A Regularized Free Form Estimator for Dark Energy

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ABSTRACT
We construct a simple, regularized estimator for the dark energy equation of state by using the recently introduced linear response approximation. We show that even a simple regularization substantially improves the performance of the free form fitting approach. The use of linear response approximation allows an analytic construction of maximum likelihood estimator, in a convenient and easy to use matrix form. We show that in principle, such regularized free form fitting can give us an unbiased estimate of the functional form of the equation of state of dark energy. We show the efficacy of this approach on a simulated SNAP class data, but it is easy to generalize this method to include other cosmological tests. We provide a possible explanation for the sweet spots seen in other reconstruction methods.

Key words: cosmology:theory – methods: statistical –cosmological parameters.

1 INTRODUCTION
One of the most exciting discovery of the last decade is the possibility that the expansion of our Universe is accelerating (Perlmutter et al. 1999; Riess et al. 1998). The simplest explanation in terms of a cosmological constant runs into to a fine tuning problem (Sahni & Starobinski 2000; Peebles & Ratra, 2002; Padmanabhan, 2002). Therefore, it has become popular to phenomenologically model the component that drives the acceleration as an ideal fluid with an equation of state given by $P = w\rho$, where the equation of state parameter $w$ is allowed to vary with time. In this parameterization the cosmological constant model corresponds to $w = -1$. In the recent years there has been a considerable interest in devising methods to extract information about the equation of state from the present and the future cosmological data.

In principle, since this information is coded directly into the distance (luminosity and angular) measures, it is possible to directly obtain $w(z)$ from the supernovae distances (Starobinsky, 1998). This requires the knowledge of up to a third derivative of noisy estimate of the distance measures with respect to the redshift. This makes such direct estimation extremely noisy. Methods based on flexible fitting functions (Saini et al. 2000; Nakamura & Chiba 2001) for the luminosity distance have been invoked to get around this problem. In such schemes the number of parameters in the fitting function is kept small, therefore, the allowed behaviour of the equation of state is restricted by the adoption of specific forms for the fitting functions. Other popular methods approximate the dark energy density or the unknown function $w(z)$ as low order polynomials (Sahni et al. 2002; Weller & Albrecht, 2002). Since the quantity of interest is the equation of state, direct expansion of $w(z)$ are better able to constrain the dark energy. Saini et al. (2003) (hereafter SPB) show that the distance measures are approximately linear functionals of the equation of state in the possible range of parameters. Using this they calculate the expectation value of the polynomial approximations for any given $w(z)$. They conclude that schemes based on polynomial expansion of the equation of state are useful since they measure certain well defined, integrated properties of the underlying, true equation of state.

Wang & Lovelace (2001) show that by considering the dark energy density in redshift bins the bias inherent in the finite parameterization of the dark energy can be easily removed. Huterer & Starkman (2002) apply a similar method to binned equation of state parameter, $w(z)$. A limitation of this approach is that due to the large number of bins required to reconstruct the precise behaviour of the dark energy, the estimated equation of state turns out to be very noisy. Huterer & Starkman (2002) find that although a direct reconstruction looks hopelessly noisy, useful information about the equation of state is still coded into the Fisher matrix. They show that by diagonalizing it, a few principle components could still be measured with good accuracy from the future experiments. They advocate the use of eigen vectors of the Fisher matrix as the optimal basis to express the unknown function $w(z)$.

Such free form reconstructions of the equation of state do not return a smooth function. Our main aim in this paper is to show that simple regularization of the free form estimation helps substantially in bringing down the noise in the reconstruction. In SPB the linear response approximation was used to formulate a similar free form reconstruc-
in a matrix form. We use this approximation in this paper to investigate the effect of introducing smoothness as a constraint. Although the accuracy of the linear response approximation is limited, we make use of it in this paper since it enables the regularization to be done analytically. Similar results hold for the exact case. We also show that an iterative scheme could in principle extend the applicability of the linear response approximation, while still retaining all the advantages of its analytical simplicity.

The plan of this paper is as follows. In Section 2 we collate the results on linear response approximation. In Section 3 we formulate a discrete version, more suited to real data and apply it to construct the free form estimator for the equation of state. We then add the regularizing terms to modify the estimator to guarantee smoothness. In Section 4 we use a simple model for dark energy to illustrate the performance of the regularized estimation and compare it to the unregularized one. Our conclusions are presented in Section 5.

