the accurate
estimation of the numerical differentiation with noise observational sample.

Recently, observational Hubble parameter data (OHD) $H(z)$ has obtained many atten-
tions on the constraint of cosmological parameters [9–11]. Ma & Zhang [12] and Zhang et
al. [13] have summarized the power and potential of OHD from statistical point of view.
At present, there are total about 28 independent measurements of $H(z)$, which are listed in
table 1.

The relation between transition redshift and $H(z)$ can be written as

$$
z_t = \left[ \frac{1}{H(z)} \frac{dH(z)}{dz} \right]_{z=z_t}^{-1} - 1.
$$

Obviously, the technique of numerical differentiation needs to be used to determine $z_t$ if
$H(z)$ sample is available. Unfortunately, unlike the SN Ia dataset, the recent OHD are too
penurious to provide valuable estimation of the transition redshift using such method. There
are some other reasons that make it invalid. The apparent uncertainty of the existing $H(z)$
will greatly increase the possibility of failure. Moreover, sparse sample will lead the optimal
functions to deviate the actuality seriously, as well as the corresponding differentiation. Lima
et al. [14] suggests three different means to obtain $H(z)$, so it is expected that such embarrassments could be overcome by ongoing and future observations to expand the volume of the sample.

3.1 Simulated $E(z)$

To extend the applications of OHD further and test the Reinsch Splines, a simulated sample of $H(z)$ will be helpful. Further, from equation (3.1) the dimensionless expansion rate $E(z)$, defined as $H(z)/H_0$, will be a better choice for the present analysis. Therefore, we will concentrate on the technique of generating a sample of $E(z)$, named as simulated-$E(z)$, in this section. Our simulation is based on the spatially flat $\Lambda$CDM model with $\Omega_m = 0.28$ and $\Omega_\Lambda = 0.72$. A Gaussian prior $H_0 = 74.2 \pm 3.6$ km·s$^{-1}$·Mpc$^{-1}$ suggested by Riess et al. [15] is adopted. The expansion rate $E(z)$ in the fiducial model can be written as

$$E_{fid}(z) = \sqrt{\Omega_m(1+z)^3 + \Omega_\Lambda}. \quad (3.2)$$

Based on the OHD listed in table 1 and equation (2.4), we can obtain the ‘observational’ expansion rate, denoted as derived-$E(z)$, and the corresponding error.
Figure 2. The model of $\sigma_{\text{sim}}(z)$. The circles represent the derived-$E(z)$ sample where the solid ones are chosen to fit the up- and down-edge. The solid line is the midline of the two edges.

The simulated-$E(z)$ sample should take the fiducial model value $E_{\text{fid}}$ as its expectation and follow the same systematic information and characteristic of the derived-$E(z)$. However, this goal is so difficult to reach, because we have quite a few real data points and almost little knowledge about the derived-$E(z)$, e.g. the distribution of the data points along the redshift-axis. Therefore, our $E(z)$ simulation includes the following two procedures:

The offset estimation $\varepsilon(z)$: To generate the simulated-$E(z)$ sample at any given redshift point, we introduce the variable $\varepsilon(z)$ satisfying

$$E_{\text{sim}}(z) = E_{\text{fid}}(z) + \varepsilon(z), \quad (3.3)$$

which represents the offset between the fiducial value and simulation at given $z$. In order to make $\langle E_{\text{sim}} \rangle = E_{\text{fid}}$, $\varepsilon(z)$ should be a random variable with respect to $z$.

Defining the offset $\hat{\varepsilon}(z) = E_{\text{der}}(z) - E_{\text{fid}}(z)$ whose absolute value is shown in figure 1. Assuming that there is no bias on the sign of it, then we can make the offset satisfy $|\hat{\varepsilon}(z)| \leq E(z)\eta$ for most derived-$E(z)$ points, where $\eta$ is a constant. The best estimate value of $\eta$ is 0.1320. From figure 1 we see that the offset curve covers most of the points of interest, ignoring only three points with extraordinary deviation. As a result, we can denote

$$\varepsilon_{\pm}(z) = \pm E_{\text{fid}}(z)\eta (\eta = 0.1320)$$
Table 1. The currently known observational Hubble parameter data. The latest four data points from Zhang et al. [16] are added. However, we do not include them to perform the simulation because of the remarkable uncertainty and the existing dense data points with relatively small deviations at low redshift.

