Uncorrelated Modes of the Nonlinear Power Spectrum

A. J. S. Hamilton
JILA and Dept. Astrophysical & Planetary Sciences, Box 440, U. Colorado, Boulder CO 80309, USA; Andrew.Hamilton@Colorado.EDU; http://casa.colorado.edu/~ajsh

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ABSTRACT
Nonlinear evolution causes the galaxy power spectrum to become broadly correlated over different wavenumbers. It is shown that prewhitening the power spectrum – transforming the power spectrum in such a way that the noise covariance becomes proportional to the unit matrix – greatly narrows the covariance of power. The eigenfunctions of the covariance of the prewhitened nonlinear power spectrum provide a set of almost uncorrelated nonlinear modes somewhat analogous to the Fourier modes of the power spectrum itself in the linear, Gaussian regime. These almost uncorrelated modes make it possible to construct a near minimum variance estimator and Fisher matrix of the prewhitened nonlinear power spectrum analogous to the Feldman-Kaiser-Peacock estimator of the linear power spectrum. The paper concludes with summary recipes, in gourmet, fine, and fastfood versions, of how to measure the prewhitened nonlinear power spectrum from a galaxy survey in the FKP approximation. An Appendix presents FFTLog, a code for taking the fast Fourier or Hankel transform of a periodic sequence of logarithmically spaced points, which proves useful in some of the manipulations.

Key words: cosmology: theory – large-scale structure of Universe

1 INTRODUCTION
Most of the information about cosmological parameters bottled inside current and coming galaxy surveys, notably the Two-Degree Field Survey (2dF) (Colless 1998; Folkes et al. 1999) and the Sloan Digital Sky Survey (SDSS) (Gunn & Weinberg 1995; Margon 1998), lies in the nonlinear regime. Even in the linear regime, nonlinearities perturb.

At large, linear scales, the power spectrum – the covariance of the density field, expressed in the Fourier representation – is the preeminent measure of large scale structure. It is a generic, though by no means universal, prediction of inflation (Turner 1997) that linear density fluctuations should be Gaussian. More generally, primordial fluctuations should be Gaussian whenever they result from superpositions of many independent processes, thanks to the central limit theorem. Observations of large scale structure are consistent with linear density fluctuations being Gaussian (Bouchet et al. 1993; Juszkiewicz, Bouchet, & Colombi 1993; Gaztañaga 1994; Gaztañaga & Frieman 1994; Nusser, Dekel & Yahil 1995; Stirling & Peacock 1996; Colley 1997; Frieman & Gaztañaga 1999) although the evidence is not definitive (White 1999). If linear density fluctuations are Gaussian, then the 3-point and higher irreducible moments are zero, so that the covariance of the density field contains complete information about the statistical properties of the field, hence all information about cosmological parameters. Compared to other measures of covariance such as the correlation function, the power spectrum has the additional advantage that estimates of power at different wavenumbers are uncorrelated, for Gaussian fluctuations. This asset of the power spectrum has the additional advantage that estimates of power at different wavenumbers are uncorrelated, for Gaussian fluctuations. This asset of the power spectrum is intimately related to the assumption that the field is statistically translation invariant, and to the fact that Fourier modes are eigenfunctions of the translation operator.

At smaller, nonlinear scales, the power spectrum loses some of its glow. Nonlinear evolution drives the density...
field away from Gaussianity, coupling Fourier modes, feeding higher order moments, and causing power at different wavenumbers to become correlated. The broad extent of the correlation of the nonlinear power spectrum has been emphasized by Melkin & White (1999) and Scoccimarro, Zar- 
darriaga & Hui (1999), and is illustrated in Figure B of the present paper.

The purpose of the present paper is to show how to unfold the nonlinear power spectrum into a set of nearly uncorrelated modes, somewhat analogous to the Fourier modes of the power spectrum itself in the linear, Gaussian regime. The present paper is a natural successor to Hamilton (1997a,b, hereafter Papers 1 and 2), which showed how to derive the minimum variance estimator and Fisher matrix of the power spectrum of a galaxy survey in the Feldman, Kaiser & Peacock (1994, hereafter FKP) approximation, for Gaussian spectrum of a galaxy survey in the Feldman, Kaiser & Pea-
cock (1994, hereafter Paper 4), describes how to complete the processing of the power spectrum itself in the linear, Gaussian regime. The procedures described in the present paper should assist future galaxy surveys will constrain cosmological parameters (Binggeli, Sandage & Tammann 1988; Willmer 1997; Tresse et al. 1999; Blanton et al. 1999; Benson et al. 1999; Bernardoe & Scha-
effer 1999; Coles, Melott & Munshi 1999). It further assumes that uncertainties arising either from the selection function (Binggeli, Sandage & Tammann 1988; Willmer 1997; Tresse 1999) or from evolution in the cosmological volume element or the galaxy population, are negligible.

Several authors have recently published estimates of how well measurements of the power spectrum from future galaxy surveys will constrain cosmological parameters (Tegmark 1997b; Goldberg & Strauss 1998; Hu, Eisenstein & Tegmark 1998; Eisenstein, Hu & Tegmark 1998, 1999). The procedures described in the present paper should assist this enterprise.

The aims of the present paper are complementary to those of Bond, Jaffe & Knox (1998b). The question Bond et al. considered was: If the power spectrum (of the Cosmic Microwave Background, specifically) is quadratically compressed (Tegmark 1997a; Tegmark et al. 1997, 1998) into a set of band-powers, then what is the best way to use those band-powers in Maximum Likelihood estimation of parameters? For example, one general procedure is to use not the band-powers themselves, but rather functions of the band-powers arranged such that their variances remain constant as the prior power is varied. Bond et al. argued that the likelihood function is then more nearly Gaussian. The pur-
pose of this paper and Paper 4 is rather to arrive at the point where one has decorrelated band-powers to work with in the first place.

The plan of this paper is as follows. Section 2 sets up the notation and defines reference material needed in subsequent sections. Section 3 goes through the difficulties one meets in attempting to measure the nonlinear power spectrum in minimum variance fashion, and describes how to overcome them. Section 4 reveals the unexpectedly nice properties of the prewhitened covariance of the power spectrum, key to the whole enterprise of this paper. Section 5 defines the prewhitened power spectrum. Sections 6 and 7 show how the approximations motivated in previous sections lead to a practical way to evaluate the Fisher matrix of the prewhitened nonlinear power, and to measure the prewhitened nonlinear power spectrum from a galaxy survey. Section 8 discusses how to evaluate the Fisher matrix and nonlinear power spectrum using the FKP approximation alone, without any additional approximation. Section 9 summarizes the results of previous sections into recipes, in gourmet, fine, and fastfood versions, for measuring nonlinear power, the end product being a set of uncorrelated prewhitened nonlinear band-powers, with error bars, over some prescribed grid of wavenumbers. Section 10 summarizes the conclusions. Appen
dix B gives details of FFTLog, a code for taking the fast Fourier or Hankel transform of a periodic sequence of logarithmically spaced points.

2 PRELIMINARIES

This section contains reference material needed in subsequent sections. The reader interested in new results may like to skip to the next section, referring back to the present section as needed.

2.1 Data, parameters

'He will, of course, use maximum likelihood because his text-
books have told him that' – E. T. Jaynes (1996, p. 624).

According to Bayes’ theorem, the probability distribution of parameters \( \theta_a \), given data \( \delta_i \), is, up to a normalization factor, the product of the prior probability with the likelihood function \( L(\delta_i|\theta_a) \). The data \( \delta_i \) in a galaxy survey can be taken to be overdensities \( \delta(r) \) at positions \( r \) in the survey

\[
\delta(r) = \frac{n(r) - \bar{n}(r)}{\bar{n}(r)}
\]

where \( n(r) \) is the observed number density of galaxies, and \( \bar{n}(r) \) is the selection function. The parameters \( \theta_a \) are, for the present purpose, some parametrization of the galaxy power spectrum; the focus of this paper is on the case where the parameters are the power spectrum \( \xi \), itself.

This paper conforms to the common convention used by cosmologists to relate the power spectrum \( \xi(k) \) in Fourier space to the correlation function \( \xi(r) \) in real space, notwithstanding the extraneous factors of \( 2\pi \) that result:

\[
\xi(k) = \int e^{ik \cdot r} \xi(r) \, d^3r = \int_0^\infty j_0(kr) \xi(r) \, 4\pi r^2 \, dr
\]

\[
\xi(r) = \int e^{-ik \cdot r} \xi(k) \frac{dk}{(2\pi)^3} = \int_0^\infty j_0(kr) \xi(k) \frac{4\pi k^2 \, dk}{(2\pi)^3}
\]

where \( j_0(x) = \sin x / x \) is a spherical Bessel function.

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2.2 Hilbert space

As in Paper 1, it is convenient to adopt a notation in which Latin indices \( i, j, \ldots \) refer to 3-dimensional positions, while Greek indices \( \alpha, \beta, \ldots \) run over the space of parameters, and more specifically over the 1-dimensional space of wavenumbers or pair separations.

For generality, brevity, and ease of manipulation, it is convenient to treat quantities such as the data vector \( \delta_i \), or the power spectrum \( \xi_\alpha \), as vectors in a Hilbert space (for a didactic exposition, see Hamilton 1998 §3.3). Such vectors have a meaning independent of the particular basis, i.e. complete set of linearly independent functions, with respect to which they might be expressed. For example, the data vector has components \( \delta_r \) when expressed in real space, or components \( \delta_k \) when expressed in Fourier space, but from a Hilbert space point of view these are the same vector, and in this paper they are both denoted by the same symbol \( \delta \).

Similarly the power spectrum \( \xi_\alpha \) has components \( \xi_k \) when expressed in Fourier space, or \( \xi_\alpha \) when expressed in real space, but again from a Hilbert space point of view these are the same vector, and in this paper they are both denoted by the same symbol \( \xi_\alpha \).

Latin indices \( i, j, \ldots \), on vectors and matrices run over the 3-dimensional space of positions \( r \), or more generally over any 3-dimensional basis of the Hilbert space. Unless stated otherwise, repeated pairs of indices signify the inner product in Hilbert space, as in

\[
a^\dagger b = \int a^\dagger(r)b(r)\,d^3r = \int a^\dagger(k)b(k)\,d^3k/(2\pi)^3.
\]

By definition, the inner product is a scalar, the same quantity independent of the choice of basis. The raised index \( a^\dagger \) denotes the Hermitian conjugate (if the basis is orthonormal) of the vector \( a \). One of the indices in an inner product is always raised, the other lowered. In this paper, all vectors in the Hilbert space are real-valued when expressed in real space, so that \( a^\dagger(r) = a(r) \) and \( a^\dagger(k) = a(-k) \).

Adhering to the raised/lowered index convention serves as a useful reminder that one of the pair of vectors in an inner product is a Hermitian conjugate (if the basis is orthonormal). In Fourier space, for example, this means using \(-k\) for one index (raised) and \(+k\) for the other index (lowered) of an inner product.

Greek indices \( \alpha, \beta, \ldots \), run over the space of 1-dimensional pair separations \( r \), or wavenumbers \( k \), or more generally over any 1-dimensional basis in the associated Hilbert space. Again, unless stated otherwise, repeated indices signify the inner product

\[
a^{\alpha\beta}b_\alpha = \int a^{\alpha\dagger}(r)b(r)\,4\pi r^2\,dr = \int a^{\alpha\dagger}(k)b(k)\,4\pi k^2dk/(2\pi)^3.
\]

which is again a scalar, the same quantity independent of the choice of basis. Again, in this paper all vectors in the Hilbert space are real-valued in real space, so \( a^{\alpha\dagger}(r) = a(r) \) and \( a^{\alpha\dagger}(k) = a(k) \). Although there is no distinction in this case between vectors with raised and lowered indices in either real or Fourier space, adhering to the raised/lowered index convention again serves as a useful reminder.

The unit matrix \( 1_\alpha^{\alpha\beta} \) in any representation is defined such that its inner product with any vector \( a_\beta \) leaves the vector unchanged,

\[
1_\alpha^{\beta\beta} a_\beta = a_\beta 1_\alpha^{\beta\beta} = a_\alpha\;.
\]

In the continuous real representation, the unit matrix is

\[
1_\alpha^{\beta\beta} = \delta_3D(r_\alpha - r_\beta)
\]

where \( \delta_3D(r_\alpha - r_\beta) \) denotes the 3-dimensional Dirac delta-function, defined such that

\[
\int \delta_3D(r_\alpha - r_\beta)\,4\pi r_\alpha^2dr_\alpha = 1\;.
\]

In the continuous Fourier representation, the unit matrix is

\[
1_\alpha^{\beta\beta} = (2\pi)^3\delta_3D(k_\alpha - k_\beta)
\]

again a 3-dimensional Dirac delta-function.

2.3 Discretization of matrices

Many of the operations in this paper involve manipulations of matrices in the 1-dimensional space of separations. Continuous matrices must be discretized to manipulate them numerically. Discretization should be done in such a way as to preserve the inner product \( \langle \xi, \xi \rangle \), so that integration over the volume element, \( 4\pi r^2dr \) in real space, or \( 4\pi k^2dk/(2\pi)^3 \) in Fourier space, translates into summation in the corresponding discrete space. This ensures that matrix operations such multiplication, diagonalization, and inversion can be done in the usual fashion.

Most of the manipulations in this paper are done in Fourier space on a logarithmically spaced grid of wavenumbers \( k_\alpha \). In this case, a continuous vector \( a(k_\alpha) \) is discretized by multiplying it by \( [4\pi k_\alpha^3\Delta\ln k/(2\pi)^3]^{1/2} \)

\[
a(k_\alpha) \to a_{k_\alpha} = a(k_\alpha)\left[4\pi k_\alpha^3\Delta\ln k/(2\pi)^3\right]^{1/2}
\]

and a continuous matrix \( A(k_\alpha, k_\beta) \) is discretized by multiplying it by \( 4\pi(k_\alpha k_\beta)^{3/2}\Delta\ln k/(2\pi)^3 \)

\[
A(k_\alpha, k_\beta) \to A_{k_\alpha k_\beta} = A(k_\alpha, k_\beta)\left[4\pi(k_\alpha k_\beta)^{3/2}\Delta\ln k/(2\pi)^3\right].
\]

The unit matrix \( (2\pi)^3\delta_3D(k_\alpha - k_\beta) \) in the continuous Fourier representation translates to the unit matrix \( 1_{\alpha\beta} \) in the discrete case

\[
(2\pi)^3\delta_3D(k_\alpha - k_\beta) \to 1_{\alpha\beta}.
\]

Similarly, a continuous vector \( a(r_\alpha) \) in real space is discretized on to a logarithmically spaced grid of separations \( r_\alpha \) by multiplying the vector by \( [4\pi r_\alpha^3\Delta\ln r]^{1/2} \)

\[
a(r_\alpha) \to a_{r_\alpha} = a(r_\alpha)\left[4\pi r_\alpha^3\Delta\ln r\right]^{1/2}
\]

and a continuous matrix \( A(r_\alpha, r_\beta) \) is discretized by multiplying it by \( 4\pi(r_\alpha r_\beta)^{3/2}\Delta\ln r \)

\[
A(r_\alpha, r_\beta) \to A_{r_\alpha r_\beta} = A(r_\alpha, r_\beta)\left[4\pi(r_\alpha r_\beta)^{3/2}\Delta\ln r\right].
\]

The unit matrix \( \delta_3D(r_\alpha - r_\beta) \) in the continuous real representation translates to the unit matrix \( 1_{\alpha\beta} \) in the discrete case

\[
\delta_3D(r_\alpha - r_\beta) \to 1_{\alpha\beta}.
\]

The transformation between Fourier and real space for logarithmically spaced wavenumbers \( k_\alpha \) and separations \( r_\alpha \) may be accomplished with FFTLog (Appendix B).
2.4 Gaussian density field

If the density distribution $\delta(r)$ were Gaussian – which is not true in the present case – then one would have the luxury of being able to write down an explicit Gaussian likelihood function

$$\mathcal{L} \propto \frac{1}{|C|^{1/2}} \exp \left( -\frac{1}{2} \delta C^{-1} \delta_j \right) \quad (16)$$

where $|C|$ and $C^{-1}$ are the determinant and inverse of the covariance matrix $C$ of overdensities $C_{ij} \equiv \langle \delta_i \delta_j \rangle$.