2 LINEARIZED LUMINOSITY DISTANCE

The exact relation between the luminosity distance and the equation of state \( w(z) \) is non-linear, however, it was shown in SPB that by considering a given equation of state as small departure from a fiducial equation of state we can approximately linearize this relation. In this section we collate the necessary expressions. In a spatially flat universe the luminosity distance is given by

\[
D_L(z) = (1 + z)(1 + g)^{1/2} \int_1^{1+z} dx \frac{x^{-3/2}}{[g + Q[w, x]]^{1/2}},
\]

where \( x = 1 + z, g = \Omega_m/\Omega_Q \), and the function containing the dark energy equation of state is given by

\[
Q[w, z] = \exp \left[ 3 \int_1^{1+z} dx w(x)/x \right].
\]

We have set \( c \) and \( H_0 \) equal to unity in these expressions. We can approximately linearize this equation about a fiducial \( w^{\text{fid}}(z) \) through

\[
D_L[w^{\text{fid}} + \delta w, z] \approx D_L[w^{\text{fid}}, z] + \delta D_L
\]

\[
\delta D_L = \int_0^z K_w(z, z') \delta w(z')dz',
\]

where the kernel \( K_w(z, z') \) is given by the functional derivative of the luminosity distance with respect to \( w(z) \), evaluated about \( w^{\text{fid}}(z) \)

\[
K_w(z, z') = \frac{\delta D_L[w^{\text{fid}}(z''), z]}{\delta w(z')},
\]

Evaluating the functional derivative for \( D_L \) given by Eq. 3 gives

\[
K_w(x, x') = \left\{ \begin{array}{ll} 
-\frac{3x(1+g)^{1/2}}{2x'} & \text{for } x < x' \\
0 & \text{for } x > x'
\end{array} \right.
\]

(5)

The accuracy of the linear response approximation was shown in SPB to be better than that achieved by the Supernova Acceleration Probe (SNAP) survey, which is expected to observe about 2000 Type 1a SNe, up to a redshift \( z \sim 1.7 \), each year (Aldering et al. 2002). By binning the supernovae in a redshift interval of \( \sim 0.02 \), SNAP is expected to give a relative error in the luminosity distance of about \( \sim 1\% \). In SPB the accuracy of the linear response approximation was shown to be better than \( 1\% \), implying that it can be used conveniently for a SNAP class data. However, there are indeed finite departures from the linear approximation and one must be careful in applying it to real data. For the purposes of this paper we use this approximation for convenience, since it enables us to regularize the free form estimation of the equation of state analytically. We shall apply the linear response approximation only to those models for which the departures from the exact expression are small. The usefulness of the linear approximation, however, can be improved by employing an iterative method described below.

3 FREE FORM RECONSTRUCTION OF \( W(Z) \)

For the purposes of this paper we simulate the luminosity distance \( D_L \) at a large number, \( N_{\text{dat},\text{exp}} \), of uniformly distributed redshifts \( z_i \), up to a maximum redshift \( z = 1.7 \). We assume a Gaussian noise equivalent to 1% relative error in the distances with \( \sigma_i \) as the variance. As a first approximation we fit the simulated data to a constant \( w \) model to obtain \( w = w_0 \). If \( \Omega_m \) is known to a good accuracy this will give us a first good approximation to the equation of state. We then linearize the luminosity distance around \( w^{\text{fid}} = w_0 \). The difference between the given noisy estimate of luminosity distance and the best fit \( D_L \) as obtained from \( w = w_0 \) model gives us the residuals \( \delta D_L \).

For modelling purposes we consider a discrete version of Eq. 3

\[
\delta D_L(z_i) \approx \delta z \sum_{j=1}^{N_{\text{bin}}} K_w(z_i, z'_j) \delta w(z'_j).
\]

(6)

To quantify departures from the constant \( w = w_0 \) we consider the equation of state to be given in \( N_{\text{bin}} \) uniformly distributed redshift bins \( z'_k \) with values \( w_k = \delta w(z'_k) \), with a
redshift spacing $\delta z$. The number and placement of bin positions for $\delta w$ is such that the the equations generated by the maximum likelihood procedure, to be described below, yield a unique solution. The value of $\delta w$ at the position of the farthest given distance cannot be inferred from the data, since it has no effect on any of the distances. In practice we also exclude those bins that are close to the farthest redshift for reconstruction, since the reconstruction is too noisy in those bins. This particular expansion is especially convenient since if we have prior knowledge about the range of $w(z)$ then it is extremely easy to code that into the reconstruction procedure.

