

# Fisher matrix decomposition for dark energy prediction

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## ABSTRACT

Within the context of constraining an expansion of the dark energy equation of state  $w(z)$ , we show that the eigendecomposition of Fisher matrices is sensitive to both the maximum order of the expansion and the basis set choice. We investigate the Fisher matrix formalism in the case that a particular function is expanded in some basis set. As an example we show results for an all-sky weak lensing tomographic experiment. We show that the set of eigenfunctions is not unique and that the best constrained functions are only reproduced accurately at very higher order  $N \gtrsim 100$ , a top-hat basis set requires an even higher order. We show that the common approach used for finding the marginalized eigenfunction errors is sensitive to the choice of non- $w(z)$  parameters and priors. The eigendecomposition of Fisher matrices is a potentially useful tool that can be used to determine the predicted accuracy with which an experiment could constrain  $w(z)$ . It also allows for the reconstruction of the redshift sensitivity of the experiment to changes in  $w(z)$ . However, the technique is sensitive to both the order and the basis set choice. Publicly available code is available as part of ICOSMO at <http://www.icosmo.org>.

**Key words:** methods: statistical – cosmological parameters.

## 1 INTRODUCTION

The Fisher matrix methodology (Fisher 1935; Jungman et al. 1996; Tegmark, Taylor & Heavens 1997) is a statistical tool that has been used with some success in predicting the ability of future experiments to constrain particular parameters of interest. In cosmology, Fisher matrices have gained some importance in predicting the potential outcome of experiments, in particular dark energy surveys, on which a large amount of resources may be spent. It is therefore of paramount importance that the way in which Fisher matrices are used should be understood and that any results that depend on this methodology should be robust and reliable.

In this article, we will outline how the techniques of decomposing a general matrix have a special interpretation when used within the Fisher matrix framework. This will be done within the context of attempting to predict constraints for an extended parameter set. We will use the specific example of attempting to constrain dark energy equation-of-state  $w(z)$  parameters (Hu 2002; Huterer & Starkman 2003; Crittenden & Pogosian 2005; Huterer & Cooray 2005; Knox, Albrecht & Song 2005; Dick, Knox & Chu 2006; Ishak, Upadhye & Spergel 2006; Simpson & Bridle 2006; Albrecht & Bernstein 2007; de Putter & Linder 2008; Sarkar et al. 2008; Tang, Abdalla & Weller 2008; Cunha, Huterer & Frieman 2009; Joudaki, Cooray &

Holz 2009; Zhan, Knox & Tyson 2009a; Zhan et al. 2009b), most recently Albrecht et al. (2009) defined a new dark energy figure of merit using a binned 36 parameter model.

We will show that the eigenfunctions obtained by diagonalizing a Fisher matrix are dependent of the basis set used in the construction of the Fisher matrix, and that the eigenfunctions only tend to be in agreement in the limit of a very large order of expansion. We will also show that the usual method of marginalizing over extra parameters – constructing the Schur complement (Zhang 2005) of the total Fisher matrix – is dependent on the choice of non- $w(z)$  parametrization and priors when also performing an eigendecomposition.

In Section 2, we will introduce the methodology. In Section 3, we will apply the approach to weak lensing tomographic survey prediction. We present conclusions in Section 4.

## 2 METHODOLOGY

For a set of parameters  $\theta$ , the Fisher matrix allows for the prediction of parameter errors given a specific experimental design and method for extracting parameters. In the case of Gaussian-distributed data where we assume that the error on the signal is not a function of parameter values  $\sigma_C \neq \sigma_C(\theta)$ , we can take the covariance of the estimated values of the parameters:

$$\text{cov}[\theta_i, \theta_j] = \langle (\theta_i - \langle \theta_i \rangle)(\theta_j - \langle \theta_j \rangle) \rangle = F_{ij}^{-1}, \quad (1)$$

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where the Fisher matrix is defined by (Tegmark et al. 1997; Jungman et al. 1996; Fisher 1935)

$$F_{ij} = \sum_x \left[ \sigma_c^{-2} \frac{\partial S}{\partial \theta_i} \frac{\partial S}{\partial \theta_j} \right], \quad (2)$$

where  $S$  is the signal. The predicted marginal errors on the parameters are given by  $\Delta\theta_i = \sqrt{(F^{-1})_{ii}}$ , this is the minimum marginal error that one can expect for the method and experimental design considered (due to the lower bound in the Cramer–Rao inequality).

If we extend the parameter set to  $\phi = (\theta, \psi)$ , then the Fisher matrix is extended to include these extra parameters

$$F^{\phi\phi} = \begin{pmatrix} F^{\theta\theta} & F^{\theta\psi} \\ F^{\psi\theta} & F^{\psi\psi} \end{pmatrix}, \quad (3)$$

and the predicted marginal errors on the parameters  $\Delta\theta_i = \sqrt{(F^{-1})_{ii}^{\phi\phi}}$  are increased due to degeneracies between the original parameters and the new parameters.

For dark energy cosmology prediction, the parameter set is commonly divided into those that contain information on the dark energy equation of state  $w(z)$  and those that do not. The usual approach taken (Hu 2002; Huterer & Starkman 2003; Crittenden & Pogosian 2005; Huterer & Cooray 2005; Knox et al. 2005; Dick et al. 2006; Ishak et al. 2006; Simpson & Bridle 2006; Albrecht & Bernstein 2007; de Putter & Linder 2008; Sarkar et al. 2008; Tang et al. 2008; Albrecht et al. 2009; Cunha et al. 2009; Joudaki et al. 2009; Zhan et al. 2009a,b) is to ‘bin’  $w(z)$  in redshift and to assign an amplitude to the value of  $w(z)$  in each bin. However,  $w(z)$  is not a directly observable quantity but can only be inferred through other integral relations, most simply the comoving distance or the Hubble parameter

$$D(z) = \frac{c}{H_0} \int_0^z dz' \frac{1}{\left\{ \Omega_m(1+z')^3 + \Omega_{de} e^{3 \int_0^{z'} dz'' [1+w(z'')]/(1+z'')} \right\}^{1/2}}, \quad (4)$$

$$H(z) = H_0 \left\{ \Omega_m(1+z)^3 + \Omega_{de} e^{3 \int_0^z dz' [1+w(z')]/(1+z')} \right\}^{1/2}. \quad (5)$$

So any binned expansion of  $w(z)$  to include extra parameters cannot be justified by arguing that the data themselves are binned in redshift.

The choice of how to expand the function  $w(z)$  is thus a purely theoretical one. In general, we will consider  $w(z)$  expanded in some complete basis set

$$1 + w(z) = \sum_{i=1}^{\infty} a_n \phi_n(z), \quad (6)$$

where  $a_n$  are the basis coefficients and  $\phi_n$  are the basis functions. Since we do not know what dark energy equation state is apt for the physical Universe, any chosen basis set is as valid as any other. Binning is a special case where the basis functions are top-hat functions in redshift

$$\phi_n^{\text{binning}}(z) = \mathcal{H}\left(z - \frac{\Delta z}{2}\right) - \mathcal{H}\left(z + \frac{\Delta z}{2}\right), \quad (7)$$

where  $\Delta z$  is the bin width and  $\mathcal{H}$  is the Heaviside (step) function.