| redshift $z$ | $H(z)$ ($km \cdot s^{-1} \cdot Mpc^{-1}$) | $\sigma_{H(z)}$ ($km \cdot s^{-1} \cdot Mpc^{-1}$) |
|-------------|---------------------------------|---------------------------------|
| 0.090       | 69                              | 12[17]                          |
| 0.170       | 83                              | 8[17]                           |
| 0.270       | 77                              | 14[17]                          |
| 0.400       | 95                              | 17[17]                          |
| 0.900       | 117                             | 23[17]                          |
| 1.300       | 168                             | 17[17]                          |
| 1.430       | 177                             | 18[17]                          |
| 1.530       | 140                             | 14[17]                          |
| 1.750       | 202                             | 40[17]                          |
| 0.480       | 97                              | 62[18]                          |
| 0.880       | 90                              | 40[18]                          |
| 0.179       | 75                              | 4[19]                           |
| 0.199       | 75                              | 5[19]                           |
| 0.352       | 83                              | 14[19]                          |
| 0.593       | 104                             | 13[19]                          |
| 0.680       | 92                              | 8[19]                           |
| 0.781       | 105                             | 12[19]                          |
| 0.875       | 125                             | 17[19]                          |
| 1.037       | 154                             | 20[19]                          |
| 0.24        | 79.69                           | 3.32[20]                        |
| 0.43        | 86.45                           | 3.27[20]                        |
| 0.44        | 82.6                            | 7.8[21]                         |
| 0.60        | 87.9                            | 6.1[21]                         |
| 0.73        | 97.3                            | 7.0[21]                         |
| 0.07        | 69.0                            | 19.6[16]                        |
| 0.12        | 68.6                            | 26.2[16]                        |
| 0.20        | 72.9                            | 29.6[16]                        |
| 0.28        | 88.8                            | 36.6[16]                        |

as the boundaries of the offset values of simulated expansion rate (see figure 1). As a random variable, $\varepsilon(z)$ follows the Gaussian distribution $N(0, \eta E_{fid}(z)/2)$ so that the probability of $\varepsilon(z)$ falling within the offset domain is 95.4%.

The uncertainty estimation $\sigma(z)$: There is an apparent trend of the errors of derived-$E(z)$: the uncertainty $\sigma_E(z)$ becomes larger as the increase of redshift $z$ except for two outliers at $z = 0.48$ and 0.88, as figure 2 shows. Ignoring the two points, we find the rest are right within the region between the lines

$$\sigma_+ = 0.2324z + 0.1365, \quad \sigma_- = 0.1091z + 0.0393.$$
And the midline between the two boundaries is
\[ \sigma_m = \frac{1}{2} (\sigma_+ + \sigma_-), \]
which represents the expectation value of the uncertainty \( \sigma_{sim} \) of the simulated expansion rate. Meanwhile, we make the \( \sigma_{sim} \) follow a Gaussian distribution \( N(\sigma_m(z), \rho(z)) \) at any given redshift, where
\[ \rho(z) = \frac{\sigma_+ - \sigma_-}{4} \]
ensuring that the simulated uncertainty \( \sigma_{sim} \) falls within the region between lines \( \sigma_+(z) \) and \( \sigma_-(z) \) with the probability of 95.4%.

According to the above two procedures, the method of generating a simulated \( E(z) \) sample is completed. First of all, we can calculate the fiducial values \( E_{fid}(z) \) from equation (3.2). A random variable \( \varepsilon(z) \) can be drawn from a Gaussian distribution, so the \( E_{sim}(z) \) is generated via equation (3.3) at a given \( z \). Finally, the corresponding uncertainty \( \sigma_{sim}(z) \) is also estimated through another Gaussian distribution. Some similar but different techniques have also been proposed by Ma & Zhang [12] and Wang & Zhang [22] to simulate OHD. Figure 3 shows the final simulation which contains total 256 data points ranging from \( 0.001 \leq z \leq 2.0 \), as well as 24 derived-\( E(z) \).