We define the normalized vector $d \equiv \{\Delta D_L(z_i)/\sigma_i\}$. Similarly we define $w \equiv \{\delta w(z_i')\}$ and $K \equiv \{\delta K(z_i, z_i')/\sigma_i\}$, where $K$ is a $N \times M$ matrix. In terms of these quantities a maximum likelihood reconstruction is equivalent to the standard procedure of minimizing the $\chi^2$ function

$$\chi^2 = (d - Kw)^T (d - Kw)$$

(7)

with respect to $w$. This can be done analytically to give

$$w = (K^T K)^{-1} K^T d,$$

(8)

as the required estimator for $w$. In general Eq 8 gives a very noisy estimate for the equation of state. This is due to the fact that too many parameters are being estimated so the estimator fits most of the noise as well, and this lack of resolution is a general feature of the free form fitting (Sivia, 1996). This formulation gives the Fisher matrix trivially as

$$F = K^T K.$$

Huterer & Starkman, (2003) diagonalize the Fisher matrix and find that only a few eigenvectors are well determined. They expand the equation of state in terms of the eigen vectors of the Fisher matrix to obtain an approximate form for the equation of state by truncating the series after the first few well determined eigenvectors. They note that truncating the series biases the estimation. They find that the badly determined eigen vectors are precisely those that peak at high redshift, therefore, throwing away those eigenvectors biases the equation to state to zero at high redshift. In the next section we describe another approach that does not have this problem and is better able to represent the equation of state at all redshifts.

3.1 Regularization

The expansion described above does not guarantee smoothness or continuity. In fact, for large $N_{\text{bin}}$ the solution fits most of the noise as well, and therefore gives a very small value of $\chi^2$. Since an acceptable model would give $\chi^2 \sim N_{\text{dat}}$ we might wish to modify the best fit $w$ to ensure some smoothness. As noted above, the amount of information contained even in a SNAP class experiment is too little to adequately constrain $w(z)$. Additional information in terms of continuity and smoothness constraints tend to fuzz information across the bins and reduces the degrees of freedom of the free form fitting function. In regions where the data is not discriminatory enough, the derived equation of state tends to extrapolate from the well constrained regions and can provide useful information. As an obvious warning we note that in general this is a dangerous thing to do since it might bias the estimator, or even create spurious signal. In our view these disadvantages are outweighed by the fact that a scheme would give us, at least, a fighting chance to infer the behavior of $w(z)$ in a way that is independent of the specific form of $w(z)$ chosen to fit the data. Regularization also reminds us that we are explicitly assuming smoothness for $w(z)$, rather than sneaking it in the form of smooth fitting functions.

To ensure continuity and smoothness we modify the $\chi^2$ above to

$$\chi^2 = \chi^2 + \lambda \sum_{i=1}^{N-1} (w_i + w_{i+1})^2$$

(10)
For our numerical explorations we adopt the following model for the dark energy as the input equation of state
\[ w(z) = w_0 + w_1 \ln(1 + z), \]
since it has the nice property that \( w_0 \) and \( w_1 \) are the present day value of \( w(z) \) and its first derivative respectively. Since this model has finite departures from the equivalent linear model it also serves to illustrate how well a regularized estimation gives information about departures from a simpler linear model. The function \( Q[w, z] \) defined in Eq (2) is calculated analytically to obtain
\[ Q[w, z] = \exp[\frac{3w_1}{2} \ln^2(1 + z)]. \]

Since the linear response approximation is an expansion about a given \( \Omega_m \), we shall assume its value to be exactly known. We generate the simulated data in \( N_{\text{dat}} = 50 \) bins up to a maximum redshift \( z = 1.7 \). For reconstruction purposes we employ \( N_{\text{bin}} = 48 \) bins for placing the binned \( w(z) \). As remarked earlier, we do not reconstruct \( w(z) \) above a redshift of \( z \sim 1.6 \) due to poor resolution.

The unregularized estimator given in Eq (3) picks up numerical noise even when the distances are exactly given. To show how unstable such an estimation is we contrast it with the regularized estimation in Fig 4 which shows the reconstructed equation of state for \( w_0 = -1 \) and \( w_1 = 0.2 \) model without added noise (but with small numerical noise due to inexact mathematical operations). The un-regularized reconstruction follows the true model quite closely but picks up numerical noise and appears noisy. The regularized reconstruction, on the other hand, follows the true equation of state quite closely. The tiny departures from it are due to the fact that the linear response approximation is not exact. This clearly shows that a reconstruction without regularization is ineffective even when the statistical noise is absent.

Since the unregularized estimator is extremely sensitive to noise, we can improve its performance by taking into account the inevitable numerical noise due to inexact mathematical operations to make the comparison fair. To a good approximation the numerical noise grows linearly with the distance. If we normalize \( d = (\delta D_L(z_i)/\sigma_i) \) and \( K = (\delta z K(z_i, z_j)/\sigma_i) \) with \( \sigma_i \propto D_r(z_i) \) then we find that the unregularized estimation is stabilized to some extent. To illustrate this effect, and to show how the reconstruction works for a model that shows strong departures from a straight line we also reconstruct the equation of state \( w(z) = -1.0 + 0.2 \sin 4z \) in Fig 4 without added statistical noise. We find that the reconstruction works better than before for the unregularized case, but the regularized estimation works better in both the cases.