Note that interpolations between delta function values at discrete redshifts, linearly or with some spline function, are *different* basis sets to binning. We clarify three broad meanings of binning that occur in the literature.

(i) Top-hat basis set: functions are not continuous, all derivatives are ill defined.

(ii) Linear interpolation: functions are continuous, first derivatives are discontinuous, second and higher order derivatives are ill defined.

(iii) Spline (e.g. quadratic spline): functions are continuous, first derivatives are continuous, second derivatives are discontinuous, third derivatives and higher are ill defined.

Of these three basis functions, only top hat forms an orthogonal basis set; though all form a complete basis set. We include interpolation in Section 3 for completeness, and because it is commonly used in the literature.

The most general condition that we could apply to the expected  $w(z)$  is that it is continuous (features could be very sharp in redshift but not physically discontinuous – the sound speed of dark energy is generally expected to be  $\leq c$ ).<sup>1</sup> We note that binning is not discrete differentiable, since at the bin boundary the gradient is infinite.

We will now investigate how the Fisher matrix should be treated when such an expanded basis set is used.

## 2.1 Basis set decomposition

The general framework with which we are now presented consists of a Fisher matrix

$$\mathbf{F} = \begin{pmatrix} F^{\theta\theta} & F^{\theta w(\phi)} \\ F^{w(\phi)\theta} & F^{w(\phi)w(\phi)} \end{pmatrix}, \quad (8)$$

where  $\theta$  are the cosmological parameters not associated with  $w(z)$ .  $w(\phi)$  is the set of parameters that describes  $w(z)$  where we have expanded  $w(z)$  using a general complete orthogonal basis set with basis functions  $\phi$ . The sub-Fisher matrix for  $w(z)$  is calculated by

$$F^{w(\phi)w(\phi)} = \sum_x \frac{1}{\sigma(x)^2} \frac{\partial S}{\partial a_i} \frac{\partial S}{\partial a_j}, \quad (9)$$

where  $\sigma(x)$  is the expected marginal error on the signal  $S$  and the errors on the coefficients of the expansion (equation 6)  $\sqrt{[F^{w(\phi)w(\phi)}]_{ii}^{-1}} = \Delta a_i$  [not marginalizing over non- $w(z)$  parameters  $\theta$ ].

A basis set is orthogonal if it satisfies the orthogonality relationship

$$\int_R \phi_m(z) \phi_n(z) M(z) dz = c_m \delta_{mn}^K, \quad (10)$$

over a range  $R$ , where  $M(z)$  is a weighting function,  $c_m$  are constants and  $\delta_{mn}^K$  is the Kronecker delta. The coefficients needed to construct an arbitrary function  $f(z)$  using the basis set  $\phi$  are given by

$$a_n = \frac{1}{c_n} \int_R f(z) \phi_n(z) M(z) dz. \quad (11)$$

In general, we can construct the Fisher matrix (equation 8) using an orthogonal basis set for  $w(z)$  [orthogonal with respect to a weight function  $M(z)$ ], but the submatrix  $F^{w(\phi)w(\phi)}$  will not be diagonal since  $w(z)$  can, at a minimum, only be observed through integral relations.<sup>2</sup>

<sup>1</sup> There are some tachyonic dark energy models (e.g. Bagla, Jassal & Padmanabhan 2003), but choosing a basis set based on these specific models would be optimistic.

<sup>2</sup> Most articles in the literature (e.g. Huterer & Starkman 2003; Crittenden & Pogosian 2005; Albrecht et al. 2009) neglect the weight function. We note that the top-hat basis set is peculiar, in that it is orthogonal with respect to any weight function.

A common approach is to look for the eigenfunctions of  $w(z)$ . The motivation for this is that the eigenfunctions are thought to form an orthogonal basis set. These functions are found by rotating the Fisher matrix such that it is diagonalized using the transformation

$$\begin{aligned}\Lambda^\phi &= \mathbf{Q}^T \mathbf{F} \mathbf{Q}, \\ \mathbf{F} &= \mathbf{Q} \Lambda^\phi \mathbf{Q}^T,\end{aligned}\quad (12)$$

where  $\mathbf{Q}$  is an orthogonal matrix,  $\mathbf{Q}^T \mathbf{Q} = I$ .

By performing this transformation, the non- $w(z)$  errors can also be affected. There are three possibilities: either  $\mathbf{F}$  is the full  $w$  and non- $w$  Fisher matrix in which case the non- $w$  parameters are clearly affected, or  $\mathbf{F}$  is the  $w$ -only Fisher matrix, or  $\mathbf{F}$  can be the marginalized  $w$ -only Fisher matrix. We discuss these latter two options in Section 2.3.

The new Fisher matrix  $\Lambda^\phi$  is a diagonal matrix. The  $\mathbf{Q}$  matrices are called the eigenmatrices (or vectors), which are a special kind of Jacobian matrix in which the original matrix is rotated such that it is diagonalized (see Appendix A). In performing this operation, we have constructed a new set of basis functions,  $e$ , that are linear combinations of the original basis set,  $\phi$ .  $w(z)$  can now be reconstructed using two equivalent forms

$$1 + w(z) = \sum_{n=1}^N a_n \phi_n(z) = \sum_{n=1}^N b_n e_n(z), \quad (13)$$

where  $N$  is the order of the sub-Fisher matrix  $F^{w(\phi)w(\phi)}$  – we have introduced this maximum order since Fisher matrices have, by definition, a finite order. The new functions,  $e$ , can be constructed using the eigenmatrix

$$e_i(z) = \sum_{j=1}^N Q_{ij} \phi_j(z), \quad (14)$$

where (Appendix A)

$$Q_{ij} = \frac{\partial b_j}{\partial a_i}. \quad (15)$$

The new Fisher matrix has diagonal elements that are related to the errors on the new functions' coefficients

$$\Lambda_{ij}^\phi = \sum_x \frac{1}{\sigma(x)^2} \frac{\partial S}{\partial b_i} \frac{\partial S}{\partial b_j} = \delta_{ij}^K \frac{1}{(\Delta b_i)^2}. \quad (16)$$

In performing such a rotation, we have effectively created a new basis set that is orthogonal with respect to a new weight function (equation 10) that takes into account the covariance in the Fisher matrix.