Angle-brackets here and throughout this paper signify averages over possible data sets $\delta$, predicted by the likelihood function

$$(t) \equiv \int t \mathcal{L}(\delta|\theta_0) d[\delta] \quad (18)$$

Maximum Likelihood (ML) estimates $\hat{\theta}_0$ of the parameters $\theta_0$ (the hat distinguishing the estimate $\hat{\theta}_0$ from the true value $\theta_0$) are given by the vanishing of the vector of partial derivatives of the log-likelihood function

$$\frac{\partial \ln \mathcal{L}}{\partial \theta_0} = \frac{1}{2} \frac{\partial C_{ij}}{\partial \theta_0} C^{-1} \delta C_{kl} \partial \theta_0$$

$$\frac{\partial \ln \mathcal{L}}{\partial \theta_0} \bigg|_{\theta_0=\hat{\theta}_0} = 0 \quad (19)$$

The covariance $(\Delta \hat{\theta}_0, \Delta \hat{\theta}_0)$ of the estimated parameters is given approximately by the inverse of the Fisher information matrix $F^{\alpha \beta}$, defined to be minus the expectation value of the matrix of second partial derivatives of the log-likelihood function

$$F^{\alpha \beta} \equiv -\langle \partial^2 \ln \mathcal{L} / \partial \theta_0^\alpha \partial \theta_0^\beta \rangle = \frac{1}{2} \frac{\partial C_{ij}}{\partial \theta_0^\alpha} C^{-1} \delta C_{kl} \partial \theta_0^\beta \partial \theta_0^\beta \quad (21)$$

$$\langle \Delta \hat{\theta}_0, \Delta \hat{\theta}_0 \rangle \approx F^{-1} \quad (22)$$

The approximation (22) is exact if the estimated parameters $\hat{\theta}_0$ are Gaussianly distributed about their expectation values. The central limit theorem asserts that the parameters become Gaussianly distributed in the asymptotic limit of a large amount of data.

It is commonly assumed, and the same assumption is adopted here, that the dominant source of variance in a galaxy survey is a combination of cosmic (sample) variance and shot-noise arising from the discrete sampling of galaxies. If the sampling of galaxies is random – a Poisson process – then the covariance $C_{ij}$ is a sum of the cosmic covariance $\xi_{ij}$ with Poisson sampling noise $N_{ij}$

$$C_{ij} = \xi_{ij} + N_{ij} \quad (23)$$

In the real representation, the cosmic covariance $\xi_{ij}$ is the correlation function

$$\xi_{ij} = \xi(|r_i - r_j|) \quad (24)$$

and the noise matrix $N_{ij}$ is the diagonal matrix

$$N_{ij} = \frac{\delta_{3D}(r_i - r_j)}{n(r_i)} \quad (25)$$

with $\delta_{3D}(r_i - r_j)$ a 3-dimensional Dirac delta-function. In the Fourier representation the cosmic covariance $\xi_{ij}$ is the diagonal matrix $\xi_{ij} = (2\pi)^3 \delta_{3D}(k_i + k_j) \xi(k_i)$

whose eigenvalues $\xi(k_i)$ constitute the power spectrum.

The focus of this paper is on the case where the parameters $\theta_0$ are the power spectrum $\xi_0$ itself (in this paper the cosmic covariance function $\xi_0$, expressed in an arbitrary representation, will often be referred to as the ‘power spectrum’, even though this name is commonly reserved for the covariance $\xi(k)$ expressed in Fourier space; no confusion should result). In this case the covariance $C_{ij}$ is a linear function of the parameters $\xi_0$

$$C_{ij} = D_{ij} \xi_0 + N_{ij} \quad (27)$$

where in real space $\xi_0 = \xi(r_0)$ is the correlation function, and

$$D_{ij} = \delta_{3D}(\langle r_i - r_j \rangle - r_0) \quad (28)$$

is a 3-dimensional Dirac delta-function, equation (15), while in Fourier space $\xi_0 = \xi(k_0)$ is the thing commonly called the power spectrum, and

$$D_{ij} = (2\pi)^3 \delta_{3D}(k_i + k_j) \delta_{3D}(k_i - k_j) \quad (29)$$

It follows from equations (19) and (20) that the ML estimator $\hat{\xi}_0$ of the power spectrum, for Gaussian fluctuations, is that solution of

$$\hat{\xi}_0 = \frac{1}{2} F^{-1} \partial \xi_0 \partial \theta_0$$

$$\partial \xi_0 \partial \theta_0 \approx F^{-1} \xi_0$$

for which the estimate is equal to the prior, $\hat{\xi}_0 = \xi_0$. The variance of the ML estimator is

$$\langle \Delta \hat{\xi}_0, \Delta \hat{\xi}_0 \rangle \approx F^{-1} \xi_0$$

and the Fisher matrix is

$$F^{\alpha \beta} = \frac{1}{2} D_{ij} \partial \xi_0 \partial \theta_0 \partial \theta_0$$

If the prior power $\xi_0$ is regarded as fixed, then equation (28) yields an estimated power $\hat{\xi}_0$ that is quadratic in overdensities $\delta$. If this estimated power is folded back into the prior, then equation (25) with the revised prior yields another estimate of power. Iterated to convergence, the result is the ML estimator of the power. It is to be noted that even without iteration, equation (28) yields a measurement of power that (as long as the prior is at least roughly correct) should already be a good approximation, since ‘if the prior matters, then you are not learning much from the data’, to quote one of the refrains from the 1997 Aspen workshop on Precision Measurement of Large Scale Structure.

The question of how to apply quadratic estimators (such as given by equation 28) to measure the power spectrum is addressed by Tegmark et al. (1998) for galaxies, and by Tegmark (1997a), Tegmark et al. (1997), and Bond, Jaffe & Knox (1998a,b) for the CMB.

2.5 Non-Gaussian density field

Ultimately, one might look forward to a wondrous $N$-body machine able to compute the probability distribution of linear initial conditions given noisy and incomplete data from a survey (Narayanan & Weinberg 1998; Monaco & Efstathiou 1999; and references therein).

In the meantime it is far from clear what to write down
as a likelihood function for the nonlinear density field (Dodelson, Hui & Jaffe 1999). Certainly it would be a bad idea to use a Gaussian likelihood function for a non-Gaussian density field, since that would lead to a serious underestimate of the true uncertainty in the measured nonlinear power spectrum.

An alternative procedure is to seek a minimum variance unbiased estimator of power. Now the power spectrum is by definition a covariance of overdensities, and by the presumption of Poisson sampling, any a priori weighted sum of quantities quadratic in observed over-densities (with self-terms excluded, to eliminate shot-noise) provides an unbiased estimate of the power spectrum linearly windowed in some fashion. It was shown in §2.3 of Paper 1 that, amongst estimators quadratic in observed over-densities $\delta$, the unbiased estimator $\hat{\xi}_a$ of the power spectrum having minimum variance is

$$\hat{\xi}_a = F_{a\beta} D_{ij} \xi^{ijkl} (\delta_h \delta_l - \bar{N}_{kl})$$

(33)

with variance

$$\langle \Delta \hat{\xi}_a \Delta \hat{\xi}_a \rangle = F_{a\beta}$$

(34)

where $F_{a\beta}$ is the Fisher matrix

$$F_{a\beta} = D_{ij} C_{ijkl} D_{kl}$$

(35)

$C_{ijkl}$ is the covariance of shot-noise-subtracted products of over-densities

$$C_{ijkl} \equiv \langle (\delta_h \delta_l - \bar{N}_{kl} - \xi_{ik}) (\delta_h \delta_l - \bar{N}_{kl} - \xi_{kl}) \rangle$$

(36)

and $C_{ijkl}$ is its inverse, meaning $C_{ijmn} C_{ijkl}^{-1} = \text{Sym}_{ijkl} 1_{ij}^\dagger 1_{kl}$. The symbol $\text{Sym}_{ijkl}$ signifies symmetrization over its under-scripts, as in

$$\text{Sym}_{ijkl} A_{ij} = \frac{1}{2} (A_{ij} + A_{ji})$$

(37)

The quantity $\bar{N}_{kl}$ in equations (33) and (34) is the ‘actual’ shot-noise, the contribution to $\delta_h \delta_l$ from self-pairs of galaxies, pairs consisting of a galaxy and itself. The actual shot-noise $N_{kl}$ in a survey is to be distinguished from its expectation value $\bar{N}_{kl} \equiv \langle \bar{N}_{kl} \rangle$. If the expected shot-noise $N_{kl}$ is used in equation (33) in place of the actual shot-noise, then additional terms (given in eq. [8] of Paper 1) appear in the covariance matrix $\mathcal{C}_{ijkl}$, increasing the variance of the estimator. Why does the ML estimator $\hat{\xi}_a$ in the Gaussian case, equation (34), involve the expected shot-noise $N_{kl}$ rather than the actual shot-noise $\bar{N}_{kl}$? Because a discretely sampled Gaussian field is not really Gaussian, except in the limit where a cubic wavelength contains many galaxies, so the assumption of a Gaussian likelihood function is not strictly correct. In fact it is plain that the Gaussian ML estimator $\hat{\xi}_a$ would also be improved if the actual shot-noise $N_{kl}$ were used in place of the expected shot-noise $\bar{N}_{kl}$ in equation (34), since using the actual shot-noise exploits additional information about the character of the Poisson sampling that is discarded by the Gaussian likelihood. However, as discussed by Tegmark et al. (1998 Appendix A), the gain from subtracting the actual versus the expected shot-noise is in practice small at linear scales, where a cubic wavelength is likely to contain many galaxies.

In the same Poisson sampling approximation as equation (37), the covariance $C_{ijkl}$ of shot-noise-subtracted products of over-densities, equation (38), is, in the real representation with no implicit summation,

$$C_{ijkl} = \xi_{ik} \xi_{jl} + \xi_{il} \xi_{jk} + \eta_{ijkl} + [N_{ik} (\xi_{jl} + \xi_{jl}) + (i \leftrightarrow j, k \leftrightarrow l)] (4 \text{ terms})$$

(38)

in which the top line is the 4-point, the middle the 3-point, and the bottom line the 2-point contribution to the covariance, as illustrated in Figure 1. For Gaussian density fluctuations equation (39) reduces to

$$C_{ijkl} = 2 \text{ Sym}_{ijkl} C_{ij} C_{jl}$$

(39)

with inverse

$$C_{ijkl}^{-1} = \frac{1}{2} \text{ Sym}_{ijkl} C_{ij}^{-1} C_{ij}^{-1}$$

(40)

It follows from equation (3) that for Gaussian fluctuations the minimum variance estimator of the power spectrum, equation (33), is the same as the ML estimator, equation (34), if the estimate is folded back into the prior and iterated to convergence (modulo the comments about shot-noise in the previous paragraph).

3 PROBLEMS

3.1 FKP approximation

Calculating the minimum variance estimate $\hat{\xi}_a$ of the power spectrum, equation (33), involves the formidable problem of inverting the pair covariance $\mathcal{C}_{ijkl}$, a rank 4 matrix of 3-dimensional quantities. Whereas for Gaussian fluctuations the rank 4 matrix $\mathcal{C}_{ijkl}$ factorizes into a product of rank 2 matrices, equation (39), for non-Gaussian fluctuations it does not factorize. Again, whereas for Gaussian fluctuations it may be possible, at least at the largest scales, to pixellize a survey into large enough pixels that brute force numerical inversion is feasible, for non-Gaussian fluctuations brute force inversion is quite impossible.

A natural way to simplify the problem is to adopt the Feldman, Kaiser & Peacock (1994, FKP) approximation, where the selection function $\bar{n}(r)$ is taken to be locally constant. The FKP approximation is expected to be valid at wavelengths much smaller than the characteristic size of the survey. Section 5 of Paper 1 terms this the ‘classical’ approximation, since it is valid to the extent that the position and wavelength of a density mode can be measured simultaneously. While the FKP approximation is liable to break down at larger scales, particularly for pencil beam or slice
surveys, it should be a good approximation at smaller, non-linear scales, especially in surveys with broad contiguous sky coverage.

Even if the selection function \( \tilde{\eta} \) is taken to be constant, the general problem of inverting the rank 4 matrix \( \mathbf{C}_{ijkl} \) remains intractible. Notice however that \( \mathbf{C}^{-1ij\beta\gamma} \) appears multiplied in both equations (43) and (45) by the matrix \( D_{ij}^{\beta} \). Now \( D_{ij}^{\beta} \) has translation and rotation symmetry, and in the FKP approximation the matrix \( \mathbf{C}_{ijkl} \) also has translation and rotation symmetry, the selection function \( \tilde{\eta} \) being constant. Indeed, inspection of equation (38) reveals that the matrix \( \mathbf{C}_{ijkl} \) remains translation and rotation invariant even if the selection functions \( \tilde{n}_i \) and \( \tilde{n}_j \) at positions \( i \) and \( j \) are two different constants. It follows that the combination \( \mathbf{C}_{ijkl}D_{ij}^{\beta} \) is likewise translation and rotation symmetric, which implies that it can be expressed in the form

\[
\mathbf{C}_{ijkl}D_{ij}^{\beta} = \mathbf{C}_{\alpha\beta}(\tilde{n}_i, \tilde{n}_j)D_{ij}^\beta
\]

for some matrix \( \mathbf{C}_{\alpha\beta} \), which we can term the ‘reduced’ covariance matrix. Equation (41) is the FKP approximation, expressed in concise mathematical form; additional details of the justification of this equation are provided in Appendix A. The reduced matrix is written in equation (41) as \( \mathbf{C}_{\alpha\beta}(\tilde{n}_i, \tilde{n}_j) \) to emphasize the fact that it is a function of the selection functions \( \tilde{n}_i \) and \( \tilde{n}_j \) at positions \( i \) and \( j \); note that no implicit summation over \( i \) or \( j \) is intended on the right hand side of equation (41). Inspection of equation (45) for \( \mathbf{C}_{ijkl} \) shows that the reduced covariance \( \mathbf{C}_{\alpha\beta}(\tilde{n}_i, \tilde{n}_j) \) takes the form

\[
\mathbf{C}_{\alpha\beta}(\tilde{n}_i, \tilde{n}_j) = 2 \left[ K_{\alpha\beta} + (\tilde{n}_i^{-1} + \tilde{n}_j^{-1})J_{\alpha\beta} + \tilde{n}_i^{-1} \tilde{n}_j^{-1}H_{\alpha\beta} \right]
\]

a linear combination of 4-point, 3-point, and 2-point contributions \( K_{\alpha\beta}, J_{\alpha\beta}, \) and \( H_{\alpha\beta} \). Multiplying equation (41) by \( \mathbf{C}^{-1\gamma\alpha\beta} \) shows that the inverse of \( \mathbf{C}_{ijkl} \) is similarly related to the inverse of the reduced matrix \( \mathbf{C}_{\alpha\beta} \).

\[
\mathbf{C}^{-1ij\beta\gamma}D_{ij}^{\alpha} = \mathbf{C}^{-1\alpha\beta}(\tilde{n}_i, \tilde{n}_j)D_{ij}^\beta.
\]

Physically, to the extent that the selection functions \( \tilde{n}_i \) and \( \tilde{n}_j \) at positions \( i \) and \( j \) are constants, the minimum variance pair-weighting attached to a pair \( ij \) should be a function only of the separation \( \alpha \) of the pair, not of their position or orientation. Just as \( \mathbf{C}_{ijkl} \) is the covariance between a pair \( ij \) and another pair \( kl \), so the reduced covariance \( \mathbf{C}_{\alpha\beta} \) is the covariance between a pair separated by \( \alpha \) and another pair separated by \( \beta \).

In the FKP approximation given by equation (41), the minimum-variance estimate (43) of the power spectrum is

\[
\hat{C}_\alpha = F_{\alpha\beta}^{-1}\mathbf{C}^{-1\beta\gamma}D_{ij}^{\gamma}(\delta_{i\delta} - \tilde{N}_{ij})
\]

and the associated Fisher matrix (45) is

\[
F_{\alpha\beta} = \mathbf{C}^{-1\alpha\gamma}D_{ij}^{\gamma}D_{ij}^{\beta}.
\]

Notice that the approximate Fisher matrix given by this equation (46) is not symmetric, whereas the original Fisher matrix, equation (43), was symmetric. The asymmetry results from the asymmetry of the FKP approximation, equation (41). The approximate expression (43) would be symmetric if the FKP approximation were exact, and in practice it should be nearly symmetric; if not, it is a signal that the FKP approximation is breaking down.

To ensure symmetry of the Fisher matrix, one might be inclined at this point to symmetrize equation (41), since after all an equally good approximation to the Fisher matrix would be the same expression (43) with the indices swapped on the right hand side, \( \alpha \leftrightarrow \beta \). However, it is desirable that the FKP estimator \( \hat{\xi}_\alpha \), equation (41), should be unbiased, meaning that

\[
\langle \hat{\xi}_\alpha \rangle = \xi_\alpha.
\]

Averaging equation (46), gives, since \( \langle \delta_i \delta_j - \tilde{N}_{ij} \rangle = D_{ij}^\alpha \xi_\alpha \)

\[
\langle \hat{\xi}_\alpha \rangle = F_{\alpha\beta}^{-1}\mathbf{C}^{-1\beta\gamma}D_{ij}^{\gamma}D_{ij}^\alpha \xi_\alpha
\]

which shows that the FKP estimator \( \xi_\alpha \) is unbiased only if the Fisher matrix in equation (44) is interpreted as satisfying the asymmetric expression (45). A detailed discussion of this issue is deferred to §4. Here it suffices to remark that, to the extent that the FKP approximation is valid, the variance of the FKP estimator \( \xi_\alpha \) is equal to the inverse of the symmetrized Fisher matrix given by equation (45)

\[
\langle \Delta \tilde{\xi}_\alpha \Delta \bar{\xi}_\beta \rangle = F_{(\alpha\beta)}^{-1}
\]

where \( F^{(\alpha\beta)} \equiv \text{Sym}_{(\alpha\beta)} F_{\alpha\beta} \) denotes the symmetrized Fisher matrix, and \( F_{(\alpha\beta)}^{-1} \) its inverse.