3.2 Numerical Results
In this section, the Reinsch Splines is applied to estimate the transition redshift with the simulated expansion rate \( E(z) \).

In order to obtain the optimal function \( f(x) \) defined as equation (2.3), we need to minimize the functional \( \Phi(f) \) (see equation (2.1)). For such noisy data, constant \( S \) plays an important role. A proper choice of the constant will substantially boost the fitting accuracy of numerical differentiation. If the underlying function to be fitted is known, the classical least-squares fitting can be used. But how to determine it without any model information, just as the model-independent tests in cosmology, and how to judge whether the chosen \( S \) can approach the real situation remain to be solved. The general practice is to set \( S \approx n \) which satisfies equation (2.2). It works fairly well when we test the method on different analytic functions with small errors. An example can also be seen Reinsch [5]. But it fails for our simulated sample because of the significant errors of \( E(z) \)!

One possible estimation of \( S \) here we introduce is to minimize
\[ \eta = \sum_{i=1}^{n-1} ||v_{i+1} - v_i||, \tag{3.4} \]
where \( v_i = (x_i, f'(x_i)) \). With this condition, we can make the numerical differentiation as smooth as possible. However, the criterion can merely ensure local smoothing. In other words, the global oscillations or undulations due to the accuracy of Reinsch Splines can not be determined by equation (3.4). In most cases, we hope that the number of times such oscillations or undulations happen should be as little as possible. One convenient way is to calculate the number of the extremum values \( N_e \) when different \( S \) is given. We can find \( N_e \) using the general definition of extremum on mathematics. Equivalently, it can be determined
through the 'nodes', corresponding to the locations of extremum or inflection points, in the region of errors, just as figure 4 shows. Utilizing the two criterions, the constant $S$ can be evaluated uniquely. In this work, the best value is $S = 76.97$.

Once $S$ is fixed, the optimal $f(x)$ can also be obtained with the algorithm presented in section 2. Figure 4 illustrates the final numerical results. The best estimate of the transition redshift is $z_t = 0.69^{+0.06}_{-0.14}$ which is moderately consistent with the observational and theoretical results. Note that we just take the statistical errors and truncation errors into consideration due to the rounding errors are negligible in our sample. Furthermore, from figure 4, we see that there are large deviations of the boundary ascribed to the selection of the boundary conditions in Reinsch Splines. However, a different version of the boundary conditions based on physical facts or some prior knowledge may be helpful to overcome the problem.

4 Conclusions

In the present work, we introduce a general numerical differentiation referred as Reinsch Splines, and preliminarily apply it to the analysis of the transition redshift $z_t$ with simulated expansion rate $E(z)$. By comparing the difference between the model value of $z_t$ and the
Figure 4. The determination of the transition redshift using simulated $E(z)$. The error bar contains both statistical errors and truncation errors. The transition redshift $z_t \sim 0.69$ estimated using Reinsch Splines. The 'nodes' showing in the region of errors correspond to the locations of extremum or inflection points of the differentiation.

estimation, some experimental characteristics of the Reinsch Splines are unfolded. The determination of constant $S$ is essential to approach the optimal $f(x)$, and we provide an effective recipe to evaluate it when the experimental error $\sigma$ is significant. Meanwhile, Reinsch Splines can also be applied to reconstruct the nonparametric dark energy equation of state $\omega(z)$ with recent supernova data. Some different techniques have been provided by Clarkson & Zunckel [1] and Holsclaw et al. [2]. By contrast, Reinsch Splines will generalize the procedures of numerical differentiation and reduce the artificial uncertainty.

The accuracy of the Reinsch Splines still remains to improve to extend its applications. One feasible method is to relax the boundary conditions when constructing the optimal spline functions $f(x)$. In addition, the errors resulting from the numerical differentiation should be dealt with carefully, and need further discussion, especially the truncation errors and rounding errors.

Acknowledgments

Liu De-Zi would like to thank Jiang Peng-Xu for his kindly help. This work was supported by the National Science Foundation of China (Grants No. 11173006), the Ministry of Science and
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