We note that an operation of the form  $\mathbf{F} = \mathbf{Q} \Lambda \mathbf{Q}^T$  (or the inverse  $\mathbf{Q}^T \mathbf{F} \mathbf{Q} = \Lambda$ ) leads to a unique  $\mathbf{Q}$  if  $\Lambda$  and  $\mathbf{F}$  are fixed. However, in general, a further operator  $P$  can be applied to the new diagonal matrix  $P \Lambda = P(\mathbf{Q}^T \mathbf{F} \mathbf{Q})$  to map a matrix  $\mathbf{F}$  to any diagonal of the same dimension, where  $P$  is also a diagonal.  $P$  acts like a 'stretching' (or compression), not a rotating, operator.  $P$  does not correspond to a change in parameters but a change in the errors on an eigenbasis parameter set. We do not consider this in the remainder of the article.

We also note that, in general, there exist operators that can rotate from a large matrix to a smaller one. For example, an  $n \times n$  diagonal matrix  $\Lambda^{\text{large}}$  can be mapped to a smaller  $m \times m$  diagonal matrix  $\Lambda^{\text{small}}$  where  $m < n$  via the operator  $\Lambda_{kk}^{\text{small}} = A_{ki} \Lambda_{ii}^{\text{large}} A_{ik}^T$ , where  $A_{ki}$  is an  $n \times m$  matrix. So if the size of the matrices is not specified, then the operation  $\mathbf{F} = A(\mathbf{Q} \Lambda \mathbf{Q}^T) A^T = R \Lambda R^T$  (where  $R = A \mathbf{Q}$ ) can map a matrix to a diagonal of smaller dimension. This is equivalent

to mapping the basis set expansion from a particular order to one of a smaller maximum order. Note that this is, in general, a one-way operation since information is lost in the minimization. In the remainder of this article, we will only consider mapping between matrices of the same dimension.

## 2.2 The non-uniqueness of the eigenfunctions

It is often assumed that an eigenfunction decomposition yields a set of functions that are *unique* (if they are not degenerate; Huterer & Starkman 2003; Crittenden & Pogosian 2005; Albrecht et al. 2009). This statement comes from the matrix theory; the diagonalization of a particular matrix can only be done one way. However, this does not mean that the eigenfunctions of  $w(z)$  from a finite Fisher matrix are unique, since we can start with different basis sets and this choice is arbitrary. This breakdown is due to the finite number of coefficients – so it is really a convergence statement.

The general minimum assumption case we are dealing with is one in which we consider two Fisher matrices calculated by expanding  $w(z)$  in two different basis sets  $\phi$  and  $\psi$ .

We can only transform one Fisher matrix  $F^\phi \rightarrow F^\psi$  to another by changing the basis sets if *all* the basis set  $\phi$  functions  $1 \rightarrow N$  can be described using *only* the functions  $1 \rightarrow N$  from the set  $\psi$ , and vice versa. For example, to rotate from basis  $\phi$  to  $\psi$ , then

$$\psi_i(x) \equiv \sum_{j=1}^N J_{ij} \phi_j(x) \quad \forall 1 \leq i \leq N \quad (17)$$

needs to be true. However, for any conceivable complete basis set for finite  $N$  this sum will always have some residual. This residual  $R_i(x)$  can be quantified by

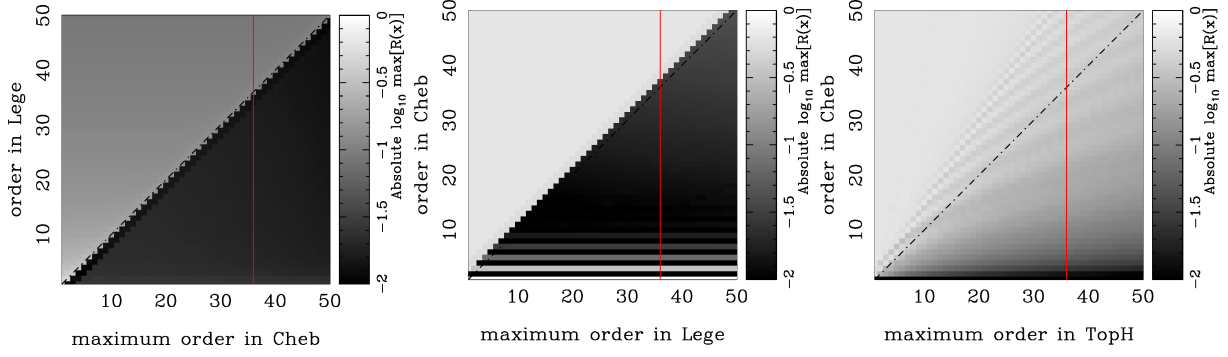
$$\begin{aligned}\psi_i(x) &= \sum_{j=1}^N J_{ij} \phi_j(x) + R_i(x), \\ R_i(x) &= \sum_{n=N+1}^{\infty} \left[ \frac{1}{c^\phi} \int_R dx' \psi_i(x') \phi_n(x') M^\phi(x') \right] \phi_n(x).\end{aligned}\quad (18)$$

The notation we use throughout is that  $\mathbf{Q}$  are explicitly eigenmatrices,  $\mathbf{J}$  are explicitly general Jacobian transformations,  $R$  are residuals and  $\mathbf{F}$  are Fisher matrices. Note however that an eigenmatrix  $\mathbf{Q}$  is a special kind of Jacobian  $\mathbf{J}$  where the result of the transformation is a diagonal.

In Appendix B, we show that if the residual is non-zero then the eigenvalues are not equal.

If the residual between any two basis sets is small, in the limit of large  $N$ , then the eigenfunctions will agree to some accuracy, and one would expect the best constrained eigenfunctions from any basis set to converge. However, for a finite  $N$ , the eigenfunctions will only *all* agree if the  $N$ th basis function in one set can be reproduced using only the functions  $1 \rightarrow N$  in other basis set.

Fig. 1 shows the residuals (equation 18) between a variety of basis sets as a function of order [in equation (18) we replaced  $\infty$  with  $10^7$  for which we find numerical convergence of the results in this figure since  $50 \ll 10^7$ ]. This plot shows that in order to have a residual of  $<0.01$  when reconstructing Legendre polynomials with Chebyshev, the order of the Chebyshev needs to be at least as high as the order of the basis function that is being reconstructed. However, in the opposite case the low-order Chebyshev polynomials are difficult to reproduce with Legendre, and the Chebyshev polynomials are difficult to reproduce with the top-hat basis set (binning). In fact, Chebyshev functions are more difficult to reproduce (especially at



**Figure 1.** An example of the residual that can occur when reconstructing a given basis sets functions with another basis set. On the y-axis is the order of the basis function to be reconstructed, on the x-axis is the maximum order of the series that is attempting to reconstruct the functions. The grey-scale shows the maximum residual (black low residual, white large residual), each function is investigated over the range  $x \in [-1, 1]$ . The left-hand plot shows the order of Chebyshev polynomials needed to reconstruct Legendre polynomials. The middle plot shows the order of Legendre polynomials needed to reconstruct Chebyshev polynomials (the inverse operation to the left-hand plot). The right-hand plot shows the order of the top-hat basis set needed to reconstruct Chebyshev polynomials. The red (grey vertical) lines are at  $N = 36$  (Albrecht et al. 2009) to guide the reader.

low order) because they are bounded in the  $y$  direction as well as the  $x$  direction.