3.2 Hierarchical model

The pair covariance matrix \( \mathbf{C}_{ijkl} \), equation (41), hence also the reduced covariance matrix \( \mathbf{C}_{\alpha\beta} \), equation (41), involves the 3-point and 4-point correlation functions \( \zeta_{ijk} \) and \( \eta_{ijkl} \). The problem here is that these correlation functions are not known precisely.

Available observational and \( N \)-body evidence (see for example the summaries by Scoccimarro & Frieman 1999 and Hui & Gaztañaga 1999) is consistent with a hierarchical model in which the 3-point and 4-point functions are, in the real representation with no implicit summation, 

\[
\zeta_{ijk} = Q (\xi_{ij}\xi_{jk} + \xi_{jk}\xi_{ki} + \xi_{ki}\xi_{ij})
\]

\[
\eta_{ijkl} = R_a [\xi_{ij}\xi_{jk}\xi_{kl} + \text{cyclic (12 snake terms)}]
\]

\[
+ R_b [\xi_{ij}\xi_{jk}\xi_{kl} + \text{cyclic (4 star terms)}]
\]

with approximately constant hierarchical amplitudes \( Q, R_a \), and \( R_b \). On the other hand it is clear that the hierarchical amplitudes do vary at some level, both as a function of scale and configuration shape.

In the translinear regime, perturbation theory predicts that the hierarchical amplitudes should vary (somewhat) with both scale and configuration, for density fluctuations growing by gravity from Gaussian initial conditions (Fry 1984; Scoccimarro et al. 1998).

In the deep nonlinear regime, predictions for the behaviour of the hierarchical amplitudes are more empirical. Scoccimarro & Frieman (1999) have recently suggested an ansatz, which they dub hyperextended perturbation theory (HEPT), that the hierarchical amplitudes in the highly nonlinear regime go over to the values predicted by perturbation theory for configurations collinear in Fourier space. For power law power spectra \( \xi(k) \propto k^n \), HEPT predicts a 3-point amplitude

\[
Q = \frac{4 - 2^n}{1 + 2^n}
\]

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and 4-point amplitudes $R_a = R_b = Q_4$ with
\[ Q_4 = \frac{54 - 27 \, 2^n + 2 \, 3^n + 6^n}{2 \, (1 + 6 \, 2^n + 3 \, 3^n + 6 \, 6^n)}. \] (52)

For simplicity, the present paper adopts the hierarchical model, with constant hierarchical amplitudes set equal to the HEPT values (51) and (52). For reasons to be discussed shortly (namely that the Schwarz inequality is violated otherwise), most of the calculations shown take
\[ R_a = -R_b = Q_4 \] (53)
although where possible results are also shown for
\[ R_a = R_b = Q_4 . \] (54)

In addition to power law power spectra, the present paper shows results for the power spectrum derived from observations by Peacock (1997), and for an observationally concordant $\Lambda$CDM model from the fitting formulae of Eisenstein & Hu (1998), nonlinearly evolved according to the procedure of the hierarchical model is consistent only for $J(\text{HEPT values}) = (51)$ and (52). For reasons to be discussed shortly, the Schwarz inequality, which requires that the absolute value of the correlation coefficient be less than or equal to unity, is violated unless $R_a = -R_b$. This problem has been remarked and discussed by Scoccimarro et al. (1999 §3.3). Scoccimarro et al. show from N-body simulations that the traditional relation $R_a \approx R_b$ holds approximately for $k_a \approx k_b$, but that indeed $R_a + R_b$ decreases systematically as $k_a$ and $k_b$ become more and more separated. Scoccimarro et al. conclude that the simple hierarchical model with constant amplitudes is not a good description of the 4-point function in the highly nonlinear regime.

For simplicity, the present paper adopts the hierarchical model with constant amplitudes, and either $R_b = -R_a$ or $R_a = R_b$. Ultimately, the latter choice leads to unphysically huge variances, plainly a consequence of the violation of the Schwarz inequality. Thus the canonical models in this paper have $R_b = -R_a$. However, where possible, intermediate results are also shown for $R_b = R_a$.

### 3.3 Prewhitening

The minimum variance estimator $\hat{\xi}_i$ and associated Fisher matrix $F_{\alpha\beta}$, equations (44) and (55), involve 6-dimensional integrals of $C^{-1\alpha\beta}(\hat{n}_i, \hat{n}_j)$ over all pairs $ij$ of volume elements in a survey. This is actually quite a feasible numerical problem. The reduced covariance matrix $C_{\alpha \beta}(\hat{n}_i, \hat{n}_j)$ is a rank 2 matrix of 1-dimensional quantities, so is straightforward to invert numerically for any particular values of the selection functions $\hat{n}_i$ and $\hat{n}_j$. If, as is typical, the selection function separates into the product of an angular mask and a radial selection function, then the angular integrals can be done analytically (Hamilton 1993), leaving a double integral of $C^{-1\alpha\beta}(\hat{n}_i, \hat{n}_j)$ over the radial directions, which is doable. This direct procedure is discussed further in §8 and forms the basis of the gourmet recipe summarized in §9.4. Still, the integration is burdensome, and it is enlightening to explore whether further simplification is possible.

Ideally what one would like is that there would exist a representation in which $C_{\alpha \beta}(\hat{n}_i, \hat{n}_j)$ were simultaneously diagonal for arbitrary values of the selection function $\hat{n}$. Precisely this situation obtains in the case of Gaussian fluctuations, for which the reduced covariance matrix $C_{\alpha \beta}$ is diagonal in Fourier space
\[ C_{\alpha \beta}(\hat{n}_i, \hat{n}_j) = 2 \, 2^n \delta_{\text{SD}}(k_a - k_b) \left[ \xi(k_a) + \hat{n}_i^{-1} \right] \left[ \xi(k_a) + \hat{n}_j^{-1} \right] \] (62)
regardless of the values $\hat{n}_i$ and $\hat{n}_j$ of the selection function.

For non-Gaussian fluctuations, the reduced covariance $C_{\alpha \beta}(\hat{n}_i, \hat{n}_j)$ is a linear combination of 4-point, 3-point, and 2-point matrices $K_{\alpha \beta}$, $J_{\alpha \beta}$, and $H_{\alpha \beta},$ according to equation (44). Finding a representation in which $C_{\alpha \beta}(\hat{n}_i, \hat{n}_j)$ is diagonal for any $\hat{n}_i$ and $\hat{n}_j$, thus means diagonalizing the three matrices $K, J,$ and $H$ simultaneously. This is of course generically impossible.

However, it is possible to diagonalize two ($K$ and $H$) of the three matrices simultaneously by the trick of prewhitening, and to cross one’s fingers on the third matrix ($J$). The term prewhitening refers to the operation of multiplying a

\[
\frac{K_{\alpha \beta}}{\langle K_{\alpha \beta} K_{\gamma \delta} \rangle^{1/2}} \rightarrow \frac{(R_a + R_b)}{2 \left( \frac{2^n + 2}{n + 2} R_a + R_b \right)} \left( \frac{k_a}{k_b} \right)^{n/2}
\] (61)

which diverges as $k_a/k_b \rightarrow \infty$ (for $-2 < n < 0$) unless $R_a = -R_b$. Thus the Schwarz inequality, which requires that the absolute value of the correlation coefficient be less than or equal to unity, is violated unless $R_a = -R_b$. This problem has been remarked and discussed by Scoccimarro et al. (1999 §3.3). Scoccimarro et al. show from N-body simulations that the traditional relation $R_a \approx R_b$ holds approximately for $k_a \approx k_b$, but that indeed $R_a + R_b$ decreases systematically as $k_a$ and $k_b$ become more and more separated. Scoccimarro et al. conclude that the simple hierarchical model with constant amplitudes is not a good description of the 4-point function in the highly nonlinear regime.

For simplicity, the present paper adopts the hierarchical model with constant amplitudes, and either $R_b = -R_a$ or $R_a = R_b$. Ultimately, the latter choice leads to unphysically huge variances, plainly a consequence of the violation of the Schwarz inequality. Thus the canonical models in this paper have $R_b = -R_a$. However, where possible, intermediate results are also shown for $R_b = R_a$.
signal by a function in such a way that the noise becomes white, or constant (Blackman & Tukey 1959 §11). Prewhitening is commonly used in the construction of Karhunen-Loève modes (signal-to-noise eigenmodes), in order to allow a signal and its noise to be diagonalized simultaneously (Vogelez & Szalay 1996; Tegmark, Taylor & Heavens 1997; Tegmark et al. 1998).

Define the prewhitened reduced covariance $\mathcal{B}_{\alpha\beta}$ to be

$$\mathcal{B} \equiv H^{-1/2} \mathcal{C} H^{-1/2}$$

and similarly define the prewhitened 4-point and 3-point matrices $M_{\alpha\beta}$ and $L_{\alpha\beta}$ to be

$$M \equiv H^{-1/2} K H^{-1/2}$$

$$L \equiv H^{-1/2} J H^{-1/2}$$

By construction, the prewhitened 2-point matrix is the unit matrix, $H^{-1/2} H H^{-1/2} = I$. In terms of the prewhitened 4-point and 3-point matrices $M_{\alpha\beta}$ and $L_{\alpha\beta}$, the prewhitened reduced covariance $\mathcal{B}_{\alpha\beta}(\mathbf{n}_1, \mathbf{n}_2)$ is (compare eq. (62))

$$\mathcal{B}_{\alpha\beta}(\mathbf{n}_1, \mathbf{n}_2) = 2 \left[ M_{\alpha\beta} + (\mathbf{n}_1^{-1} + \mathbf{n}_2^{-1}) L_{\alpha\beta} + \mathbf{n}_1^{-1} \mathbf{n}_2^{-1} L_{\alpha\beta} \right].$$

The properties of the prewhitened 4-point and 3-point matrices $M$ and $L$ are examined in 3.4 FFTLog

3.4 FFTLog

Several of the manipulations described in this paper involve transforming between real and Fourier space. Ideally, one would like to be able to cover several orders of magnitude in separation or wavenumber. The SDSS, for example, should be able to probe scales from $10^{-2} h^{-1} \text{Mpc}$ to $10^3 h^{-1} \text{Mpc}$, a range of $10^5$. If the Fourier transforms were done using standard Fast Fourier Transform (FFT) techniques, which require linearly spaced points, covering such a range would require $10^5$ points. The trouble with this is that one would then have to manipulate $10^5 \times 10^5$ matrices. Clearly this is a problem of the shoe not fitting the foot; that is, a linear spacing of points is not well suited to the case at hand: while the difference between separations of 0.01 $h^{-1} \text{Mpc}$ and 0.02 $h^{-1} \text{Mpc}$ may be significant, the difference between 1000.01 $h^{-1} \text{Mpc}$ and 1000.02 $h^{-1} \text{Mpc}$ is practically irrelevant.

The problem may be solved by using an FFT method originally proposed by Talman (1978), that works for logarithmically spaced points, and which I have implemented in a code FFTLog. FFTLog is analogous to the normal FFT in that it gives the exact Fourier transform of a discrete sequence that is uniformly spaced and periodic in logarithmic space. More generally, FFTLog yields Fast Hankel (= Fourier-Bessel) Transforms of arbitrary order, including both integral and 1/2-integral orders. FFTLog, like the normal FFT, suffers from the usual problems of ringing (response to sudden steps) and aliasing (periodic folding of frequencies), but under appropriate circumstances and with suitable precautions, discussed in Appendix B, it yields reliable Fourier transforms covering ranges of many orders of magnitude with modest numbers of points.

Appendix B gives further details of FFTLog. The code may be downloaded from http://casa.colorado.edu/~ajsh/FFTLog/.

4 PREWHITENED 4-POINT AND 3-POINT COVARIANCE MATRICES

4.1 Computation

Before showing pictures, it is helpful to comment on the numerical computation of the 4-point and 3-point covariance matrices $K_{\alpha\beta}$ and $J_{\alpha\beta}$ and their prewhitened counterparts $M_{\alpha\beta}$ and $L_{\alpha\beta}$.

Equations (55) and (56) give expressions for the 4-point and 3-point matrices $K(k_x, k_y)$ and $J(k_x, k_y)$ in Fourier space, for the hierarchical model with constant hierarchical amplitudes. These are discretized as described in 3.3.

An issue here is the calculation of the subsidiary matrix $A(k_x, k_y)$. This matrix $A_{\alpha\beta}$ is diagonal in real space with diagonal entries $\xi(r_\alpha)$, equation (64), so one way to calculate $A(k_x, k_y)$ is to start with the diagonal matrix $A(r_\alpha, r_\beta)$ in real space, and then Fourier transform it into Fourier space. Unfortunately the resulting Fourier transformed matrix $A(k_x, k_y)$ shows evident signs of ringing and aliasing, which is true whether the wavenumbers $k_x$, $k_y$ are linearly spaced (FFT) or logarithmically spaced (FFTLog). Part of the difficulty is that the diagonal matrix $A(r_\alpha, r_\beta)$ is liable to vary by several orders of magnitude along the diagonal; since the FFT (or FFTLog) assumes that the matrix is periodic, the matrix appears to have a sharp step at its boundary. These problems can be reduced by padding the matrix, and in the case of FFTLog by biasing the matrix with a suitable power law (see Appendix B). Still, artefacts from the FFT remain a concern.

A more robust procedure, the one used in this paper, is to avoid FFTs altogether, and to calculate the matrix $A(k_x, k_y)$ directly from its Fourier expression (59).

A similar issue arises when prewhitening the 4-point and 3-point matrices $K$ and $J$. The prewhitening matrix $H^{-1/2} = (1 + A)^{-1/2}$ is again diagonal in real space, with diagonal entries $[1 + \xi(r)]^{-1/2}$. Thus one way to prewhiten $K$ (say) is to start with $K(k_x, k_y)$ in Fourier space, Fourier transform it into real space, prewhiten $M(r_\alpha, r_\beta) = [1 + \xi(r_\alpha)]^{-1/2} K(r_\alpha, r_\beta) [1 + \xi(r_\beta)]^{-1/2}$, and then Fourier transform back into Fourier space. Once again the resulting matrix $M(k_x, k_y)$ shows signs of ringing and aliasing.

Again, a more robust procedure, the one used in this paper, is to avoid FFTs, and to calculate the prewhitening matrix $H^{-1/2} = (1 + A)^{-1/2}$ directly in Fourier space. Specifically, take the Fourier expression (55) for $A(k_x, k_y)$, add the unit matrix $I$ to form $H$, and evaluate the inverse positive square root $H^{-1/2}$ via an intermediate diagonalization. This yields the prewhitening matrix $H^{-1/2}$ in Fourier space, which can be used directly to prewhiten the 4-point and 3-point covariances matrices $K$ or $J$ in Fourier space. This manner of constructing $H^{-1/2}$ guarantees that the prewhitened 2-point covariance matrix $H^{-1/2} H^{-1/2}$ is numerically equal to the unit matrix $I$, as it should be. Although this procedure is slower than using FFTs, it yields results that are robust with respect to range, resolution, and linear or logarithmic binning, and consistent with the results from FFTs if due care is taken with the latter.

4.2 Prewhitened 4-point covariance matrix

Figure 3 shows the correlation coefficient $K_{\alpha\beta}/(K_{\alpha\alpha} K_{\beta\beta})^{1/2}$ (no implicit summation) of the 4-point contribution $K_{\alpha\beta}$ to
Figure 4. Correlation coefficients (top) $K(k_\alpha,k_\beta)/[K(k_\alpha,k_\alpha)K(k_\beta,k_\beta)]^{1/2}$ of the prewhitened covariance, and (bottom) $M(k_\alpha,k_\beta)/[M(k_\alpha,k_\alpha)M(k_\beta,k_\beta)]^{1/2}$ of the covariance of the power spectrum in four different models of the power spectrum. Each curve is the correlation coefficient at fixed $k_\beta = 1 h^{-1}{\text{Mpc}}$, plotted as a function of $k_\alpha$. The three sets of panels starting from the left are for power law power spectra with correlation functions $\xi(r) = (r/5 h^{-1}{\text{Mpc}})^{-\gamma}$ with indices $\gamma = 1.1$, 1.8, and 2.9, while the rightmost panel is for the $\Lambda$CDM power spectrum of Eisenstein & Hu (1998) with $\Omega_\Lambda = 0.7$, $\Omega_m = 0.3$, $\Omega_bh^2 = 0.02$, and $h = 0.65$, nonlinearly evolved by the procedure of Peacock & Dodds (1996). The two lines on each line are for 4-point hierarchical amplitudes (solid) $R_\beta = R_\alpha$, and (long-dash) $R_\beta = -R_\alpha$. Lines are dotted where the correlation coefficient is negative. The Schwarz inequality, which requires that the correlation coefficient be $\leq 1$, is violated by the hierarchical model with $R_\beta = R_\alpha$ at values $k \ll k'$ and $k \gg k'$. The resolution is 128 points per decade, the same as in Figures 2 and 3.