To quantify how the regularized estimator works for noisy data we add a 1% Gaussian noise to the previous model \( (\sigma_i = 0.1 \times D_L(z_i)) \). We fixed the weights \( \lambda \) and \( \beta \) to ensure a reasonable \( \chi^2 \) for this experiment. Fig 4 shows the outcome for 10 realizations of the noisy data. The reconstructed equation of state typically has a scatter of about \( \sim 0.2 \) at low redshift. At large redshifts the reconstruction is poor but remain unbiased. To see the effect of decreasing noise we lower it by ten times for Fig 4. The reconstruction now works much better, as expected. The scatter at the large redshift is still substantial, however, the equation

\[ \chi^2 = \chi^2_w + \lambda w^T F w + \beta w(S^T S) w \]
\[ = (K^T K + \lambda F^T F + \beta S^T S)^{-1} K^T d, \]

In terms of this new regularized \( \chi^2 \) the solution Eq (3) is modified to
\[ w = (K^T K + \lambda F^T F + \beta S^T S)^{-1} K^T d, \]
of state is reconstructed very well up to \( z \sim 0.7 \). We also find that the reconstruction recovers the shape of \( w(z) \), even up to large redshifts in many cases. In part this success is due to the fact that regularization extrapolates from the well determined low redshift \( w(z) \).

### 4.1 Noise Estimation

Quantifying errors on the reconstructed equation of state is not simple in this approach. One way to do this is to use the reconstructed equation of state to calculate the Fisher matrix in Eq \( \text{[1]} \). The inverse of that would yield the required covariance matrix. This would be equivalent to assuming a Gaussian distribution for the estimator in Eq \( \text{[1]} \). Our numerical experiments show that the distribution of equation of states generated for different realizations of noise by the regularized estimator is not close to Gaussian. In fact, as Fig \( \text{[2]} \) shows, the curves fill the space in a very complex fashion so the distribution of \( w \) values at any given redshift are not well approximated by the Gaussian distribution. To take into account this effect we generate 1000 realizations of data and plot the envelope of all the curves obtained from different realizations. The scatter is, of course, more concentrated around the true equation of state. The result is shown in Fig \( \text{[3]} \), where for comparison we have plotted the same for different realizations. The scatter is, of course, more concentrated around the true equation of state. The result is shown in Fig \( \text{[3]} \), where for comparison we have plotted the same for the case where \( \beta \) is kept equal to zero. The figure shows that the when \( \beta \neq 0 \) the noise goes down in the estimation at all redshifts. This is what we would expect since this term adds information about the second derivative in the estimation.

The envelope for \( \beta = 0 \) shows a weak sweet spot at \( z \sim 0.1 \) while the one with a non-zero \( \beta \) the sweet spot becomes stronger and moves to \( z \sim 0.2 \). In fact, if we consider the Fisher matrix of the unregularized estimation in Eq \( \text{[1]} \) we find that no sweet spot appears anywhere. This is indeed as it should be since the \( w \) values at small redshifts affect the distances at all the higher redshifts, so should be better constrained. If we increase \( \beta \) the sweet spot moves to \( z \sim 0.3 \) and becomes stronger. This behaviour suggests that the sweet spot is, in general, an artifact of the particular method employed in the estimation. The demand that the \( w(z) \) have a small second derivative cannot fit the data at all redshifts adequately, so it develops an anchor at an intermediate redshift, as is seen in Fig \( \text{[3]} \). Huterer & Starkman (2003) express similar views on the origin of the sweet spot in their paper.

### 5 CONCLUSIONS

We have shown that the limitations of the free form estimation of dark energy can be overcome by simple regularization, which substantially improves its performance. Our regularizing terms incorporate smoothness of the equation of state and its first derivative, but can be easily generalized to take into account further information about the equation of state. We have explicitly constructed an analytic form for the regularized estimator for the equation of state by employing the recently introduced linear response approximation which allows the maximum likelihood estimation to be performed analytically. Although the linear response approximation is not perfect, its applicability can be extended by iteration. The major uncertainty in the determination of the properties of dark energy is the present day density in the form of pressureless dark matter. The results in this paper assume this density to be known but can be easily generalized to take this into account properly. Due to its analytical simplicity and due to the fact that by construction it is unbiased, the regularized free form estimation is superior to all others. However, we do find that artifacts of regularization appear in the form of sweet spots. It is fair to say that at the level of accuracy that a SNAP class experiment will achieve it seems unlikely that this method will give any more information than that given by simple polynomial fits to the equation of state. Since this method is well suited for combining supernovae data with other cosmological tests it might yet prove to be a more useful way of constraining the properties of dark energy.

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