If one chooses a maximum order of  $N = 36$  (Albrecht et al. 2009), for example, then there would be  $>0.01$  residual in reconstructing Chebyshev, Legendre and top-hat basis sets from each other. As a result, the reconstructed eigenfunctions would not agree. We will investigate this further in Section 3.

To summarize this section.

- (i) The eigenfunctions created using two different basis sets and a finite order will only agree if the residual between the reconstruction of the basis functions is zero.
- (ii) For a finite order, there will always exist some eigenfunctions from a given basis set that cannot be reproduced using another. So for finite order, the set of eigenfunctions is non-unique.
- (iii) For a large finite order, we expect the best constrained eigenfunctions to tend to agreement, and for this agreement to improve as the order is increased.<sup>3</sup>

### 2.3 Marginalization

Another difficulty in constructing robust eigenfunctions is deciding what to do with the non- $w(z)$  parameters. A common approach is to marginalize over these other parameters and then perform the eigenfunction decomposition. This in effect mixes all of these parameters with the equation-of-state expansion.

Referring to equation (8), if we want to know the errors on the expanded  $w(z)$  parameters, then we can marginalize over the other parameters  $\theta$  by constructing the Schur complement (Zhang 2005) of the  $F^{w(\phi)w(\phi)}$  submatrix

$$F_{1S}^{w(\phi)w(\phi)} = F^{w(\phi)w(\phi)} - F^{w(\phi)\theta} (F^{\theta\theta})^{-1} F^{\theta w(\phi)}. \quad (19)$$

The new Fisher matrix  $F_{1S}^{w(\phi)w(\phi)}$  will then give errors on the  $w(z)$  parameters already marginalized over the extra parameters.

We can now diagonalize  $F_{1S}^{w(\phi)w(\phi)}$  like

$$\begin{aligned} \text{diag} \left[ F_{1S}^{w(\phi)w(\phi)} \right] &= (Q^{\text{mixed}})^T F^{w(\phi)w(\phi)} Q^{\text{mixed}} \\ &\quad - (Q^{\text{mixed}})^T F^{\theta w(\phi)} (F^{\theta\theta})^{-1} F^{w(\phi)\theta} Q^{\text{mixed}} \\ &= \Lambda^{\text{mixed}}, \end{aligned} \quad (20)$$

<sup>3</sup> The full proof of this involves Weyl's matrix inequality and is beyond the scope of this article. We demonstrate convergence in Section 3.

where  $\Lambda^{\text{mixed}}$  is a diagonal matrix and  $Q^{\text{mixed}}$  is the eigenmatrix of the Schur complement. Note that it is the sum of the terms on the right-hand side that forms a diagonal not necessarily the individual terms themselves.

Alternatively, we can diagonalize  $F^{w(\phi)w(\phi)}$  without marginalizing so that  $(Q^w)^T F^{w(\phi)w(\phi)} Q^w = \Lambda^w$ , where  $\Lambda^w$  is diagonal. In this case, we can construct the new full Fisher matrix in equation (3) for which the  $F^{w(\phi)w(\phi)}$  component is now diagonal

$$\mathbf{F} = \begin{pmatrix} F^{\theta\theta} & (Q^w)^T F^{\theta w(\phi)} \\ F^{w(\phi)\theta} Q^w & (Q^w)^T F^{w(\phi)w(\phi)} Q^w \end{pmatrix}. \quad (21)$$

The cross terms need to be modified so that the correlations between  $\theta$  and  $w(\phi)$  are correct. We can now write the new marginalized errors on the new diagonalized  $w(\phi)$  vectors like equation (19) so that

$$\begin{aligned} F_{2S}^{w(\phi)w(\phi)} &= (Q^w)^T F^{w(\phi)w(\phi)} Q^w \\ &\quad - (Q^w)^T F^{\theta w(\phi)} (F^{\theta\theta})^{-1} F^{w(\phi)\theta} Q^w. \end{aligned} \quad (22)$$

Note that the  $(Q^w)^T F^{w(\phi)\theta}$  effectively acts like rotation on  $(F^{\theta\theta})^{-1}$  and that since the  $w(\phi)$  are independent parameters to the  $\theta$ , there is no reason to generally expect that the second term is diagonal – why should  $(Q^w)^T F^{w(\phi)\theta}$  be the eigenmatrix of  $(F^{\theta\theta})^{-1}$  when the  $\theta$  are independent of the  $w(\phi)$ ? Hence, the  $F_{2S}^{w(\phi)w(\phi)} \neq \text{diag}[F_{1S}^{w(\phi)w(\phi)}]$  in general and the full eigenfunctions are not equal to the  $w(\phi)$  eigenfunctions  $Q^{\text{mixed}} \neq Q^w$ , comparing equations (20) and (22).

If equation (20) is used to create eigenfunctions, then the reconstructed functions will contain the eigenfunctions of the  $w(z)$  parameters mixed with the eigenfunctions from the non- $w(z)$  parameters.

Our concern is that if the eigenfunctions are mixed, then any statements on the redshift sensitivity to  $w(z)$  are dependant on the non- $w(z)$  parametrization and the true  $w(z)$ -only sensitivity is masked. For example, if flatness was assumed, if a spectral index is included or its running, or if massive neutrinos were included (to name a few cases), then conclusions made using the mixed eigenfunctions will be different.

What we propose as an alternative is to find the  $w(z)$ -only eigenfunctions – which are robust to the non- $w(z)$  parametrization – and to include the marginalization in a consistent way to find the marginalized errors on the  $w(z)$ -only eigenfunctions.

- (i) Find the eigenfunctions of  $w(\phi)$  by diagonalizing  $F^{w(\phi)}$ .
- (ii) Calculate the new full matrix like equation (21).

(iii) Find the marginal errors on the  $w(\phi)$  eigenfunctions by marginalizing over the other parameters like equation (22).

We note that using this approach the errors on the eigenfunction coefficients will be correlated after marginalizing over the non- $w(z)$  parameters. But that these marginalized eigenfunction errors will be robust to the non- $w(z)$  choices made.

## 2.4 Priors

One can add a prior before the eigendecomposition or afterwards. Depending on the nature of the prior, this can affect the eigenfunctions themselves. Adding a general non-diagonal prior before diagonalization will act to modify the eigenfunctions in a similar way as described in Section 2.3.