Figure 2. Correlation coefficient $K(k_\alpha,k_\beta)/[K(k_\alpha,k_\alpha)K(k_\beta,k_\beta)]^{1/2}$ of the 4-point contribution $K(k_\alpha,k_\beta)$ to the covariance of the power (i.e. the covariance without shot-noise) in the case of a power law power spectrum with correlation function $\xi(r) = (r/5 h^{-1}{\text{Mpc}})^{-1.8}$. Each line is the correlation coefficient for a fixed $k_\beta$, and each line peaks at $k_\alpha = k_\beta$, where the value is unity. The hierarchical amplitudes are $R_\alpha = -R_\beta = 4.195$. The resolution is 128 points per decade, $\Delta \log k = 1/128$.

Figure 3. Correlation coefficient $M(k_\alpha,k_\beta)/[M(k_\alpha,k_\alpha)M(k_\beta,k_\beta)]^{1/2}$ of the 4-point contribution $M(k_\alpha,k_\beta)$ to the prewhitened covariance of a power law power spectrum with correlation function $\xi(r) = (r/5 h^{-1}{\text{Mpc}})^{-1.8}$. Lines are dotted where the correlation coefficient is negative. This is the same as Figure 2 except that the covariance is prewhitened.

The (unprewhitened) reduced covariance matrix $\mathbf{C}_{\alpha\beta}$, equation (12), for the case of a power law power spectrum having correlation function $\xi(r) = (r/5 h^{-1}{\text{Mpc}})^{-1.8}$. Physically, the quantity plotted is the (correlation coefficient of) the covariance of estimates of power in the case of a perfect survey with no shot-noise, $n \to \infty$.

The correlation coefficient offers a good way to visualize the covariance, since a value of $(-)1$ means two quantities are perfectly (anti-)correlated, and the Schwarz inequality requires that the absolute value of the correlation coefficient always be less than or equal to unity.

The Gaussian spikes evident in the curves on the leftward, linear, side of Figure 2 reflect the fact that the covariance of power becomes diagonal in the linear, Gaussian regime. In the nonlinear regime, the hierarchical contribution to the covariance dominates, and the covariance of power becomes quite broad, a point previously made by Meiksin & White (1999) and Scoccimarro et al. (1999).
It should be borne in mind that the shape of the correlation coefficient shown in Figure 3 depends on the resolution in wavenumber \( k \), a point emphasized by Scoccimarro et al. (1999). In Figure 4 the points are logarithmically spaced with 128 points per decade, so \( \Delta \log k = 1/128 \). However, the correlation coefficient varies in an unsurprising way: as the resolution increases, the Gaussian spikes get spikier, tending in principle to a Dirac delta-function in the limit of infinite resolution.

Figure 3 shows the correlation coefficient \( M_{\alpha \beta}/(M_{\alpha \alpha} M_{\beta \beta})^{1/2} \) of the 4-point contribution \( M_{\alpha \beta} \) to the prewhitened reduced covariance \( B_{\alpha \beta} \), equations (3) and (2), again for the case of a power law power spectrum having correlation function \( \xi(r) = (r/5 \ h^{-1} \text{Mpc})^{-1.8} \). The only difference between this Figure and Figure 3 is that the covariance is now prewhitened.

The prewhitened covariance \( M \) plotted in Figure 3 appears to be remarkably narrow, certainly substantially narrower than the covariance shown in Figure 3. The Gaussian spikes again show up in the linear regime, and again the hierarchical contribution to the prewhitened covariance dominates in the nonlinear regime. The hierarchical contribution appears empirically to have a constant width of \( \Delta k \approx \pi/\rho_0 \approx 1 \ h \text{Mpc}^{-1} \), where \( \rho_0 = 5 \ h^{-1} \text{Mpc} \) is the correlation length. Thus the prewhitened covariance appears to become relatively narrower at large wavenumber \( k \).

Figure 4 shows the correlation coefficients of the covariance of the power, both straight \( K \) and prewhitened \( M \), for several other power spectra. In each case the covariance of power with the power at \( k = 1 \ h \text{Mpc}^{-1} \) is plotted, which is essentially the ‘worst case’, where the prewhitened covariance \( M \) is relatively broadest.

The solid lines in Figure 4 are for 4-point hierarchical amplitudes \( R_b = -R_a \), while the dashed lines are for \( R_b = R_a \). As discussed in §3.2, the hierarchical model violates the Schwarz inequality at \( k_\alpha > k_\beta \) (or \( k_\alpha < k_\beta \)) unless \( R_b = -R_a \).

Figure 4 illustrates that the pattern encountered in Figures 3 and 5 is remarkably robust over different power spectra. That is, while the covariance of the power is itself broad, in all cases the covariance of the prewhitened power is substantially narrower, at least for \( R_b = -R_a \) (solid lines). Note that the power law power spectra illustrated in Figure 4 cover essentially the full range of indices, \( 1 < \gamma < 3 \), allowed by the hierarchical model.

The situation for \( R_b = R_a \) is muddier. Although the core of the prewhitened covariance is for the most part reasonably narrow also in this case, the off-diagonal covariances at \( k_\alpha \gg k_\beta \) (or \( k_\alpha \ll k_\beta \)) are starting to become worrying large in several cases. Some of this behaviour is undoubtedly inherited from the unphysical (Schwarz-inequality-violating) behaviour of the ordinary covariance, and is surely not realistic. Here I leave the problem with the comment that further investigation is clearly required, along the lines being pioneered by Scoccimarro et al. (1999).

**4.3 Prewhitened 3-point covariance matrix**

As discussed in §3.3, it would be ideal if the prewhitened 3-point contribution \( L_{\alpha \beta} \) to the covariance of power were diagonal in the same representation as the 4-point contribution \( M_{\alpha \beta} \).
pair-weighting will raise the variance quadratically from its
be precisely minimum variance. But a linear error in the
weighting that emerges from assuming diagonality will not
variance as long as minimum, so the pair-weighting should be close to minimum
L is not too far from being diagonal. In
is indeed diagonal. In
not precisely diagonal, then the ‘minimum variance’ pair-
weighting that emerges from assuming diagonality will not be minimum variance. But a linear error in the
pair-weighting will raise the variance quadratically from its minimum, so the pair-weighting should be close to minimum variance as long as $L$ is not too far from being diagonal. In any case, as discussed in (27), the estimate of power remains unbiased whatever approximations are made.

Figure 6 shows the correlation coefficient of the prewhitened 3-point covariance $L_{\alpha\beta}$ in the representation of eigenfunctions $\phi_\alpha$ of the prewhitened 4-point covariance $M_{\alpha\beta}$, at a representative nominal wavenumber $k_\beta = 1 \ h \ Mpc^{-1}$. The horizontal axis is the nominal wavenumber $k_\alpha$, which labels the 4-point eigenfunctions $\phi_\alpha$ ordered by eigenvalue. The three sets of panels starting from the left are for power law power spectra with correlation functions $\xi(r) = (r/5 \ h^{-1} \ Mpc)^{-\gamma}$ with indices $\gamma = 1.1$, 1.8, and 2.9, while the rightmost panel is for the ΛCDM power spectrum of Eisenstein & Hu (1998) with $\Omega_M = 0.7$, $\Omega_L = 0.3$, $\Omega_B h^2 = 0.02$, and $h = 0.65$.

Figure 7 shows the ratio $\mu_\alpha/\xi(k_\alpha)$, at a representative nominal wavenumber $k_\alpha = 1 \ h \ Mpc^{-1}$. The Figure illustrates that this correlation coefficient remains remarkably diagonal for all power spectra. Again, the range of power law power spectra shown covers essentially the full range $1 < \gamma < 3$ allowed by the hierarchical model.

4.4 4-point and 3-point eigenvalues

Denote the eigenvalues of the 4-point and 3-point prewhitened covariance matrices $M$ and $L$ by

$$M \phi_\alpha = \mu_\alpha \phi_\alpha \quad (67)$$

$$L \varphi_\alpha = \lambda_\alpha \varphi_\alpha \quad (68)$$

(no implicit summation on the right hand side) so that for Gaussian fluctuations the eigenvalues $\mu_\alpha$ and $\lambda_\alpha$ would be

$\mu_\alpha = \lambda_\alpha = \xi(k_\alpha)$. 

Figure 8 shows the ratio $\mu_\alpha/\xi(k_\alpha)$ of the 4-point eigenvalues $\mu_\alpha$ to the nonlinear power spectrum $\xi(k_\alpha)$, plotted as a function of the nominal wavenumber $k_\alpha$, which labels the eigenfunctions $\phi_\alpha$ ordered by eigenvalue, for a power law power spectrum with correlation function $\xi(r) = (r/5 \ h^{-1} \ Mpc)^{-1.8}$. The eigenvalue is comparable to the power spectrum at all wavenumbers, $\mu_\alpha \sim \xi(k_\alpha)$. In the
Gaussian, small \( k_\alpha \) regime the eigenvalue is equal to the power spectrum, \( \mu_\alpha = \xi(k_\alpha) \), as expected, while in the hierarchical, large \( k_\alpha \) regime the eigenvalue asymptotes to close to \( 2^{1/2} R_\alpha \) times the power spectrum, \( \mu_\alpha \approx 2^{1/2} R_\alpha^{1/2} \xi(k_\alpha) \). Similar behaviour is found for other power spectra (not plotted), and for the 3-point eigenvalue \( \lambda_\alpha \), which in the hierarchical regime asymptotes to \( \lambda_\alpha \approx 2Q \xi(k_\alpha) \).

Figure 8 shows the ratio \( \lambda_\alpha/\mu_\alpha \) of 3-point to 4-point eigenvalues, as a function of the nominal wavenumber \( k_\alpha \), for various power spectra. The two lines in each case are for 4-point hierarchical amplitudes (solid) \( R_b = -R_a \), and (long-dash) \( R_b = R_a \). The horizontal axis is the nominal wavenumber \( k_\alpha \), which labels the 3-point and 4-point eigenfunctions \( \varphi_\alpha \) and \( \phi_\alpha \) ordered by eigenvalue. The relation between eigenvalue and nominal wavenumber varies with resolution. The resolution is \( \Delta \log k = 1/32 \), except for a high resolution case shown for \( \gamma = 1.8 \), where \( \Delta \log k = 1/128 \).

Curiously, the ratios \( \mu_\alpha/\xi(k_\alpha) \) and \( \lambda_\alpha/\xi(k_\alpha) \), regarded as functions of the nominal wavenumber \( k_\alpha \), vary with the resolution \( \Delta \log k \) of the matrix, as illustrated in Figures 7 and 8 for the case \( \gamma = 1.8 \). In the Gaussian limit of small \( k_\alpha \), the ratios do not change with resolution, but in the hierarchical limit of large \( k_\alpha \), the ratios seems to shift (to the right on the Figures, as the resolution increases) in such a way that the ratios are functions of the product \( k_\alpha \Delta \log k \). At intermediate \( k_\alpha \), the shift is intermediate. Now the wavenumber \( k_\alpha \) is only a nominal wavenumber, a labelling of the eigenfunctions ordered by eigenvalue, and it is only in the Gaussian regime that the eigenmodes are Fourier modes and the correspondence between nominal and true wavenumber is precise. Still, the shift seems surprising: for example, in the limit of infinite resolution \( \Delta \log k \to 0 \), the ratio \( \mu_\alpha/\xi(k_\alpha) \) plotted in Figure 8 would shift to the right so far that \( \mu_\alpha/\xi(k_\alpha) \) would equal 1 at all finite wavenumbers. Similarly, the ratio \( \lambda_\alpha/\mu_\alpha \) plotted in Figure 8 would shift to the right so far that \( \lambda_\alpha/\mu_\alpha \) would equal 1 at all finite wavenumbers. Numerically, to the limit that I have tested it (\( \Delta \log k = 1/1024 \)), this is indeed what seems to happen: both \( \mu_\alpha/\xi(k_\alpha) \) and \( \lambda_\alpha/\xi(k_\alpha) \), hence also their ratio \( \lambda_\alpha/\mu_\alpha \), shift to the right together as the resolution increases, for all power spectra.

This does not appear to be a numerical error, because ‘observable’ quantities computed via the eigenfunctions \( \phi_\alpha \) and their eigenvalues \( \mu_\alpha \), such as the error bars attached to the prewhitened power spectrum \( X(k) \) in Fourier space (§), appear robust against changes in resolution.
\[ X(r) = \frac{2\xi(r)}{1 + [1 + \xi(r)]^{1/2}}. \]  

The expression (69) is equivalent to \( X(r) \equiv 2[1+\xi(r)]^{1/2} - 2 \), but the former expression (68) is numerically stabler to evaluate when \( \xi(r) \) is small. Similarly, define an estimator \( \hat{X}_\alpha \) of the prewhitened power in terms of the minimum variance estimator \( \xi_\alpha \), equation (68), of the power spectrum by, again in the real space representation,

\[ \hat{X}(r) = \frac{2\hat{\xi}(r)}{1 + [1 + \hat{\xi}(r)]^{1/2}}. \]  

which by construction has the property that for small \( \Delta \hat{X}(r) \), as should be true in the limit of a large amount of data (the following equation is essentially the derivative of eq. (68)),

\[ \Delta \hat{X}(r) = \frac{\Delta \hat{\xi}(r)}{[1 + \Delta \hat{\xi}(r)]^{1/2}}. \]  

The covariance of the estimate \( \hat{X}_\alpha \) of the prewhitened power spectrum is given by

\[ \langle \Delta \hat{X}_\alpha, \Delta \hat{X}_\beta \rangle = (H^{-1/2})_\alpha^\beta \langle \Delta \xi_\alpha, \Delta \xi_\beta \rangle (H^{-1/2})_\beta^\alpha = E_{\alpha\beta}^{-1} \]  

where the Fisher matrix \( E^{\alpha\beta} \) of the prewhitened power equals the prewhitened Fisher matrix of the power, equation (63),

\[ E^{\alpha\beta} = (H^{1/2})_\alpha^\gamma F^{\gamma\delta} (H^{1/2})_\delta^\beta. \]  

In § it will be found convenient to deal with another prewhitened estimator \( \hat{Y}_\alpha \) defined by

\[ \hat{Y}_\alpha \equiv (H^{-1/2})_\alpha^\beta \hat{\xi}_\beta. \]  

The prewhitened estimator \( \hat{Y}_\alpha \) has the same covariance as \( \hat{X}_\alpha \)

\[ \langle \Delta \hat{Y}_\alpha, \Delta \hat{Y}_\beta \rangle = \langle \Delta \hat{X}_\alpha, \Delta \hat{X}_\beta \rangle = E_{\alpha\beta}^{-1}. \]  

So why not define \( \hat{Y}_\alpha \) to be the prewhitened power? The problem with the estimator \( \hat{Y}_\alpha \) is that it depends explicitly on the prior power spectrum \( \xi_\alpha \). That is, \( \hat{Y}_\alpha \) in real space is

\[ \hat{Y}(r) = \frac{\hat{\xi}(r)}{1 + \hat{\xi}(r)}^{1/2} \]  

which involves an estimated quantity \( \hat{\xi}(r) \) in the numerator and the prior quantity \( \xi(r) \) in the denominator. Imagine plotting \( \hat{Y}_\alpha \) on a graph. What is this quantity supposed to be an estimate of? Obviously \( \hat{Y}_\alpha \) is an estimate of \( \langle Y_\alpha \rangle \equiv (H^{-1/2})_\alpha^\beta \xi_\beta \). But if one wanted to attach error bars to the estimate, then to be fair one should include the full covariance of the quantity being estimated, including the covariance that arises from the denominator \([1 + \xi(r)]^{1/2}\) in equation (67), not just the covariance \( \langle \Delta Y_\alpha, \Delta Y_\beta \rangle \) with the denominator held fixed. Indeed, if one goes through the usual ML cycle of permitting the data to inform the prior, so that the estimated \( \hat{\xi}(r) \) is inserted into the denominator of equation (67), then it becomes abundantly evident that it would be correct to include covariance arising from the denominator.

To avoid confusion, it should be understood that the quantities \( \hat{Y}_\alpha \) are of course perfectly fine for carrying out ML estimation of parameters. In ML estimation, error bars

5 PREWHITENED POWER SPECTRUM

5.1 Definition

Given the nice properties of the prewhitened covariance of power established in the previous section, it makes sense to define a prewhitened power spectrum \( \hat{X}_\alpha \), and a corresponding estimator \( \hat{X}_\alpha \) thereof, with the property that the covariance of the prewhitened power equals the prewhitened covariance of power.

