I. INTRODUCTION

Dark energy is a premier mystery of cosmology and high energy physics. To address this, NASA and the Department of Energy (DOE) are funding the Joint Dark Energy Mission (JDEM). Because the physical nature of dark energy is so unknown, it is challenging to quantify simply and accurately the science requirements for learning about the physical origin. To assess approaches to a figure of merit for the dark energy science reach of different JDEM architectures, NASA and DOE formed the Figure of Merit Science Working Group (FOMSWG).

FOMSWG found in a preliminary report\(^1\) that the figure of merit used by the Dark Energy Task Force\(^2\), given by the inverse area of the likelihood contour in the dark energy equation of state plane \(w_0-w_a\), was reasonable for the task. Here the equation of state (EOS) as a function of scale factor is given by \(w(a) = w_0 + w_a(1-a)\). This form has been tested for physical accuracy and against bias, and has been shown to faithfully reproduce relations for observables such as distances and Hubble parameters to an accuracy of \(10^{-3}\), better than needed for JDEM.

These results, and especially the calibration relations of \(\alpha\), should substantially allay concerns about using a particular functional form. Recall that the current issue is how to project simulated constraints of various JDEM scenarios; once the data are in hand one will carry out the analysis through a diversity of methods, and test specific models directly against the data without an intermediate form. Nevertheless, one can reasonably consider an additional (not replacement) approach to build confidence that the conclusions on science design were robust. An example is principal component analysis (see, e.g., \(\alpha\) for application to dark energy), which has the capability of covering a wide variety of functional forms.

The assessment of whether principal components (PCs) add new insights to JDEM design projections depends on appropriate scientific criteria. Here we present brief cautions about possible oversimplifications of interpretation, titling the following section headings with some of the possible misunderstandings.

II. UNCERTAINTIES ARE SMALL, SO WE KNOW THE ANSWER?

The principal components compose the EOS through

\[
\begin{align*}
\epsilon_i(a) &= \sum_i \alpha_i \epsilon_i(a), \\
\end{align*}
\]

where \(w_b\) is the baseline EOS to compare to (e.g. \(w = -1\)), \(\epsilon_i\) are the eigenmodes of the Fisher matrix for the particular experiment, and \(\alpha_i\) are the mode coefficients.

Given the information from some (simulated) experiment, one forms the Fisher information matrix and diagonalizes it. The rows of the diagonalization matrix are the eigenvectors, or modes \(\epsilon_i(a)\). If the Fisher matrix was formed with respect to the baseline model, then the expectation value of the coefficients \(\langle \alpha_i \rangle = 0\). The rms about the mean is \(\sigma_i = \sigma(\alpha_i)\), i.e. the inverse square root of the eigenvalues.

One of the key misapprehensions of PCA is the physical interpretation of the uncertainties on the amplitudes \(\alpha_i\) of each mode. Although PCs are often ordered by the uncertainties, these values \(\sigma_i\) have no physical meaning by themselves. One has to interpret their magnitude in terms of some distance between models. One possibility is adopting the range of \(w \in [-1,0]\), valid for many models (with the upper limit to avoid disrupting early matter domination), and considering values of \(\sigma_i\) as useful if they are smaller than one. For example, FOMSWG imposes priors on the EOS such that \(\sigma_i\) cannot exceed one. This prescription is equivalent to a redefinition

\[
\sigma_{\text{true}} \rightarrow \sigma_{\text{FOM}} = \frac{\sigma_{\text{true}}}{\sqrt{1 + \sigma_{\text{true}}^2}},
\]

One might choose to form a figure of merit given as the reciprocal of the product of all the \(\sigma_i\)'s. This appears similar to a multi-dimensional extension (cf. \(\text{5, 6, 7}\)) of the DETF figure of merit written in terms of \(1/[\sigma(w_p) \sigma(w_a)]\) where \(w_p\) is the pivot EOS value. However, none of this addresses the meaning. Since every PC by construction has an uncertainty smaller than or equal to one, does this mean that all give physical insight? As argued by \(\text{6, 8, 9}\), the \(\sigma_i\)'s alone capture no physics. The imposition of a prior does define a goal for “smallness” of the uncertainty, if somewhat artificially. However, just as in most astronomy, the true information is held by the signal-to-noise ratio,

\[
S/N = \left[ \sum \frac{\alpha^2}{\sigma^2} \right]^{1/2},
\]

Using PCA: Principal Components and Dark Energy

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where each mode contributes \( \alpha_i/\sigma_i \) worth of \( S/N \). This is equivalent to the \( \chi^2 \) comparison of mode coefficients between a model and the baseline. So the important quantity is not \( \sigma_i \) but \( \sigma_i/\alpha_i \).

Consider if one misestimated the value of some PC coefficient \( \alpha_i \) by \( \sigma_i \) (i.e. 1\( \sigma \)) – would it change the physics conclusion? In particular, the cosmological constant corresponds to \( \alpha_i = 0 \) for all PCs. If some \( \alpha_i \) is within 1\( \sigma \) (or some other confidence level) of zero, then that PC is not effectively contributing to distinction of the physics from a cosmological constant, since there is a high statistical probability that \( \alpha_i \) is consistent with zero. (This can of course be generalized to differences between any two models.)

Therefore, how many PCs truly contribute to distinguishing some model from the cosmological constant \( \Lambda \)? We test this for a continuum of models, over various model classes, assuming an imaginary experiment giving 0.3% distance measurements between \( z = 0 - 3 \), plus Planck CMB information. Every one of 36 PCs between \( a = 0.1 - 1 \) have \( \sigma_i \)'s less than one, by the construction of Eq. 2. However, when we carry out the test for various model parameters, and model classes, below, we find generically that only \( \sim2-3 \) PCs have \( \sigma_i/\alpha_i < 1/2 \), i.e. a 2\( \sigma \) deviation from the cosmological constant, even with the extraordinary assumptions of experimental accuracy. This is in agreement with the multiple studies of this issue by [8].