If we add a diagonal prior  $P$  (no correlation between the prior errors) before diagonalization, then in general this will affect the eigenfunctions since if  $\mathbf{QFQ}^T = \Lambda_F$ , then  $\mathbf{QFQ}^T + \mathbf{PQQ}^T \neq$  diagonal. There is a special case of adding a unity matrix as the prior, in this case the eigenfunctions are unaffected since  $\mathbf{QFQ}^T + \mathbf{QIQ}^T = \mathbf{QFQ}^T + \mathbf{I} = \Lambda_F + \mathbf{I}$ , and adding the prior before or after the diagonalization has the same effect.

Throughout the remainder of this article, we will not add any priors to any parameters. In Albrecht et al. 2009, they suggest adding a prior of unity to all  $w(z)$  binned parameters. We note that this does not have an effect on the eigenfunctions and in the case of survey optimization and comparison adds a common floor to all the scenarios and does not affect the relative merit of any survey/method.

## 3 APPLICATION

We will now investigate the effect of choosing different basis sets for the expansion of  $w(z)$ . We will use the example of weak lensing tomography (described in Amara & Refregier 2007) where a photometric survey is split into redshift bins, and the auto- and cross-correlation power spectra of the shear fields are used to infer cosmological parameter likelihoods. We will present predictions for an Euclid/DUNE-like survey (Refregier et al. 2006) – a 20 000 deg<sup>2</sup> photometric survey in five bands with a number density of 35 galaxies per arcmin<sup>2</sup> and a median redshift of  $\bar{z} = 1$ , we use 10 tomographic bins in the range  $0 \leq z \leq 5.0$ . We have extended the publicly available *ICOSMO* (Refregier et al. 2008; Kitching et al. 2009) package to include basis set expansion of  $w(z)$ , these additions will be available in version 1.2 (<http://icosmo.pbworks.com>).

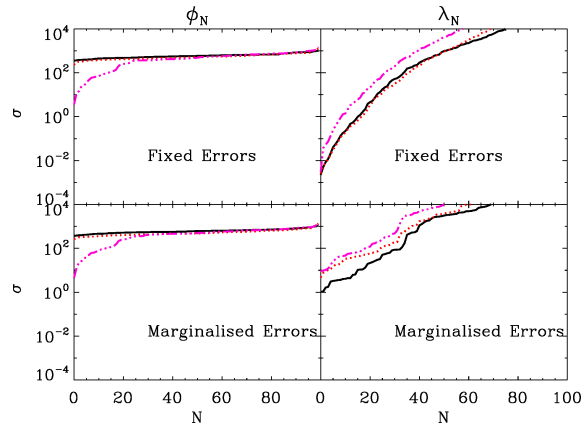
We will investigate six different basis sets summarized in Table 1. We expand these basis sets to a maximum order such that

$$1 + w(z) = \sum_{N=1}^{\text{Order}} a_N \phi_N(z), \quad (23)$$

where the fiducial cosmology is  $\Lambda$  cold dark matter, i.e. the fiducial values are  $a_N = 0$  for all basis sets. In performing such a calculation, the fiducial  $w(z)$  function must be the one that all the basis sets can reproduce.

### 3.1 Parameter errors

Fig. 2 shows the expected  $w(z)$  conditional errors on the original basis function coefficients and on the eigenfunctions. It can be seen that by rotating into an eigenbasis set the distribution of errors is skewed to produce more well-defined functions as well as

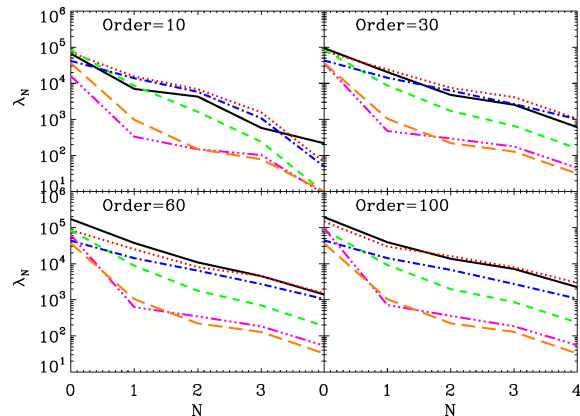


**Figure 2.** The lines show the predicted fixed errors on the basis set coefficients for the original basis set  $\phi_N$  and for the rotated, eigenfunctions,  $\lambda_N$  for a maximum order of 100. We have ordered the errors in the increasing order of magnitude for clarity, so that the  $N$ th function in the top panel does not correspond to the  $N$ th basis function, but is the  $N$ th best constrained. The top two panels show the error for  $w(z)$  not marginalized over any other cosmological parameters. The bottom two panels show the errors including marginalization over the other non- $w(z)$  parameters using the method outlined in Section 2.3 (equation 22). The key to the line styles is given in Table 1 – here we show the Fourier, Chebyshev and top-hat basis sets.

more poorly constrained functions in comparison to the non-rotated set.

It can be seen from the left-hand panels of Fig. 2 that the best constrained eigenfunctions have a similar error (the variance between the lines is small) but for the poorest constrained functions the variance between the basis sets is larger. This is because the most well-constrained eigenfunctions are similar for each basis set whereas the poorest constrained have very different functional forms. As shown in Section 2.2, the set of eigenfunctions is not unique.

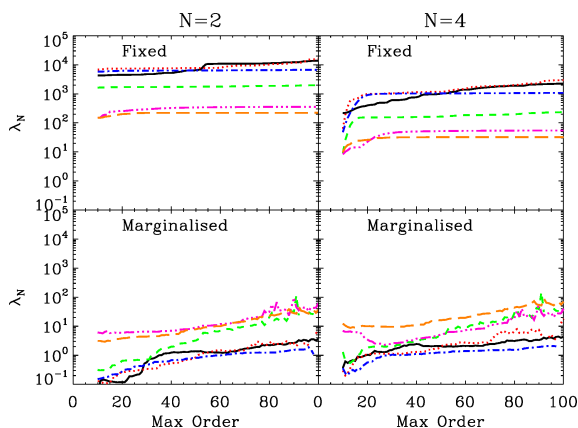
We also show the errors marginalized over the non- $w(z)$  parameters. For the eigenvalue case, this is done using equation (22) where the eigenfunctions are the  $w(z)$ -only eigenfunctions. In all cases, the best constrained eigenfunctions are those that are also the most degenerate with the other cosmological parameters, and marginalizing over these can increase the error on the eigenfunctions by an order of magnitude.



**Figure 3.** The five largest eigenvalues as a function of the maximum order of expansion. Each line represents a different basis set, the key to the line styles is given in Table 1.

**Table 1.** A summary of the basis sets investigated. The sets are complete over a range  $R$  and orthogonal with respect to the weight function  $M(z)$ . Top hat is equivalent to binning. Interpolation means a linear interpolation between delta functions, where  $m = \frac{y_2 - y_1}{x_2 - x_1}$  and  $c = y_1 - mx_1$  for the nearest two delta functions  $x_1 \leq x < x_2$  to  $x$ .<sup>\*</sup> interpolation is not an orthogonal basis set, we include it here since this is a commonly adopted expansion.