Define, therefore, the prewhitened power spectrum \( \hat{X}_\alpha \) by, in the real space representation,
The linear power spectra \( \xi(k) \), nonlinear power spectra \( \xi(k) \), and prewhitened nonlinear power spectrum \( X(k) \) for (left) the \( \Omega_m = 0.3 \) power spectrum derived from observations by Peacock (1997), and (right) the COBE-normalized \( \Lambda \)CDM power spectrum from the fitting formulae of Eisenstein & Hu (1998), with parameters as listed on the graph. The nonlinear power spectra were computed from the linear power spectra according to the formula of Peacock & Dodds (1996). The \( \Lambda \)CDM power spectrum is the one used in Figures 10 and 11, and Figure 12.

The alternative of using the wiggly slope has the additional demerit that it amplifies baryonic wiggles in the nonlinear regime, which is opposite to the suppression of baryonic wiggles in the nonlinear regime observed in N-body simulations by Meiksin, White & Peacock (1999).

The prewhitened power spectra \( X(k) \) shown in Figure 10 were computed by transforming the nonlinear power spectrum \( \xi(k) \) into real space using FFTLog (see Appendix B, Fig. 12), constructing the prewhitened power \( X(r) \) from \( \xi(r) \) according to equation (70), and Fourier transforming back.

The prewhitened power spectra shown in Figure 10 appear to be interestingly close to the linear power spectra, \( X(k) \approx \xi_L(k) \), another one-eyebrow-raising property of the prewhitened power spectrum. But surely this is just coincidence, since for a primordial power spectrum \( \xi(k) \propto k^n \) the prewhitened correlation in the highly nonlinear regime should go as \( X(r) \propto 2 \xi(r)^{1/2} \propto r^{-(n+3)/2(n+5)} \) assuming stable clustering (Peebles 1980, eq. [73.12]), whereas the linear power spectrum would go as \( r^{-(n+3)} \), whose power law exponents agree only in the limiting case \( n \to -3 \). Still, the coincidence is curious.

Figure 10 points up one defect of the prewhitened power spectrum, which is that, surprisingly enough, it does not reproduce the linear power spectrum at the very largest scales (small \( k \)). Indeed the prewhitened power goes negative in the Peacock (1997) case at \( k \approx 0.0023 \) h Mpc\(^{-1} \), and in the \( \Lambda \)CDM case at \( k \approx 0.00021 \) h Mpc\(^{-1} \). This turns out to be a generic feature of the prewhitened power spectrum if the true power spectrum goes to zero at zero wavenumber, as is true for Harrison-Zel’dovich models, \( \xi(k) \propto k \) as \( k \to 0 \). For it is true that the power spectrum \( \xi(k) \) goes to zero at zero wavenumber \( k \)

\[
\lim_{k \to 0} \xi(k) = \int_0^\infty \xi(r) 4\pi r^2 dr = 0 \quad (77)
\]

are attached to the model, not to the data', to quote another of the refrains from the 1997 Aspen workshop on Precision Measurement of Large Scale Structure. Whereas in ML parameter estimation with \( \hat{X}_n \) one might form a likelihood from \( \hat{Y}_n \), another one-eyebrow-raising property of the prewhitened power spectrum. But surely this is just coincidence, since for a primordial power spectrum \( \hat{X}(k) \propto k^n \) the prewhitened correlation in the highly nonlinear regime should go as \( \hat{Y}(r) \propto 2 \hat{X}(r)^{1/2} \propto r^{-(n+3)/2(n+5)} \) assuming stable clustering (Peebles 1980, eq. [73.12]), whereas the linear power spectrum would go as \( r^{-(n+3)} \), whose power law exponents agree only in the limiting case \( n \to -3 \). Still, the coincidence is curious.

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then it follows that the prewhitened power must go to a constant negative at zero wavenumber
\[
\lim_{k \to 0} X(k) = \int_0^\infty \frac{2 \xi(r)}{1 + [1 + \xi(r)]^{1/2}} 4\pi r^2 dr < 0 \tag{78}
\]
since the factor \(2/[1 + [1 + \xi(r)]^{1/2}]\) in the integrand is less than one for all positive \(\xi(r)\), and greater than one for all negative \(\xi(r)\). It is not clear what to do about this, if indeed anything needs to be done. Adding a constant to \(X(k)\) and \(\hat{X}(k)\) (which would leave \(\Delta X\), hence the covariance \((\Delta \bar{X} \Delta \bar{X})\), unchanged) would spoil the nice behaviour of the prewhitened power in the nonlinear regime.

6 FISHER MATRIX OF PREWHITENED NONLINEAR POWER IN A SURVEY

It was found in \(\S 4\) that the prewhitened reduced covariance \(\mathcal{B}\) of power appears to have some unexpectedly pleasant properties: first, the prewhitened covariance is surprisingly narrow in Fourier space; second, the 4-point and 3-point contributions \(M\) and \(L\), equation (62), to the prewhitened reduced covariance \(\mathcal{B}\) are almost simultaneously diagonal (the 2-point contribution is by construction the unit matrix, so is automatically diagonal in any representation); third, the 4-point and 3-point eigenvalues \(\mu_\alpha\) and \(\lambda_\alpha\), as defined by equations (57) and (58), are approximately equal; and fourth, all these results hold for all power spectra tested.

It should be emphasized that the pleasant properties of the prewhitened power are not perfect, and that they are premised on the validity of the hierarchical model with constant hierarchical amplitudes, which as discussed in \(\S 4.2\) is certainly wrong at some level.

These properties lead to an approximate expression, equation (63), for the Fisher matrix of the prewhitened nonlinear power spectrum of a galaxy survey, which looks the same as the FKP approximation to the Fisher matrix of the power in the linear, Gaussian case, with the difference that the eigenmodes of the prewhitened covariance \(M\) of the nonlinear power take the place of the Fourier modes in the linear case.

6.1 Fisher matrix

To the further extent that the prewhitened 4-point and 3-point matrices \(M\) and \(L\) are simultaneously diagonal, the prewhitened reduced covariance matrix \(\mathcal{B}_{\alpha\beta}(\bar{n}_i, \bar{n}_j)\) is diagonal in the representation of eigenfunctions \(\phi_\alpha\) of \(M\) and \(L\), with
\[
\mathcal{B}_{\alpha\beta}(\bar{n}_i, \bar{n}_j) \approx 2 \alpha_{\alpha\beta} \left[ \mu_\alpha + (\bar{n}_i^{-1} + \bar{n}_j^{-1}) \lambda_\alpha + \bar{n}_i^{-1} \bar{n}_j^{-1} \right] \tag{79}
\]
To the further extent that \(\lambda_\alpha \approx \mu_\alpha\), the prewhitened covariance matrix \(\mathcal{B}_{\alpha\beta}(\bar{n}_i, \bar{n}_j)\) is just
\[
\mathcal{B}_{\alpha\beta}(\bar{n}_i, \bar{n}_j) \approx 2 \alpha_{\alpha\beta} (\mu_\alpha + \bar{n}_i^{-1}) (\mu_\alpha + \bar{n}_j^{-1}) \tag{80}
\]

The Fisher matrix \(F_{\alpha\beta}\) of the power spectrum is given in the FKP approximation by equation (42). In terms of the prewhitened reduced covariance \(\mathcal{B}_{\alpha\beta}\), the Fisher matrix \(F_{\alpha\beta}\) is
\[
F_{\alpha\beta} = (H^{-1/2})_\beta^\alpha \mathcal{B}^{-1} (H^{-1/2})_\alpha^\beta D_{ij}^\beta D_{ij}^\alpha \tag{81}
\]
Now \((H^{-1/2})_\beta^\alpha\) commutes with \(D_{ij}^\beta D_{ij}^\alpha\), since both are simultaneously diagonal in real space. It follows that the Fisher matrix \(E \equiv H^{-1/2} F H^{-1/2}\) of the prewhitened power, equation (66), is, in the FKP approximation,
\[
E_{\alpha\beta} = \mathcal{B}^{-1/2} D_{ij}^\beta D_{ij}^\alpha \tag{82}
\]
Like \(F_{\alpha\beta}\), the prewhitened Fisher matrix \(E_{\alpha\beta}\) is asymmetric, inheriting its asymmetry from the FKP approximation, equation (44).

To the extent that the approximation (42) to \(\mathcal{B}\) is true, it follows from equation (63) that the Fisher matrix \(E_{\alpha\beta}\) of prewhitened power in the FKP approximation is, in the representation of eigenfunctions \(\phi_\alpha\) of the prewhitened covariance,
\[
E_{\alpha\beta} = \int_0^\infty \phi_\alpha(r) \phi_\beta(r) R(r; \mu_\alpha) 4\pi r^2 dr \tag{83}
\]
where \(R(r; \mu_\alpha)\) are FKP-weighted pair integrals (commonly denoted \(RR\) in the literature, for Random-Random)
\[
R(r; \mu_\alpha) = \int \frac{\delta_0 (r_{ij} - r)}{2 [\mu_\alpha + \bar{n}(r_i) - r][\mu_\alpha + \bar{n}(r_j) - r]} d^3 r_i d^3 r_j \tag{84}
\]
the integration being taken over all pairs of volume elements \(ij\) separated by \(r_{ij} \equiv |r_i - r_j| = r\) in the survey.

The FKP approximation to the Fisher matrix \(E_{\alpha\beta}\) of prewhitened power, equation (63), takes the same form as the FKP approximation to the Fisher matrix of the power spectrum for Gaussian fluctuations derived in \(\S 5\) of Paper 1 and computed in \(\S 3\) of Paper 2. The difference is that the eigenfunctions \(\phi_\alpha(r)\) and their eigenvalues \(\mu_\alpha\) here take the place of the Fourier eigenfunctions \(j_0(k \cdot r)\) and their eigenvalues \(\xi(k_\alpha)\) in the Gaussian case.

6.2 Numerics

Equation (63) for \(E_{\alpha\beta}\) involves the eigenfunctions \(\phi_\alpha(r)\) of the prewhitened 4-point matrix \(M\) in real space, whereas in \(\S 4.2\) it was suggested that the most robust way to compute \(M\) is in Fourier space. The problem is that FFTing the matrix \(M\) from Fourier into real space is liable to introduce ringing and aliasing, which one would like to avoid.

A more robust procedure is not to FFT \(M\) into real space, but rather to FFT the pair integrals \(R(r; \mu_\alpha)\) into Fourier space; this is the same procedure adopted in \(\S 3\) of Paper 2 (except that \(R\) here is 1/2 that of Paper 2). If \(\mu_\alpha\) is treated, temporarily, as a constant, then equation (63) can be transformed into real space to yield the diagonal matrix
\[
E(r, r'; \mu_\alpha) = \delta_{0D}(r - r') R(r; \mu_\alpha) \tag{85}
\]
Beware of equation (83)! It does not signify that the Fisher matrix is diagonal in real space, because the constant \(\mu_\alpha\) is different for each row of the Fisher matrix \(E_{\alpha\beta}\). The Fourier transform of \(E(r, r'; \mu_\alpha)\) is \(E(k, k'; \mu_\alpha) = \int j_0(kr) j_0(k'r) R(r; \mu_\alpha) 4\pi r^2 dr\), which simplifies to
\[
E(k, k'; \mu_\alpha) = \pi \frac{\kappa}{k'k} \left[ \tilde{R}(k - k'; \mu_\alpha) - \tilde{R}(k + k'; \mu_\alpha) \right] \tag{86}
\]
where \(\tilde{R}(k; \mu_\alpha)\) is the 1-dimensional cosine transform of \(R(r; \mu_\alpha)\)
\[
\tilde{R}(k; \mu_\alpha) \equiv 2 \int_0^\infty \cos(kr) R(r; \mu_\alpha) dr \tag{87}
\]
Transforming $E(k, k'; \mu_\alpha)$ into $\phi_\alpha$-space gives

$$E_{\alpha\beta} = \int \phi_\alpha(k) \phi_\beta(k') E(k, k'; \mu_\alpha) \frac{4\pi k^2 dk' 4\pi k'^2 dk'}{(2\pi)^6). (88)}$$

The cosine transform $\tilde{R}(k; \mu_\alpha)$, equation (89), can be done with either FFT or FFTLog; both work well. To ensure that $\tilde{R}(k; \mu_\alpha)$ remains accurate at large (and small) wavenumbers $k$, it helps to extrapolate $R(r; \mu_\alpha)$ to small (and large) separations $r$ before transforming. The transformation into $\phi_\alpha$ space, equation (88), is done by discrete summations.

Evaluating the Fisher matrix $E_{\alpha\beta}$ with equations (88)–(89) successfully eliminates ringing and aliasing, but it introduces another problem. The problem is that equation (88) is liable to overestimate the value of $E(k, k'; \mu_\alpha)$ along the diagonal $k = k'$ if the gridding in $k$-space is too coarse to resolve the diagonal properly, as typically occurs at moderate and large $k$ with logarithmic gridding. What is important is that the integral of $E(k, k'; \mu_\alpha)$ over the diagonal be correct. Integrating $E(k, k'; \mu_\alpha)$ over $k'$ yields

$$\int_0^\infty E(k, k'; \mu_\alpha) k' dk' = \frac{2\pi}{k} \int_0^k \tilde{R}(k'; \mu_\alpha) dk'. (89)$$

The integral on the right can be done conveniently and reliably by sine transforming (with FFT or FFTLog) the pair integral

$$\int_0^k \tilde{R}(k'; \mu_\alpha) dk' = \frac{2\pi}{k} \int_0^\infty \sin(kr) \frac{R(r; \mu_\alpha)}{r} dr. (90)$$

Discretized (88) on a logarithmic grid of wavenumbers $k$, the continuous matrix $E(k, k'; \mu_\alpha)$ becomes $E_{kk'}(\mu_\alpha) = E(k, k'; \mu_\alpha) 4\pi(kk')^{3/2} \ln k/(2\pi)^3$, and equation (88) becomes

$$\sum_{k'} (k'/k)^{3/2} E_{kk'}(\mu_\alpha) = \frac{1}{\pi} \int_0^k \tilde{R}(k'; \mu_\alpha) dk'. (91)$$

Numerically, if the left hand side of equation (88), with $E_{kk'}(\mu_\alpha)$ discretized from equation (88), exceeds the right hand side of equation (91), evaluated by equation (90), then the value of the diagonal element $E_{kk}(\mu_\alpha)$ should be reduced so that the sum is satisfied. Ultimately, this procedure yields error bars on decorrelated band-powers (Paper 4) that are robust with respect to range, resolution, and linear or logarithmic binning.

### 6.3 Coarse gridding

Typically the pair integral $R(r; \mu_\alpha)$ is broad in real space, so its cosine transform $\tilde{R}(k; \mu_\alpha)$ is a narrow window about $k \approx 0$ with a width comparable to the inverse scale length of the survey. It follows that the matrix $E(k, k'; \mu_\alpha)$ given by equation (88) is likewise narrow in $k$-space, with a width comparable to the inverse scale length of the survey. Moreover the sum in equation (91) approximates $R(0; \mu_\alpha)$ at wavenumbers exceeding the inverse scale length of the survey, which is to say at all except the largest accessible wavelengths:

$$\sum_{k'} (k'/k)^{3/2} E_{kk'}(\mu_\alpha) \approx R(0; \mu_\alpha) \quad \text{for} \quad k \gg \text{scale}^{-1} (92)$$

where $R(0; \mu_\alpha)$ is the pair integral at zero separation

$$R(0; \mu_\alpha) = \int \frac{d^3r}{2 \mu_\alpha + n(r)^{-1/2}.} (93)$$

Thus if the matrix $E_{kk'}(\mu_\alpha)$ is discretized on a grid that is coarse compared to the inverse scale length of the survey, then it is approximately proportional to the unit matrix

$$E_{kk'}(\mu_\alpha) \approx 1_{kk'} R(0; \mu_\alpha). (94)$$

The resulting discrete Fisher matrix $E_{\alpha\beta}$, equation (88), is diagonal in the $\phi_\alpha$-representation

$$E_{\alpha\beta} \approx 1_{\alpha\beta} R(0; \mu_\alpha). (95)$$

The result (95) is analogous to that obtained by FKP for Gaussian fluctuations.

Of course if this diagonal Fisher matrix, equation (95), is transformed back into Fourier space, then it is no longer diagonal. That is, equation (95) asserts that the Fisher matrix of the prewhitened nonlinear power spectrum is approximately diagonal in $\phi_\alpha$-space, not in Fourier space.

### 7 ESTIMATE OF PREWHITENED NONLINEAR POWER IN A SURVEY

#### 7.1 Unbiased estimate

‘In the case of a Gaussian distribution... rather than removing the bias we should approximately double it, in order to minimize the mean square sampling error’ – E. T. Jaynes (1996, sentence containing eq. 17-13).