Figures 1–2 illustrate the physical discriminating power of this idealized experiment as a function of cosmological model. For most models viable under current data, 2-3 PCs have sufficient \( S/N \) to be useful in distinguishing between the true cosmology and the cosmological constant. Of course as the model approaches the cosmological constant, distinction becomes more difficult.

To exhibit robustness of these results against the specific assumed model, we scan over model parameters for classes of qualitatively different dark energy physics, representing the thawing class, freezing class, and a non-monotonic EOS. In the last case, we see that the ability of PCA not to be locked into a particular functional form, e.g. a monotonic parametrization, does not make more degrees of freedom significant.

Again, what we really care about is the \( S/N \). In Table I we list the fraction of the total \( S/N \) (Eq. 3) contributed by the two best modes – for the case for each dark energy class where higher modes contribute the most. For the thawing class the higher modes add less than 0.3% to the total, and for the freezing class less than 2.8% in the most sensitive case, dropping to less than 0.5% for modes above the third. And recall this was for a highly idealized experiment. In the oscillating model, an ad hoc case designed to be especially PCA-friendly, the most extreme case with oscillations reaching \( w = 0 \) allows higher modes to contribute up to 14% (8% for above the third mode). These are actually overestimates of the importance of high modes because as discussed in the next section the \( S/N \) of the higher modes degrades when \( w(z > 9) \) is marginalized over rather than fixed. Interestingly, fitting \( w_0-w_a \) rather than using PCA pro-
we also note that assumptions about the high redshift EOS behavior have significant effects. In practice, the PCs are often computed assuming a cut off at some maximum redshift to avoid complications in calculating the cosmic microwave background (CMB) primordial power spectra and the initial conditions for growth of matter perturbations. At higher redshifts one must therefore choose a particular form or value for the EOS. FOM-SWG fixes $w(z > 9) = -1$. One justification is that for the cosmological constant the dark energy density fades away quickly into the past, so the exact value of $w$ there is unimportant. However, we have no guarantee that the cosmological constant is the correct model, nor even essentially any current information on the behavior of the EOS at $z > 1$. Assumptions about the high redshift behavior can lead to significant biases and improper conclusions about the nature of dark energy (see, e.g., [6]).

Bias should not be as severe a problem for a high transition redshift, $z = 9$, and with many redshift bins at $z > 3$ the extra degrees of freedom should ameliorate bias from the prior at $z > 9$. However, fixing $w(z > 9) = -1$ does demonstrably influence the PCs: for example some of the uncertainties $\sigma_i / \alpha_i$ that are apparently tightly determined can degrade by a factor three when $w(z > 9)$ is not fixed. The modes themselves also change shape, as we discuss next.

Thus, what happens at high redshift does not stay at high redshift, but can affect some important aspects of the principal component analysis.

### IV. HIGHEST IS BEST?

Does the location in redshift of the maximum of a PC, say the first one, say something fundamental about the science reach of the survey or probe employed? No – as is clear from Eq. (4) the EOS constraints follow from the sum – with both positive and negative contributions – over all the PCs, not any single one.

Moreover, Figure 3 demonstrates that artificially fixing the high redshift EOS behavior changes the PC shape and peak location. This shift has nothing to do with the experimental design and so the peak location is not a signpost to experiment optimization. Assumptions on $w(z > 9)$ can affect probes differently: e.g. supernova distances do not involve $w(z > 9)$ while baryon acoustic oscillations, being tied to high redshift, do.

Finally, even if a PC peak did mean that the experiment is most sensitive to the dark energy EOS at a higher redshift, say, that would not imply that the experiment is most sensitive to the nature of dark energy. For example, dark energy is most influential today, so perhaps one wants an experiment most sensitive to the low redshift behavior. (We emphasize that understanding dark energy at low redshift still requires measuring expansion and growth to high redshift, to break degeneracies.) At best, one could say that probes that weight the dark energy differently in redshift have some complementarity.

### III. WHAT HAPPENS AT HIGH REDSHIFTS, STAYS AT HIGH REDSHIFTS?

While the previous demonstration of PC uncertainties and signal-to-noise is the most important of this paper, it provides distinction from the cosmological constant at the 1σ (2σ) level for $|\omega_a| = 0.13$ (0.24) – very comparable to the PCA approach. That is, the second parameter becomes useful at almost the same values as in the top panel of Fig. 1 for the PCA freezing case, and is more sensitive than in the bottom panel for the PCA thawing case. Both methods demonstrate that significant physical constraints on the dark energy EOS are described by of order two quantities.

The main point though is that the important information is not in $\sigma_i$, but $\sigma_i / \alpha_i$. Just because PCA may say uncertainties $\sigma_i$ are small, this does not mean that we know the physics answer.
FIG. 3: The location and shape of peaks in principal component modes depend on the high redshift treatment of the EOS. The peak location therefore does not in itself translate into the science impact of a given experiment. Note the effects are more severe for a more realistic experiment.

But there is no justification for claiming that the probe with the highest peak, or with the peak at the highest redshift, is the best probe.

V. CONCLUSIONS

Principal component analysis is a valid technique, used appropriately. Oversimplifying PCA interpretation or inadequately appreciating the effect of assumptions employed can lead to misunderstandings and false beliefs. We present cautionary examples of three apparently plausible but unjustified extrapolations. While data should be analyzed in every reasonable manner, for understanding the generic cosmology reach the more complicated PCA approach demonstrates no extraordinary advantage over the well-tested and highly calibrated phase space dynamics approach of $w_0 - w_a$.

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