Basis	Functions	Range $R$	Weight $M(x)$	Plot key
Fourier	$\cos(nx)$ and $\sin(nx)$	$[-\pi, \pi]$	1	—
Chebyshev	$T_n(x) = \cos[n \arccos(x)]$	$[-1, 1]$	$(1-x^2)^{-\frac{1}{2}}$	.....
Legendre	$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} [(x^2-1)^n]$	$[-1, 1]$	1	-----
Laguerre	$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} (e^{-x} x^n)$	$[0, \infty]$	$e^{-x}$	-----
Top hat	$\mathcal{H}(x - \frac{\Delta x}{2}) - \mathcal{H}(x + \frac{\Delta x}{2})$	$[-\infty, \infty]$	1	-----
Interpolation	$mx + c$	$[-\infty, \infty]$	$1^*$	-----



**Figure 4.** The eigenvalues as a function of the maximum order in the basis set expansion. The key to the different basis sets lines is given in Table 1. The upper panels show the eigenvalues for the second and fourth best constrained eigenfunctions and not marginalizing over the non- $w(z)$  parameters. The lower panels show the eigenvalues for the second and fourth best constrained eigenfunctions marginalizing over the non- $w(z)$  parameters using the method outlined in Section 2.3 (equation 22).

Fig. 3 shows how the largest five eigenvalues change as a function of the maximum order in the expansion. It can be seen that a stable regime is found in which the values do not change substantially as the order is increased. We expand this in Fig. 4 where we show how the eigenvalues for the second and fourth eigenfunctions change as a function of maximum order. The Fourier and Chebyshev values agree at higher order, the other basis sets – particularly interpolations and top hat – are very slow to converge. Even for a maximum order of  $N = 100$ , there remains a large variance between the basis sets and that this variance increases as the eigenvalues decrease. The eigenvalues are related to the eigenfunction errors by  $\sigma = 1/\sqrt{\lambda}$ , we show these errors in Fig. 2. The best constrained  $N = 0$  eigenfunction has a similar error (for top hat, Chebyshev and Fourier basis sets), but by  $N \geq 2$  the errors can vary by a factor of  $\gtrsim 10$ .

There is a large range of eigenvalues between the basis sets, the most notable outliers being the top-hat and interpolation basis sets. This is related to the fact that the residual, even at a maximum order of 100, between the reconstructed eigenfunctions and the true eigenfunctions is significant. We investigate this further in Section 3.2. When we marginalize over the non- $w(z)$  parameters, the variance between the basis sets remains but each basis set’s errors are affected in different ways since the basis functions are degenerate with the non- $w(z)$  parameters to different degrees.

We have performed a numerical test that checks that the eigen-decomposition of the Fisher matrix is working correctly. First, we find the eigenfunctions by diagonalizing the  $w(z)$  sub-Fisher matrix. We then use the eigenfunctions as a new basis set. We create a new Fisher matrix which takes derivatives with respect to the coefficients of the new (eigenbasis set). This new Fisher matrix should be diagonal and should have diagonal elements that are equal to the original Fisher matrices’ eigenvalues. We find that the code used in this article successfully passes this numerical check. The code used is available as part of `icosmo v1.2` and later.

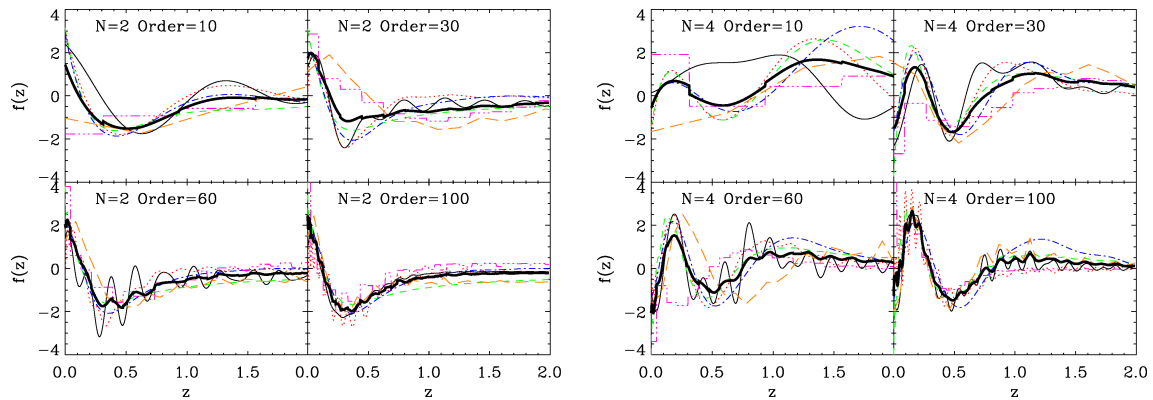
### 3.2 Eigenfunctions

The eigenfunctions are reconstructed from the eigenmatrix  $\mathbf{Q}$  using equation (14). Fig. 5 shows the second and fourth best constrained eigenfunctions for different maximum orders in the expansion for each basis set. In the absence of any way to reconstruct the ‘true’ eigenmatrix, we also show the mean eigenfunction averaged over basis sets for each order – in the limit of a high order, we expect the eigenfunctions to converge.

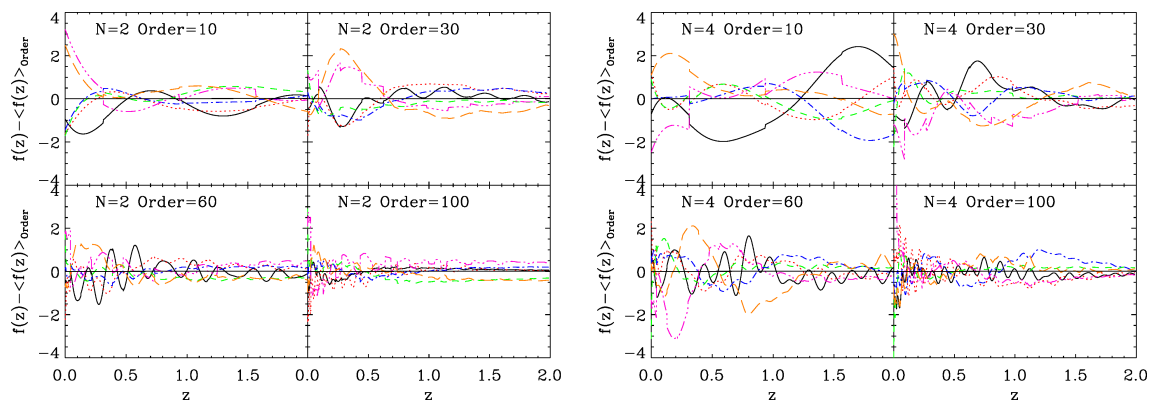
It can be seen that at order = 40, for example, there is still a significant variation between basis sets. The variance between basis sets decreases as the maximum order is increased, but for the  $N = 4$  function the top-hat basis set varies significantly from the mean. We show the difference between each basis set eigenfunction and the mean in Fig. 6.