It is convenient to start out by considering the prewhitened estimator $\hat{Y}_\alpha$ defined by equation (96). The minimum variance estimator $\hat{\xi}_\alpha$ of the power spectrum in the FKP approximation is given by equation (14). Translating this equation into prewhitened quantities, one concludes that

$$\hat{Y}_\alpha = E_{\alpha\beta}^{-1/2} \mathcal{B}^{-1/2} \langle H^{-1/2} \rangle \delta_i \delta_j - \hat{N}_{ij} \hat{\xi}_\beta \rangle. (96)$$

The estimator $\hat{Y}_\alpha$ is minimum variance if and only if $\hat{\xi}_\alpha$ is minimum variance, since $\hat{Y}_\alpha \equiv (H^{-1/2})^{\alpha\beta} \hat{\xi}_\beta$ is a linear combination of $\hat{\xi}_\alpha$.

Now the estimator $\hat{Y}_\alpha$, equation (96), is intended to be an estimate of $Y_\alpha \equiv (H^{-1/2})^{\alpha\beta} \xi_\beta$. But is that really true, given the various approximations? It will be true provided that the estimator is unbiased, meaning that the expectation value of the estimator is equal to the true value

$$\langle \hat{Y}_\alpha \rangle = Y_\alpha. (97)$$

The expectation value of the estimator $\hat{Y}_\alpha$ given by equation (96) is, since $\langle \delta_i \delta_j - \hat{N}_{ij} \rangle = D_{ij}^{\alpha\beta} \xi_\beta$ according to equation (23),

$$\langle \hat{Y}_\alpha \rangle = E_{\alpha\beta}^{-1/2} \mathcal{B}^{-1/2} \langle H^{-1/2} \rangle \langle D_{ij}^{\alpha\beta} \rangle \langle D_{ij}^{\alpha\beta} \rangle \xi_\beta = E_{\alpha\beta}^{-1} \mathcal{B}^{-1/2} \langle D_{ij}^{\alpha\beta} \rangle \langle D_{ij}^{\alpha\beta} \rangle Y_\alpha, (98)$$

where the second line follows because $(H^{-1/2})^{\alpha\beta}$ commutes with $D_{ij}^{\alpha\beta}$, both being diagonal in real space. It follows that the estimator $\hat{Y}_\alpha$ will be unbiased, $\langle \hat{Y}_\alpha \rangle = Y_\alpha$, provided...
that the Fisher matrix $E^{\alpha\beta}$ is taken to satisfy the asymmetric equation (82), not, for example, a symmetrized version of that equation.

An important point to recognize here is that an estimate $\hat{Y}_a$ of the form (99) will be unbiased for any a priori choice of the matrix $\mathfrak{Y}$, regardless of the choice of prior power $\xi(k)$, regardless of the hierarchical model, regardless of the FKP approximation, and regardless of the approximation (such as eq. 31) to $\mathfrak{Y}$, just so long as the matrix $E$ in the estimator is interpreted as satisfying the unsymmetrized equation (32). Ultimately this property of being unbiased is inherited from the basic prior assumption that galaxies constitute a random, Poisson sampling of an underlying statistically homogeneous, isotropic density field, so that the product of overdensities $\delta_i \delta_j$ at any pair of points $i$ and $j$ separated by $r_{ij}$ provides an unbiased estimate of the correlation function $\xi(r_{ij})$. Note that the presumption here is that the galaxies sampled are an unbiased tracer of the galaxy density itself, not necessarily of the mass density.

Interpreting the estimator $\hat{Y}_a$, equation (100), as involving the asymmetric matrix $E^{\alpha\beta}$, equation (32), should be regarded not as changing the estimator to make it unbiased, but rather as interpreting the estimator correctly. If instead the estimator $\hat{Y}_a$ were interpreted as involving the symmetrized Fisher matrix $E^{\alpha\beta} \equiv \text{Sym}_{\alpha\beta} E^{\alpha\beta}$, for example, then the expectation value of the estimator would be $\langle \hat{Y}_a \rangle = E^{\alpha\beta} Y_\alpha$, which is not the same as $Y_\alpha$, although of course it should be almost to the same extent that $E^{\alpha\beta}$ is almost symmetric.

It is convenient to introduce yet another estimator $\hat{Z}^\alpha$ related to the estimator $\hat{Y}_a$ by

$$\hat{Y}_a = E^{\alpha\beta} \hat{Z}^\beta.$$ (99)

In the FKP approximation, the estimator $\hat{Z}^\alpha$ is

$$\hat{Z}^\alpha = \mathfrak{Y}^{-1} (H^{-1/2})^\alpha \{D(r_{ij}) - \bar{N}_{ij}\}.$$ (100)

If the approximation (84) to the prewhitened covariance $\mathfrak{Y}$ is used in the estimate (100) of $\bar{Z}$, then, in the representation of eigenfunctions $\phi_a$,

$$\bar{Z}_a = \int_0^\infty \phi_a(r) \tilde{S}(r; \mu_a) \frac{1}{1 + \xi(r)^{1/2}} 4\pi r^2 dr$$ (101)

where $\tilde{S}(r; \mu_a)$ is the FKP-weighted integral over pairs of overdensities $\delta(r_i) \delta(r_j)$ at points $i$ and $j$ separated by $r_{ij}$ = $r$ (commonly denoted $(DD) - 2(DF) + (RR)$ in the literature, $D$ for data, $R$ for random)

$$\tilde{S}(r; \mu_a) = \int \frac{\delta_{DD}(r_{ij} - r) \delta(r_i) \delta(r_j)}{2 [\mu_a + n(r_i)^{-1} + n(r_j)^{-1}]} d^3r_id^3r_j.$$ (102)

The shot-noise $\bar{N}_{ij}$ is excluded from equation (102) by excluding from the integration the contribution from self-pairs of galaxies, which of course have zero separation. The associated asymmetric Fisher matrix $E^{\alpha\beta}$ is given by equation (33).

Equation (102) is expressed as an integral over pairs of overdensities $\delta(r_i) \delta(r_j)$ in real space. One could just as well express $\tilde{S}$ as an integral over pairs of overdensities $\delta(k_i) \delta(k_j)$ in Fourier space, or pairs of overdensities $\delta(k_i, \ell_i, m_i) \delta(k_j, \ell_j, m_j)$ in spherical harmonic space, if one found it more convenient.

7.2 Numerics

As in [82], to avoid potential problems of ringing and aliasing, it is probably better to evaluate the estimator $\hat{Z}_a$, equation (101), by means of an expression that involves the eigenfunctions $\phi_a(k)$ in Fourier space rather than the eigenfunctions $\phi_a(r)$ in real space.

If $\mu_a$ is treated, temporarily, as a constant, then transforming equation (101) into real space yields

$$\hat{Z}(r; \mu_a) = \frac{\tilde{S}(r; \mu_a)}{1 + \xi(r)^{1/2}}.$$ (103)

The Fourier transform of this is

$$\hat{Z}(k; \mu_a) = \int_0^\infty j_0(kr) \tilde{S}(r; \mu_a) 4\pi r^2 dr$$ (104)

in terms of which the estimator $\hat{Z}_a$, equation (101), is

$$\hat{Z}_a = \int_0^\infty \phi_a(k) \hat{Z}(k; \mu_a) \frac{4\pi k^2 dk}{(2\pi)^2}.$$ (105)

The transformation into $\phi_a$ space, equation (105), is done by discrete summation.

The advantage of equation (104) over the nominally equivalent equation (101) is that in equation (104) it is the data that are Fourier transformed, $\hat{Z}(r; \mu_a) \rightarrow \hat{Z}(k; \mu_a)$, equation (104), whereas in equation (101) it is the eigenfunctions of the matrix $M$ that must be transformed, $\phi_a(k) \rightarrow \phi_a(r)$. While the two methods would yield identical results for $\hat{Z}_a$ if the same unitary Fourier transform were applied in both cases, in reality it may be advantageous to have the freedom to Fourier transform the data the best way one can, without regard to the irrelevant question of how the eigenfunctions $\phi_a$ behave when Fourier transformed.

7.3 The covariance of $\hat{Z}_a$

It will now be argued that the covariances of the estimators $\hat{Z}_a$ and $\hat{Y}_a$ are approximately equal to, respectively, the symmetrized Fisher matrix $E^{\alpha\beta}$, and its inverse, equations (109) and (113). It seems worthwhile to go through the arguments rather carefully. As a general rule, one should estimate error bars as accurately as possible; but if some approximation is necessary, then one would prefer to err on the conservative side of overestimating the true errors.

Equation (109) will now be derived, commentary on the derivation being deferred to the end. The covariance of the estimate $\hat{Z}_a$ is, from equation (101),

$$\langle \Delta \hat{Z}_a \Delta \hat{Z}_b \rangle = \mathfrak{Y}^{-1} \epsilon_{ijkl} (H^{-1/2})_i^j D_i^k D_j^l$$ (106)

where $\mathfrak{Y}$ is the approximate prewhitened reduced covariance matrix (86) used to construct the estimate $\hat{Z}_a$, equation (101), while $\epsilon_{ijkl}$ is the true covariance matrix, equation (88). To the extent that the FKP approximation, equation (41), is valid for $\epsilon_{ijkl}$, equation (104) reduces to

$$\langle \Delta \hat{Z}_a \Delta \hat{Z}_b \rangle = \mathfrak{Y}^{-1} \epsilon_{ijkl} (H^{-1/2})_i^j D_i^k D_j^l$$ (107)
where \( \mathcal{C}_{\text{FKP}} \) is the FKP covariance, equation (93), and \( \mathfrak{B}_{\text{FKP}} \equiv H^{-1/2} \mathcal{C}_{\text{FKP}} H^{-1/2} \) is its prewhitened counterpart, equation (100). Note that going from equation (104) to the second expression in equation (107) includes, as part of the FKP approximation, the assumption that \( \bar{\eta}_i \) and \( \bar{\eta}_j \) are approximately constant. The expressions on the right hand side of equation (107) are not symmetric in \( \alpha \beta \), because of the asymmetry of the FKP approximation (1). To the further extent that the prewhitened covariance \( \mathfrak{B}_{\text{FKP}} \) equals the approximation \( \mathfrak{B} \), equation (84), the covariance \( \langle \Delta \tilde{Z}^{\alpha} \Delta \tilde{Z}^{\beta} \rangle \) reduces to the asymmetric matrix \( E \) given by equation (84).

\[
(\Delta \tilde{Z}^{\alpha} \Delta \tilde{Z}^{\beta}) = E^{\alpha \beta} \quad (108)
\]

the asymmetry of the right hand side being inherited from the FKP approximation. An equally good approximation to the covariance would be the same expression (105) with the indices swapped on the right hand side, \( \alpha \leftrightarrow \beta \). Thus it seems reasonable to conclude that the covariance \( \langle \Delta \tilde{Z}^{\alpha} \Delta \tilde{Z}^{\beta} \rangle \) should be approximately equal to the the symmetrized Fisher matrix \( E^{(\alpha \beta)} \).

\[
(\Delta \tilde{Z}^{\alpha} \Delta \tilde{Z}^{\beta}) = E^{(\alpha \beta)} = \text{Sym} E^{\alpha \beta}. \quad (109)
\]

Several comments can be made about the accuracy of the approximations made in the above derivation.

Firstly, one partial test of the validity of the FKP approximation is the degree of asymmetry of the asymmetric Fisher matrix \( E^{\alpha \beta} \), equation (84). If the survey is broad in real space, which is the condition for the FKP approximation to hold, then the pair integral \( R(x, \mu_\alpha) \) in the integrand on the right hand side of equation (84) will be a slowly varying function of pair separation \( r \), so that the matrix \( E^{\alpha \beta} \) will be nearly diagonal, hence symmetric. The test is not definitive because \( E^{\alpha \beta} \) would be symmetric in any case if \( \mu_\alpha = \mu_\beta \). But in practice \( \mu_\alpha \approx \xi(k_\alpha) \) in both linear and nonlinear regimes, Figure 4, and realistically the power spectrum \( \xi(k) \) varies substantially, so the consistency test should be indicative.

Secondly, one of the weaknesses of the FKP approximation is that it fails to deal with sharp edges — as typically occur at the angular boundaries of a survey — correctly. The FKP approximation tends to overestimate the variance contributed by regions near boundaries, since it assumes that those regions are accompanied by more correlated neighbours than is actually the case. Thus, at least as regards edge effects, the FKP approximate covariance, equation (107), should tend to overestimate the exact covariance, equation (106), of the approximate estimate \( \tilde{Z}^\alpha \).

Thirdly, it is possible to check the accuracy of the approximation made in going from equation (107) to equation (108). The approximation involves setting \( \mathfrak{B}_{\text{FKP}} \mathfrak{B}^{-1} = 1 \), whereas comparing equation (84) for \( \mathfrak{B}_{\text{FKP}} \) to the approximation (83) for \( \mathfrak{B} \) shows that this quantity is in fact, in the representation of eigenfunctions \( \phi_\alpha \) of the 4-point matrix \( M \), \( \mathfrak{B}_{\alpha \beta}(\bar{\eta}_i, \bar{\eta}_j) \mathfrak{B}^{-1 \gamma}(\bar{\eta}_i, \bar{\eta}_j) = \text{Sym} E^{\alpha \beta} \).

\[
\text{Sym} E^{\alpha \beta} = \frac{(\bar{\eta}_i \bar{\eta}_j^{-1} + \bar{\eta}_i^{-1} \bar{\eta}_j)}{(\mu_\alpha + \bar{\eta}_i^{-1})(\mu_\alpha + \bar{\eta}_j^{-1})} (L_{\alpha} - \mu_\alpha L_{\beta}) \quad \text{Sym} E^{\alpha \beta}. \quad (110)
\]

The correction term on the right hand side of equation (110) should be small to the extent that the 3-point matrix \( L_{\alpha \beta} \) is near diagonal in this 4-point representation, with eigenvalues \( \lambda_\alpha \approx \mu_\alpha \), as was found to be the case in §4.

If desired, one could use the expression on the right hand side of equation (110) to compute a more accurate approximation to the covariance of \( \tilde{Z}^\alpha \), based on equation (107) rather than on equation (108). However, if one were willing to go to the trouble of computing a correction from equation (110), then one would probably be willing to revert to equation (104) and to integrate \( \mathfrak{B}_{\alpha \beta}^{-1 \gamma}(\bar{\eta}_i, \bar{\eta}_j) \) numerically over all pairs of volume elements \( ij \) in the survey, inverting \( \mathfrak{B} \) numerically for each pair \( \bar{\eta}_i, \bar{\eta}_j \), of values of the selection function. This latter procedure is in fact the gourmet recipe of §0.1.

Fourthly, the approximation \( \mu_\alpha \approx \mu_\beta \) adopted in the approximation (83) to \( \mathfrak{B} \) tends to overestimate the true eigenvalues \( \lambda_\alpha \) of the 3-point matrix \( L \), according to Figure 3. This should lead to a slight overestimate of the variance. In the realistic ΛCDM case, Figure 3, the approximation \( \mu_\alpha \approx \mu_\beta \) overestimates the true eigenvalues \( \lambda_\alpha \) by at worst 20 percent, at moderately nonlinear wavenumbers \( k \). This 20 percent overestimate is diluted to at worst 10 percent because the 3-point variance contributes at most half of the combined 2-point, 3-point, and 4-point variance, where the selection function satisfies \( \bar{\eta}^{-1} = \mu_\alpha \). The overestimate is further diluted because in practice the selection function varies, and is unlikely to sit everywhere near the worst value.

The conclusion is that the covariance of the approximate estimator \( \hat{Z}_\alpha \), equation (101) or (103), should be given approximately, equation (109), by the symmetrized Fisher matrix \( E^{(\alpha \beta)} \) of equation (83), and that if anything this covariance is likely to be on the conservative side of the true covariance.

### 7.4 The covariance of \( \hat{Y}_\alpha \)

From the expression (104) for the covariance of \( \tilde{Z}^\alpha \), one might conclude (falsely) that the covariance of \( \hat{Y}_\alpha \), equation (94), is

\[
(\Delta \hat{Y}_\alpha \Delta \hat{Y}_\beta) = E^{-1}(\alpha \gamma) E^{-1}(\gamma \beta). \quad (111)
\]

A more direct derivation of the covariance of \( \hat{Y}_\alpha \), along the lines of equations (106)–(107), leads to the same (false) conclusion. The analogue of equation (109) is

\[
(\Delta \hat{Y}_\alpha \Delta \hat{Y}_\beta) = E^{-1}(\alpha \beta). \quad (112)
\]

with the asymmetric matrix \( E \) on the right hand side. At this point one might be inclined to symmetrize this equation (112), as was done for \( \langle \Delta \tilde{Z}^\alpha \Delta \tilde{Z}^\beta \rangle \) in equation (107), writing

\[
(\Delta \hat{Y}_\alpha \Delta \hat{Y}_\beta) = \text{Sym} E^{-1}(\alpha \beta). \quad (113)
\]

The symmetrized inverse \( \text{Sym}(\alpha \beta) E^{-1}(\alpha \beta) \) of the asymmetric Fisher matrix is to be distinguished from the inverse \( E^{-1}(\alpha \beta) \) of the symmetrized Fisher matrix. But it is not hard to show that

\[
\text{Sym} E^{-1}(\alpha \beta) = E^{-1}(\alpha \gamma) E^{-1}(\gamma \beta). \quad (114)
\]

Thus equations (113) and (114) are identical. However, both equations are wrong.