In Fig. 7, we show the variance between the functions for a given basis set and order and the mean eigenfunctions for  $N = 100$ . In general, as the order increases the variance between the basis sets decreases. For some basis sets, such as Chebyshev, Laguerre and Legendre polynomials, there is already convergence even at a low order of  $\sim 40$ . At very low order  $N \lesssim 10$ , the eigenfunctions are very noisy. Other basis sets, such as Fourier and interpolation, reach convergence at a high order  $\sim 100$ . The Fourier basis set is noisy since high-order functions can introduce highly oscillatory modes into the eigenfunctions, this can also be seen in the  $N = 60$  panel in Fig. 5. The top-hat basis set requires an even higher order.<sup>4</sup> We note that there would be even better agreement between the non-top-hat basis sets and the mean if we excluded the top-hat basis set from this analysis.

<sup>4</sup> We have not extended this calculation to even higher order, since numerical effects involved in inverting (nearly singular) matrices of very high order start to become important; we choose a safe maximum order of 100 for this exercise.



**Figure 5.** The second and fourth best constrained eigenfunctions for the weak lensing tomographic survey considered. We show how the functions change as the maximum order in the expansion is varied. The thin lines are for each individual basis set – the key is given in Table 1. The thick black solid line shows the mean function over all basis sets at each order.



**Figure 6.** The difference between the eigenfunctions for each basis set and the mean eigenfunction (over all basis sets) for each order. We show this residual for the second and fourth best constrained eigenfunctions for the weak lensing tomographic survey considered. Each panel matches to the corresponding panel in Fig. 5, and the key is given in Table 1.

## 4 CONCLUSION

We have found that there is some ambiguity in the use of eigendecomposition in the literature to date and have aimed to clarify this situation. By investigating an arbitrary basis set expansion of  $w(z)$ , we have found that the technique of finding the eigenfunctions of  $w(z)$  from the Fisher matrix is sensitive to the basis set choice and the order of the truncated expansion.

We used the example of a weak lensing tomographic survey to demonstrate how the eigenfunction decomposition is sensitive to these choices. We find that for an Euclid/DUNE-like survey the best constrained eigenfunctions could be determined to an accuracy of  $\leq 1$  per cent using lensing alone (no priors).

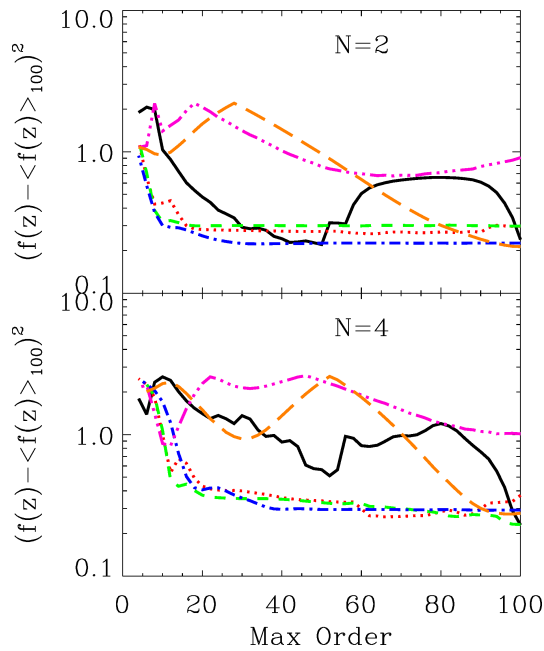
de Putter & Linder (2008) also presented a critique of the eigendecomposition approach which sheds further doubt on the technique’s validity, especially at low truncated order. They note that whilst the noise term on an eigenfunction can be predicted, it is in fact the signal-to-noise ratio that will be important for future surveys. We note then that a low-order expansion in a particular basis set is not robust and also has uncertain relevance in gauging the predicted performance of a future survey.

Because of these ambiguities in the reconstruction of  $w(z)$ , we recommend a move towards using physically motivated functional forms based on models. Physical parameters can be constrained

and models compared using evidence calculations (e.g. Heavens, Kitching & Verde 2007; Trotta 2007 for a link with Fisher matrices).

We summarize our conclusions here.

- (i) The parametrization of  $w(z)$  is an arbitrary basis set choice, and since we do not know the nature of dark energy in general any choice is valid.
- (ii) When using orthogonal basis sets, it is important to self-consistently include the weight function.
- (iii) When one refers to ‘binning’, one is actually referring to a top-hat basis set. Interpolation is also valid but should not be confused with binning.
- (iv) The set of eigenfunctions for a finite truncated basis set is not unique. There will always exist some eigenfunctions that are not common to all (truncated) eigenfunction sets.
- (v) When different basis sets are truncated to high order, the best constrained eigenfunctions will tend to agreement.
- (vi) When marginalizing over extra cosmological parameters, we show that finding the eigenfunctions of the full Fisher matrix leads to mixed non- $w(z)$  and  $w(z)$  eigenfunctions that are dependent on the non- $w(z)$  parametrization. We propose an alternative in which the marginalization affects the  $w(z)$  eigenvalues only, but not the functions themselves, by finding the eigenfunctions of the  $w(z)$  submatrix.



**Figure 7.** The variance between the eigenfunctions, reconstructed using a maximum order in the basis set expansion, and the mean eigenfunction using an order of 100. The key to the different basis sets lines is given in Table 1. The upper panel shows the variance for the second best constrained eigenfunctions, and the lower panel show the variance for the fourth best constrained eigenfunction.

(vii) To find agreement between the top  $\sim 4$  eigenfunctions, an order of at least 100 is required, for some basis set choices this is higher.

The convergence of the eigenfunctions depends on the original choice of basis sets – some converge more quickly than others. We find that Chebyshev, Legendre and Laguerre polynomials reach convergence more quickly than interpolation, top-hat or Fourier basis sets.

Even with an order of 100, the residuals between the reconstructed eigenfunctions cause the associated errors to vary by as much as a factor of 1–10 for the best  $\sim 4$  constrained functions.

We note that the dark energy figure of merit suggested by Albrecht et al. (2009) uses a top-hat basis set with 36 parameters.

We recommend that if an eigenfunction Fisher matrix analysis is needed, then a robust procedure should be followed with respect to marginalization such that results are not affected by non-dark energy assumptions and priors and that a very high order of expansion is needed. The convergence can be tested by investigating a variety of basis sets – using only a single basis set is insufficient.

The code used in the article will form part of the `ICOSMO` open source package and will be available in version 1.2 at <http://www.icosmo.org>.