The problem is that, while the Fisher matrix \( E \) remains well-behaved in the presence of loud noise, with near zero
eigenvalues, its inverse \( E^{-1} \) becomes almost singular. Consider the example of some noisy mode, for which the eigenvalue of the Fisher matrix is almost zero. It may well happen that the asymmetric Fisher matrix \( E^{\alpha\beta} \) is numerically non-singular, but that, because of approximations or numerics, the computed eigenvalue of the symmetrized Fisher matrix \( E^{(\alpha\beta)} \) is exactly zero. Equation (11) would then say that the variance of the noisy mode is zero (for if the determinant of the symmetrized Fisher matrix is zero, \(|E^{(\alpha\beta)}| = 0\), while the determinant of the asymmetric Fisher matrix is finite, \(|E^{\alpha\beta}| \neq 0\), then the determinant of the variance in eq. (11) is zero). This is plainly absurd.

It is safer to take the covariance of \( \hat{Y}_\alpha \) to be approximately equal to the inverse of the symmetrized Fisher matrix \( E^{(\alpha\beta)} \),

\[
(\Delta \hat{Y}_\alpha \Delta \hat{Y}_\beta) = E^{(\alpha\beta)^{-1}}. 
\] (115)

Here a noisy mode will always reveal itself by its small eigenvalue.

7.5 Convert to \( \hat{X}_\alpha \)

For the purpose of constructing uncorrelated quantities to be plotted on a graph, it is desirable to compute the prewhitened power spectrum \( \hat{X}_\alpha \).

To compute \( \hat{X}_\alpha \), start from the estimate \( \hat{Z}_\alpha \) given by equation (103), transform this into \( \hat{Y}_\alpha = E^{1/2} \hat{Z}^\beta \), equation (99), thence into the power spectrum \( \xi_\alpha = (H^{-1/2})^2 \hat{Y}_\beta \), equation (45), and thence into the prewhitened power spectrum \( \hat{X}_\alpha \), equation (70).

The covariance of the prewhitened power \( \hat{X}_\alpha \) is, by construction, the same as that of \( \hat{Y}_\alpha \), equation (115).

\[
(\Delta \hat{X}_\alpha \Delta \hat{X}_\beta) = E^{-1}(\alpha\beta) 
\] (116)

the inverse of the symmetrized Fisher matrix of the prewhitened power.

The estimator \( \hat{X}_\alpha \) of prewhitened power, equation (70), is a nonlinear transformation of the estimator \( \xi_\alpha \) of power, and is therefore biased if \( \xi_\alpha \) is unbiased. However, the estimator \( \hat{X}_\alpha \) is unbiased in the asymptotic limit of a large quantity of data.

7.6 Decorrelate

One final step remains, which is to process the measured prewhitened power spectrum \( \hat{X}_\alpha \) into a set of decorrelated band-powers. How to accomplish such decorrelation is described in Paper 4.

One possibility would be to decorrelate the power spectrum \( \xi(k) \) itself. This is a bad idea, because the power spectrum is highly correlated in the nonlinear regime, so the decorrelation matrices would be broad, with large negative off-diagonal entries, making it impossible to interpret the decorrelated band-powers as representing the power spectrum over some narrow band.

Another possibility would be to decorrelate the prewhitened power \( \hat{X}_\alpha \) not in Fourier space but rather in the representation of eigenfunctions \( \phi_\alpha \) of the prewhitened 4-point matrix \( M \). Again this seems not so good an idea, in the first place because the physical meaning of this representation is obscure, and in the second place because the eigenfunctions can mix where their eigenvalues \( \mu_\alpha \) are degenerate. Since \( \mu_\alpha \approx \xi(k_\alpha) \), such mixing in practice occurs between wavenumbers \( k_\alpha \), where the power \( \xi(k_\alpha) \) is the same, which happens to either side of the peak in the power spectrum.

Figure 11. Perhaps in the future a better understanding of the eigenfunctions \( \phi_\alpha \) will emerge, amongst other things allowing mixing to avoid, but in the meantime these problems remain.

The natural solution is to decorrelate the prewhitened power \( \hat{X}(k) \) in Fourier space. As seen in (11) the covariance of the prewhitened power is encouragingly narrow in Fourier space, narrow enough that the decorrelation matrices will be narrow, so that the decorrelated band-powers can be interpreted as estimates of the prewhitened power over narrow intervals of wavenumber \( k \). In contrast to the prewhitened power \( \hat{X}_\alpha \) in the \( \phi_\alpha \)-representation, the prewhitened power \( \hat{X}(k) \) in Fourier space has a clear interpretation, and there is no problem arising from mixing of eigenfunctions.

8 THE FULL FKP

Sections 3 and 4 invoked not only the FKP approximation, but also the simplifying approximation (80) to the prewhitened reduced covariance \( \mathcal{B} \). How much more work would it take to compute the minimum variance estimator and Fisher matrix of nonlinear power making only the FKP approximation and no other approximation? The question is of both didactic and practical interest.

8.1 Fisher matrix

The FKP approximation to the Fisher matrix of the power spectrum, equation (13), looks simplest expressed in real space:

\[
F(r_\alpha, r_\beta) = \mathbb{C}^{-1}(r_\alpha, r_\beta; \tilde{n}_i, \tilde{n}_j) \delta_D(r_{ij} - r_\beta) d^3 r_i d^3 r_j. \tag{117}
\]

The corresponding expression for the FKP approximation to the Fisher matrix of the prewhitened power spectrum, equation (82), is

\[
E(r_\alpha, r_\beta) = \mathbb{B}^{-1}(r_\alpha, r_\beta; \tilde{n}_i, \tilde{n}_j) \delta_D(r_{ij} - r_\beta) d^3 r_i d^3 r_j. \tag{118}
\]

These are 5-dimensional (thanks to the Dirac delta-function) integrals over pairs of volume elements \( ij \) separated by \( r_{ij} \equiv |r_i - r_j| = r_\beta \) in the survey. The integrals are actually quite doable. If, as is typical, the selection function \( n(r) \) separates into the product of an angular mask and a radial selection function, then the 3-dimensional angular integrals can be done analytically (Hamilton 1993), leaving a double integral of \( \mathbb{C}^{-1}(r_\alpha, r_\beta; \tilde{n}_i, \tilde{n}_j) \) or \( \mathbb{B}^{-1}(r_\alpha, r_\beta; \tilde{n}_i, \tilde{n}_j) \) over the radial directions. The matrices \( \mathbb{C}(r_\alpha, r_\beta; \tilde{n}_i, \tilde{n}_j) \) or \( \mathbb{B}(r_\alpha, r_\beta; \tilde{n}_i, \tilde{n}_j) \), discretized (12) over a grid of separations \( r_\alpha \) and \( r_\beta \), can be inverted numerically for each pair of values of the selection functions \( \tilde{n}_i \) and \( \tilde{n}_j \).

The problem with equations (117) or (118) is that experience (12, 8.3) suggests that discretization of the matrix \( \mathbb{C}(r_\alpha, r_\beta; \tilde{n}_i, \tilde{n}_j) \) or \( \mathbb{B}(r_\alpha, r_\beta; \tilde{n}_i, \tilde{n}_j) \) in real space is liable to introduce ringing and aliasing in Fourier space, defeating the
aim of constructing an accurate Fisher matrix of the power spectrum.

A possibly more robust procedure would be to follow more closely the program described in [8] and [7]. In Fourier space, the FKP approximation to the prewhitened Fisher matrix, equation (12), is

\[ E(k_\alpha, k_\beta) = \mathcal{B}^{-1}(k_\alpha, k_\beta; \bar{n}_i, \bar{n}_j) \delta_{ij}(r_i - r_j) \frac{4\pi k^2 dk_\gamma}{(2\pi)^3} . \]  

(119)

This integral might be evaluated as follows (since I have not actually carried through this program, I cannot say for sure that it would work without a hitch). Firstly, compute the matrix of pair integrals

\[ R(r; k_\alpha, k_\beta) = \int \mathcal{B}^{-1}(k_\alpha, k_\beta; \bar{n}_i, \bar{n}_j) \delta_{ij}(r_i - r_j) \frac{4\pi k^2 dk_\gamma}{(2\pi)^3} . \]  

(120)

for many pair separations \( r_{ij} = r \). These pair integrals \( R(r; k_\alpha, k_\beta) \), equation (120), are analogous to the FKP-weighted pair integrals \( \tilde{R}(r; \mu_\alpha) \), equation (43). Next, cosine transform (e.g. with FFTLog) the pair integrals

\[ \tilde{R}(k; k_\alpha, k_\beta) = 2 \int_0^{\infty} \cos(kr) R(r; k_\alpha, k_\beta) dr \]  

(121)

analogously to \( \tilde{R}(k; \mu_\alpha) \), equation (53). Finally, compute the prewhitened Fisher matrix \( E(k_\alpha, k_\beta) \) by integrating

\[ E(k_\alpha, k_\beta) = \frac{1}{2\pi k_\beta} \int_0^{\infty} \left[ \tilde{R}(k_\gamma - k_\beta; k_\alpha, k_\gamma) - \tilde{R}(k_\gamma + k_\beta; k_\alpha, k_\gamma) \right] k_\gamma dk_\gamma . \]  

(122)

In practice, the matrix \( \mathcal{B}(k_\alpha, k_\beta; \bar{n}_i, \bar{n}_j) \) in equation (120) must be inverted on a discrete grid of wavenumbers \( k \). Similarly, the integral over \( k_\gamma \) in equation (122) should be done as a discrete sum. Specifically, if the matrices are discretized (2,3) on a logarithmic grid of wavenumbers, so that \( \tilde{R}(k; k_\alpha, k_\beta) \) discretizes to \( R_{k_\alpha, k_\beta}(k) = R(k; k_\alpha, k_\beta) \) \( 4\pi \langle k_\alpha k_\beta \rangle^{3/2} \Delta \ln k/(2\pi)^3 \), and the Fisher matrix \( E(k_\alpha, k_\beta) \) discretizes to \( E_{k_\alpha, k_\beta} = E(k_\alpha, k_\beta) 4\pi \langle k_\alpha k_\beta \rangle^{3/2} \Delta \ln k/(2\pi)^3 \), then equation (122) becomes

\[ E_{k_\alpha, k_\beta} = \sum_{k_\gamma} \langle k_\beta k_\gamma k_\alpha \rangle^{1/2} \frac{1}{2\pi} \left[ \hat{R}_{k_\alpha, k_\gamma}(k_\gamma - k_\beta) - \hat{R}_{k_\alpha, k_\gamma}(k_\gamma + k_\beta) \right] . \]  

(123)

It may be anticipated that, as in [22, equation (123)], this will tend to overestimate the diagonal elements \( E_{k_\alpha, k_\alpha} \) if the gridding of the matrix is too coarse to resolve the diagonal properly. Integrating the continuous Fisher matrix \( E(k_\alpha, k_\beta) \), equation (122), over \( k_\beta \) yields

\[ \int_0^{\infty} E(k_\alpha, k_\beta) k_\beta dk_\beta = \frac{1}{\pi} \int_0^{k_\alpha} \hat{R}(k; k_\alpha, k_\gamma) dk_\gamma . \]  

(124)

Discretized, equation (124) becomes

\[ \sum_{k_\beta} \langle k_\beta k_\alpha \rangle^{1/2} E_{k_\alpha, k_\beta} = \frac{1}{\pi} \sum_{k_\gamma} \langle k_\gamma k_\alpha \rangle^{1/2} \int_0^{k_\alpha} \hat{R}_{k_\alpha, k_\gamma}(k) dk . \]  

(125)

The integral over \( k_\gamma \) on the right hand side of equation (125) can be done conveniently as a sine transform (e.g. with FFTLog) of the pair integral

\[ \int_0^{k_\alpha} \hat{R}_{k_\alpha, k_\gamma}(k) dk = 2 \int_0^{\infty} \sin(kr) \hat{R}_{k_\alpha, k_\gamma}(r) dr . \]  

(126)

If the sum on the left hand side of equation (123) exceeds the right hand side, then reduce the diagonal elements \( E_{k_\alpha, k_\beta} \) so that the sum is satisfied. It is fine to evaluate the sum on the right hand side of equation (123) as a discrete sum over \( k_\gamma \), rather than as a continuous integral, because \( R_{k_\alpha, k_\beta}(k) \), equation (124), inherits its behaviour from \( \mathcal{B}_{k_\alpha, k_\beta} \), which, if constructed, equation (124), from the 4-point and 3-point matrices \( M \) and \( L \) as discussed in [14], should behave correctly near the diagonal even if the resolution is too coarse to resolve the diagonal.

8.2 Estimate of power

The FKP approximation to the minimum variance estimator of the power spectrum, equation (13), again looks simplest when expressed in real space:

\[ \hat{\xi}_\alpha = F^{-1}_{\alpha \beta} \tilde{\xi}_\beta . \]  

(127)

with

\[ \tilde{\xi}(r) = \int \mathcal{C}^{-1}(r; \bar{n}_i, \bar{n}_j) \delta(r_i) \delta(r_j) \frac{d^3 r_i d^3 r_j}{[1 + \xi(r_i)]^{1/2}} . \]  

(128)

As usual, the prewhitened estimator \( \hat{\tilde{Y}} \equiv H^{-1/2} \tilde{\xi} \), equation (74), is related to the estimator \( \tilde{Z} \) by \( \hat{\tilde{Y}} = E^{-1} \tilde{Y} \), equation (109). The FKP approximation to the estimator \( \hat{\tilde{Y}} \) is, equation (109),

\[ \hat{\tilde{Z}}(r) = \int \mathcal{B}^{-1}(r; \bar{n}_i, \bar{n}_j) \delta(r_i) \delta(r_j) \frac{d^3 r_i d^3 r_j}{[1 + \xi(r_i)]^{1/2}} . \]  

(129)

Equations (128) and (129) are 6-dimensional integrals over pairs of volume elements \( ij \) in the survey. But once again one may anticipate that discretization of the matrices \( \mathcal{C}(r_i, r_j; \bar{n}_i, \bar{n}_j) \) or \( \mathcal{B}(r_i, r_j; \bar{n}_i, \bar{n}_j) \) in real space would introduce ringing and aliasing in Fourier space, defeating the aim of constructing an accurate estimator of the power spectrum.

Again, it seems likely that it would be more robust to work with prewhitened quantities in Fourier space. In Fourier space, the FKP approximation to the estimator \( \hat{Z} \) is, equation (109),

\[ \hat{Z}(k_\alpha, k_\beta) = \int \mathcal{B}^{-1}(k_\alpha, k_\beta; \bar{n}_i, \bar{n}_j) \delta(r_i) \delta(r_j) \frac{d^3 r_i d^3 r_j 4\pi k^2 dk_\gamma}{[1 + \xi(r_i)]^{1/2}} . \]  

(130)

One way to evaluate this integral might be as follows. Firstly, compute the matrix \( \hat{S}(r; k_\alpha, k_\beta) \) of integrals over pairs of overdensities \( \delta(r_i) \delta(r_j) \) at many separations \( r_{ij} = r \)

\[ \hat{S}(r; k_\alpha, k_\beta) = \int \mathcal{B}^{-1}(r; k_\alpha, k_\beta; \bar{n}_i, \bar{n}_j) \delta_{ij}(r_i - r_j) \delta(r_i) \delta(r_j) \frac{d^3 r_i d^3 r_j}{[1 + \xi(r_i)]^{1/2}} . \]  

(131)

which may be compared to equation (102). Next, prewhiten (compare eq. [104])

\[ \tilde{Z}(r; k_\alpha, k_\beta) = \hat{S}(r; k_\alpha, k_\beta) \frac{1}{[1 + \xi(r)]^{1/2}} . \]  

(132)

and Fourier transform, e.g. with FFTLog, (compare eq. [104])

\[ \tilde{Z}(k; k_\alpha, k_\beta) = \int_{-\infty}^{\infty} j_0(kr) \tilde{Z}(r; k_\alpha, k_\beta) 4\pi r^2 dr . \]  

(133)
Actually it suffices to do this Fourier transform for \( k = k_\beta \) only. Finally, the estimator \( \hat{Z}(k_\alpha) \), equation (133), is
\[
\hat{Z}(k_\alpha) = \int_0^\infty \hat{Z}(k_\beta; k_\alpha, k_\beta) \frac{4\pi k_\beta^3 k_\alpha^3}{(2\pi)^3} \, dk_\beta.
\]
(134)
The integral in equation (134) should be done as a discrete sum. If discretized on a logarithmic grid of wavenumbers, so that \( \hat{Z}(k_\alpha) \) discretizes to \( \hat{Z}_k \), \( \hat{Z}_k = \hat{Z}(k_\alpha | \{4\pi k_\alpha^3 \Delta \ln k/(2\pi)^3\}^{1/2} \) and \( \hat{Z}(k; k_\alpha, k_\beta) \) discretizes to \( \hat{Z}_k \hat{Z}_k \), then equation (134) is
\[
\hat{Z}_k = \sum_{k_\beta} \hat{Z}_k \hat{Z}_k \frac{4\pi k_\beta^3 \Delta \ln k}{(2\pi)^3} \right)^{1/2}.
\]
(135)

9 RECIPES

This section summarizes the results of previous sections into logical sequences of practical steps needed to estimate the prewhitened nonlinear power spectrum from an actual galaxy survey. The end result is a set of uncorrelated prewhitened nonlinear band-powers with error bars, over some prescribed grid of wavenumbers \( k \).