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## APPENDIX A: EQUIVALENCE OF EIGENMATRICES AND JACOBIAN MATRICES

In this Appendix, we will show that the eigenmatrix is equal to a Jacobian matrix. The eigenvalue decomposition of a matrix can be written like

$$\mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T = \mathbf{F}. \quad (\text{A1})$$

The Jacobian transform of a Fisher matrix maps from one parameter set  $a_i$  to another  $b_i$

$$\mathbf{J}\mathbf{\Lambda}\mathbf{J}^T = \mathbf{F}, \quad (\text{A2})$$

where the matrix  $\mathbf{J}$  in this case maps from the set  $b$  to  $a$ . Where  $\mathbf{\Lambda}$  and  $\mathbf{F}$  are defined as

$$F_{ij} = \sum_x \left[ \sigma_c^{-2} \frac{\partial C(\phi; x)}{\partial a_i} \frac{\partial C(\phi; x)}{\partial a_j} \right]$$

$$\Lambda_{ij} = \sum_x \left[ \sigma_c^{-2} \frac{\partial C(\psi; x)}{\partial b_i} \frac{\partial C(\psi; x)}{\partial b_j} \right], \quad (\text{A3})$$

and the signal is parametrized in as

$$C(\phi; x) = \sum_i a_i \phi_i(x)$$

$$C(\psi; x) = \sum_i b_i \psi_i(x) \quad (\text{A4})$$



in  $\mathbf{F}$  and  $\Lambda$ , respectively. The elements of the Jacobian are

$$J_{ij} = \frac{\partial b_j}{\partial a_i}. \quad (\text{A5})$$

When transforming from one basis set to another, we can write the following:

$$\begin{aligned} a_n &= \frac{1}{c_n} \int_R f(x) \phi_n(x) M(x) dx \\ &= \frac{1}{c_n} \int_R \left[ \sum_m b_m \psi_m(x) \right] \phi_n(x) M(x) dx, \end{aligned} \quad (\text{A6})$$

so that the Jacobian can be written as

$$\frac{\partial a_n}{\partial b_m} = \frac{1}{c_n^\phi} \int_R \psi_m(x) \phi_n(x) M_\phi(x) dx, \quad (\text{A7})$$

where the weight  $M$  and constant  $c$  are for the  $\phi$  basis set.

If we assume that  $\psi$  are eigenfunctions of the  $\phi$ , then they can be reconstructed using linear combinations of the original basis functions

$$\psi_i(x) = \sum_j Q_{ij} \phi_j(x). \quad (\text{A8})$$

Since the decomposition of a matrix  $\mathbf{F}$  to a diagonal matrix  $\Lambda$  in equations (A1) and (A2) is unique, it can easily be seen that the eigenmatrix is in fact a Jacobian. This can be shown in the following way. The Jacobian is written like

$$\frac{\partial a_n}{\partial b_m} = \frac{1}{c_n^\phi} \int_R \psi_m(x) \phi_n(x) M_\phi(x) dx. \quad (\text{A9})$$

We construct new basis sets as linear combinations of the old so that

$$\frac{\partial a_n}{\partial b_m} = \frac{1}{c_n^\phi} \int_R Q_{mk} \phi_k(x) \phi_n(x) M_\phi(x) dx, \quad (\text{A10})$$

this leads to

$$\begin{aligned} \frac{\partial a_n}{\partial b_m} &= \frac{1}{c_n^\phi} Q_{mk} \int_R \phi_k(x) \phi_n(x) M_\phi(x) dx \\ &= \frac{1}{c_n^\phi} Q_{mk} \delta_{kn} c_n^\phi \\ J_{mn} &= Q_{mn}. \end{aligned} \quad (\text{A11})$$

## APPENDIX B: NON-UNIQUENESS OF THE EIGENVALUES

Here, we will show that if the residual between the reconstruction of a basis set using another is non-zero, then the eigenvalues obtained

from each set via an eigenvalue decomposition of the Fisher matrices are not equal.

The rotation matrix from basis  $\phi$  to  $\psi$  can be written as

$$J_{ij} = \frac{1}{c^\phi} \int_R dx \psi_i(x) \phi_j(x) M^\phi(x). \quad (\text{B1})$$

We now assume that the new basis functions can be written as the sum of some linear combination of the old basis functions plus some residual (equation 18)

$$J_{ij} = \frac{1}{c^\phi} \int_R dx [J_{ik}^A \phi_k(x) + R_i(x)] \phi_j(x) M^\phi(x), \quad (\text{B2})$$

where the rotation matrix  $J^A$  rotates the old Fisher matrix to the new Fisher matrix assuming no residual. This can now be written like

$$\begin{aligned} J_{ij} &= J_{ij}^A + T_{ij} \\ T_{ij} &= \frac{1}{c^\phi} \int_R dx R_i(x) \phi_j(x) M^\phi(x). \end{aligned} \quad (\text{B3})$$

In the following, we will use subscripts for the basis for clarity. We now rotate from  $\phi$  to  $\psi$ , then diagonalize the Fisher matrix of  $\psi$  to get  $\Lambda_\psi$ , this can be written as

$$J_{\psi\Lambda\psi}^{-1} (J_{\phi\psi}^A + T_{\phi\psi})^{-1} F_{\phi\phi} (J_{\phi\psi}^A + T_{\phi\psi}) J_{\psi\Lambda\psi} = \Lambda_\psi. \quad (\text{B4})$$

We can also diagonalize  $F_{\phi\phi}$  directly to get  $\Lambda_\phi$

$$J_{\phi\Lambda\phi}^{-1} F_{\phi\phi} J_{\phi\Lambda\phi} = \Lambda_\phi. \quad (\text{B5})$$

If we assume that  $\Lambda_\psi = \Lambda_\phi = \Lambda$ , then comparing equations (B4) and (B5) the following must be true:

$$\begin{aligned} (J_{\phi\psi}^A + T_{\phi\psi}) J_{\psi\Lambda} &= J_{\phi\Lambda} \\ J_{\phi\psi}^A J_{\psi\Lambda} + T_{\phi\psi} J_{\psi\Lambda} &= J_{\phi\Lambda}, \end{aligned} \quad (\text{B6})$$

since we have assumed  $\Lambda_\psi = \Lambda_\phi$  the first pair of rotation matrices commutes that (however in general this is not true)  $J_{\phi\psi} J_{\psi\Lambda} = J_{\phi\Lambda}$ , and we have

$$J_{\phi\Lambda} + T_{\phi\psi} J_{\psi\Lambda} = J_{\phi\Lambda} \quad (\text{B7})$$

which leads to

$$\begin{aligned} T_{\phi\psi} J_{\psi\Lambda} &= 0 \\ T_{\phi\psi} &= 0. \end{aligned} \quad (\text{B8})$$

So if  $\Lambda_\psi = \Lambda_\phi$ , then  $T_{\psi\phi} = 0$ . By deduction we can then assert that if  $T_{\psi\phi} \neq 0$ , then  $\Lambda_\psi \neq \Lambda_\phi$  and the eigenvalues are not unique.

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