There are three versions of the recipe, gourmet (§9.1), fine (§9.2), and fastfood (§9.3). All the methods use the FKP approximation, equation (132). Thus one should imagine that there is also a haute-cuisine method, which might be brute-force, or it might be some clever procedure that apodizes edges.

First a disclaimer. The methods described herein do not take into account redshift distortions, whose effects on the power spectrum are at least as great as those of nonlinearity. There is no point in using these methods as they stand, without also taking into account redshift distortions. However, given that a full-blown procedure including redshift distortions may well be based on this method, it seems worthwhile to lay out the steps required to implement them.

9.1 Gourmet

This version of the recipe is conceptually the simplest, but it takes the most computing power (a supercomputer would be handy). The procedure is a direct implementation of the FKP approximation to the minimum variance estimator of prewhitened power and the associated Fisher matrix, as described in §6.

Naturally, if one were going to the trouble of using the gourmet recipe, then one would want to use the best possible model of the 3-point and 4-point correlation functions, not just the hierarchical model with constant amplitudes.

Steps 1 and 2 below require knowledge of the selection function of a survey, but no actual data. Steps 3–5 require actual data from a galaxy survey.

Step 1. Compute the FKP approximation to the asymmetric Fisher matrix \( E^{\alpha\beta} \) of the prewhitened nonlinear power spectrum, as described in §6.1, equations (121)–(122). Equation (121) involves a 5-dimensional integral over pairs \( ij \) of volume elements separated by \( r_{ij} = r \) in the survey. If the selection function \( n(r) \) separates into the product of an angular mask and a radial selection function, then the 3-dimensional angular integrals can be done analytically (Hamilton 1993), leaving a double integral of \( \Sigma^{-1}(k_\alpha, k_\beta, \bar{n}_i, \bar{n}_j) \) over the radial directions.

Step 2. The covariance matrix \( (\Delta \hat{X}_\alpha, \Delta \hat{X}_\beta) \) of the prewhitened power is equal, equation (111), to the inverse \( E^{-1}(\alpha, \beta) \) of the symmetrized Fisher matrix. Use this covariance matrix to construct decorrelation matrices \( W \), as described in Paper 4, with the property that \( W (\Delta X \Delta X^\top) W^\top \) is diagonal in Fourier space (cf. Paper 4 eq. [20]). The diagonal elements of this diagonal matrix are the expected variances of the decorrelated band-powers \( \hat{B} = W X \) to be computed in Step 5.

Step 3. Compute the estimator \( \hat{Z}_X \) as described in §8.2 equations (131)–(133).

Step 4. Transform \( Z^\alpha \) into the prewhitened power \( \hat{X}_\alpha \), using equations (99), (74), and (70), as stated in §7.3.

Step 5. Decorrelate the estimated prewhitened power spectrum \( \hat{X} \) into a set of uncorrelated band-powers \( \hat{B} = W \hat{X} \) using the decorrelation matrices \( W \) computed in Step 2. Bear in mind that, as usual in ML fitting, the error bars should of course be interpreted as being attached to the model, the prior band-powers \( B \), rather than to the data, the estimated band-powers \( \hat{B} \).

9.2 Fine

This method adopts the approximation made in §6 and §9.1 that the prewhitened reduced covariance matrix \( \hat{B} \) takes the simplified form \( \hat{B} \). According to the results of §6, this approximation to \( \hat{B} \) should be quite good. If it is, then the fine method should yield results close to the gourmet method of §9.1 at a considerable saving in computer time.

Steps 1–5 below do not require any actual data; the steps can be used to determine in advance how well the prewhitened power spectrum might be measured from a survey. Steps 6–9 require actual data from a galaxy survey.

Step 1. Compute a table of FKP-weighted pair integrals \( R(r; \mu) \) at many separations \( r \) and several FKP constants \( \mu \). Calculating the pair integrals \( R(r; \mu) \) requires knowing the selection function \( \bar{n}(r) \) of a galaxy survey, but does not require actual data. This pair integral, commonly denoted \( RR \), is commonly computed by Monte Carlo integration, but I find it faster, more accurate, and more convenient (since the program was already written) to compute the integral directly, using the procedures described by Hamilton (1993).

Step 2. Compute the prewhitened 4-point contribution \( M = H^{-1/2} K H^{-1/2} \) to the reduced covariance of the nonlinear power spectrum. This involves adopting a prior power spectrum \( \xi(k) \), and a model of the 4-point correlation function \( \eta_{ij} \). For the hierarchical model, the covariance matrices \( K \) and \( H \) are given by equations (53) and (57). Some numerical issues concerning the computation of the matrix \( M \) are discussed in §4.4.

Step 3. Compute the eigenfunctions \( \phi_n \) and eigenvalues \( \mu_n^2 \), equation (53), by diagonalizing the prewhitened 4-point matrix \( M \).

Step 4. Compute the asymmetric Fisher matrix \( E^{\alpha\beta} \), equation (53), of the prewhitened nonlinear power spectrum of the survey, in the representation of eigenfunctions \( \phi_n \) of the
prewhitened 4-point matrix $M$. This is where the pair integral $R(r,\mu)$ computed in Step 1 is needed. Numerical issues are discussed in [36].

Step 5. Same as Step 2 of the gourmet method: from the inverse $E^{-1}_{(\alpha\beta)}$ of the symmetrized Fisher matrix, construct decorrelation matrices $W$ such that the covariance of the band-powers $B = W \tilde{X}$ is diagonal. Decorrelation is the subject of Paper 4.

Step 6. Compute a table of FKP-weighted pair densities $\tilde{S}(r;\mu)$, equation (102), at many separations $r$ and several FKP constants $\mu$. Calculating $\tilde{S}(r;\mu)$, commonly denoted $(DD) - 2(\hat{D}R) + (RR)$, requires actual data from a survey.

Step 7. From $\tilde{S}(r;\mu_{\alpha})$, compute the estimate $\tilde{Z}^{\alpha}$, equation (105), in the representation of eigenfunctions $\phi_{\alpha}$, as described in §7.4.

Step 8. Same as Step 4 of the gourmet method: transform $\tilde{Z}^{\alpha}$ into the prewhitened power $\tilde{X}_{\alpha}$ using equations (20), (4), and (70), as stated in §7.4. The transformations may be done in whatever representation proves most convenient or numerically reliable. Ultimately, one wants the prewhitened power spectrum $\tilde{X}(k)$ in Fourier space.

Step 9. Same as Step 5 of the gourmet method: decorrelate the prewhitened power spectrum $\tilde{X}$ into a set of uncorrelated band-powers $\tilde{B} = W \tilde{X}$, using the decorrelation matrices $W$ computed in Step 5 above.

9.3 Fastfood

For some purposes a simplified, approximate version of the procedure in §9.2 may be considered adequate.

The basic simplifying approximation here is that the covariance $\langle \Delta \tilde{X}(k_{\alpha}) \Delta \tilde{X}(k_{\beta}) \rangle$ of the prewhitened power spectrum may be considered to be diagonal in Fourier space without further refinement. The procedure then becomes the same as the FKP procedure for Gaussian fluctuations, with the differences that (a) it is the prewhitened power spectrum $\tilde{X}(k)$, equation (29), rather than the power spectrum $\xi(k)$ that is being estimated; and (b) the FKP constants $\mu(k)$ in the FKP pair-weightings are modified from the Gaussian case where $\mu(k) = \xi(k)$.

Figure 11 shows the ratio $\mu(k)/\xi(k)$ of the effective FKP constant $\mu(k)$ to the nonlinear power spectrum $\xi(k)$, as a function of wavenumber $k$, for several different power spectra. The ratios should be regarded as indicative rather than definitive, because they depend on the validity of the hierarchical model (see text). The numbered curves are for power law power spectra with correlation functions $\xi(r) = (r/5h^{-1}{\text{Mpc}})^{-\gamma}$, the number label being the index $\gamma$. The curve labelled P97 is for the $\Omega_m = 0.3$ power spectrum derived from observations by Peacock (1997), while that labelled ACDM is for the ACDM power spectrum of Eisenstein & Hu (1998).

whose inverse gives the covariance of the prewhitened power $\tilde{X}$

$$\langle \Delta \tilde{X}_{\alpha} \Delta \tilde{X}_{\beta} \rangle = \frac{2}{V} M_{\alpha\beta}.$$ (137)

Decorrelating this covariance, equation (135), in Fourier space, as described in Paper 4, yields band-powers $B(k)$ whose covariance is by construction diagonal. The diagonal values of the diagonal covariance matrix of the band-powers can be taken to define the effective FKP constants $\mu(k)$

$$\langle \Delta \tilde{B}(k_{\alpha}) \Delta \tilde{B}(k_{\beta}) \rangle = 1_{\alpha\beta} \frac{2}{V} \frac{\mu(k_{\alpha})^2}{\xi(k_{\alpha})^2}.$$ (138)

With the effective FKP constants $\mu(k)$ taken as given by Figure 11 the shortcut recipe is then as follows.

Step 1. Compute the effective spatial volume $V(k)$ of the survey for modes at wavenumber $k$

$$V(k) = \frac{2}{M} \xi(k) \frac{d^3r}{[1 + \delta^2(r)^{-1} \mu(k)^{-1}]}.$$ (139)

Step 2. The Fisher matrix (33) of the prewhitened power reduces to

$$E(k_{\alpha},k_{\beta}) = \frac{1}{2} \int_{0}^{\infty} j_0(k_{\alpha}r) j_0(k_{\beta}r) R(r;\mu_{\alpha}) 4\pi r^2dr.$$ (140)

If the prewhitened power is averaged over sufficiently broad shells in $k$-space, then, by arguments similar to those in §8.4, the Fisher matrix is approximately diagonal (compare eq. 28)

$$E(k_{\alpha},k_{\beta}) \approx (2\pi)^3 \delta_{\alpha\beta} (k_{\alpha} - k_{\beta}) \frac{V(k_{\alpha})}{2 \mu(k_{\alpha})^2}$$ (141)

where $V(k_{\alpha})$ is the effective volume given by equation (139).
For the approximation \(\hat{M} \) to be valid, the shells in \(k\)-space must be broad not only compared to the inverse scale of the survey (as in the Gaussian case), but also compared to the width of the 4-point matrix \(M\) plotted in Figures 3 and 4. In the large \( k \), hierarchical limit, the width of the matrix \( M \) in \( k \)-space is comparable to an inverse correlation length, \( \Delta k \sim \pi / r_0 \).

**Step 3.** The covariance \( \langle \hat{X}(k_a) \hat{X}(k_b) \rangle \) of the prewhitened power equals the inverse of the Fisher matrix \( E(k_a, k_b) \) given by equation (141)

\[
\langle \hat{X}(k_a) \hat{X}(k_b) \rangle \approx (2\pi)^3 \delta_{4D}(k_a - k_b) \frac{2 \mu(k_a)^2}{V(k_a)} .
\]

Define prewhitened band-powers \( \hat{B}(k) \) to be the prewhitened power spectrum \( \hat{X}(k) \) averaged over broad (as in Step 2) shells of volume \( V_k \) about \( k \)

\[
\hat{B}(k) \equiv V_k^{-1} \int \hat{\xi}(k) \, dV_k
\]

where \( dV_k \equiv 4\pi k^2 dk/(2\pi)^3 \). The variance of the shell-averaged prewhitened band-powers is

\[
\langle \hat{B}(k)^2 \rangle \approx \frac{2 \mu(k_a)^2}{V(k)} V_k
\]

which is \( 2 \mu(k_a)^2 \) divided by the effective phase volume, the product of the effective spatial volume \( V(k) \), equation (139), with the Fourier volume \( V_k \) of the shell in \( k \)-space.

**Step 4.** Same as Step 6 of §4.2, compute FKP-weighted pair densities \( \hat{S}(r; \mu) \), equation (102).

**Step 5.** Compute the estimator \( \hat{Z}(k) \)

\[
\hat{Z}(k) = \int_0^{\infty} \frac{\mu(k r) \hat{S}(r; \mu)}{[1 + \hat{\xi}(r)]^{1/2}} 4\pi^2 dr
\]

which may be compared to equation (104).

**Step 6.** Same as Step 8 of §4.2, transform \( \hat{Z}(k) \) to \( \hat{X}(k) \) using equations (94), (74), and (70). The estimator \( \hat{Y} = E^{-1}Z \) is

\[
\hat{Y}(k) = \frac{2 \mu(k)^2}{V(k)} \hat{Z}(k) .
\]

**Step 7.** Form prewhitented band powers \( \hat{B}(k) \) by averaging \( \hat{X}(k) \) over sufficiently broad shells in \( k \)-space, equation (143).

**10 CONCLUSIONS**

The main finding of this paper is that the prewhitened nonlinear power spectrum \( X_\alpha \) defined by equation (67) has surprisingly sweet properties.

Firstly, the covariance of the prewhitened nonlinear power is substantially narrower in Fourier space than the covariance of the nonlinear power spectrum itself, Figures 5 and 6.

Secondly, in the FKP approximation, the 4-point and 3-point contributions \( M \) and \( L \) to the covariance of prewhitened power are almost simultaneously diagonal (the 2-point contribution is by construction the unit matrix, so is automatically diagonal), Figures 9 and 10. Thus the eigenmodes of the covariance of prewhitened nonlinear power form a set of almost uncorrelated modes somewhat analogous to the Fourier modes of power in the Gaussian case.

Thirdly, the eigenvalues \( \mu_\alpha \) and \( \lambda_\alpha \), as defined by equations (17) and (18), of the 4-point and 3-point prewhitened matrices \( M \) and \( L \) are almost equal, \( \mu_\alpha \approx \lambda_\alpha \). Figure 8, which is similar to the Gaussian case where \( \mu(k) = \lambda(k) = \xi(k) \).

The second and third points above together make it possible to construct a near-minimum variance estimator, §4.2 and Fisher matrix, §4.3 of the prewhitened nonlinear power spectrum similar to the FKP estimator and Fisher matrix of the linear power spectrum in the Gaussian case.

Fourthly, all the above properties hold for all power spectra tested, including power law nonlinear power spectra \( \xi(k) \propto k^n \) with indices \( -2 < n < 0 \) over the full range allowed by the hierarchical model, and including realistic power spectra, such as the observationally derived power spectrum of Peacock (1997), and an observationally concordant ΛCDM model of Eisenstein & Hu (1998), nonlinearly evolved according to the Peacock & Dodds (1996) formula.

Fifthly, in the realistic cases of the Peacock (1997) and Eisenstein & Hu (1998) power spectra, the prewhitened nonlinear power spectrum \( X(k) \) appears to be curiously close to the linear power spectrum \( \xi_L(k) \), Figure 10.

This having been said, it should be emphasized that the above properties are all premised on the hierarchical model with constant hierarchical amplitudes, §3.2 which as discussed in §2.2 and by Scoccimarro et al. (1999 §3.3) is certainly wrong at some level. Clearly it will be important to test how well these results stand up in \( N \)-body simulations.

In the meantime, the results of this paper raise questions. Is there some physical reason underlying the seemingly unreasonably pretty properties of the prewhitened nonlinear power spectrum? In general, modes may be statistically uncorrelated without being dynamically independent. But the fact that the covariance of the prewhitened power is narrow for all power spectra is suggestive: do the eigenmodes of the covariance of prewhitened power somehow encode the information in the linear power spectrum that is ravelled by nonlinear evolution in the power spectrum itself? And is there somehow a connection to the mapping between linear and nonlinear power spectra found by Hamilton et al. (1991)?

I conclude with a repeat of the warning that this paper has ignored redshift distortions, light-to-mass bias, and evolution, and it has assumed that the only sources of variance are cosmic variance and shot-noise variance arising from Poisson sampling of galaxies. In real galaxy surveys, all these problems must be grappled with.

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**REFERENCES**
APPENDIX A: JUSTIFICATION OF EQUATION (??)

Equation (11) is the FKP approximation, expressed in concise mathematical form. This appendix offers further details justifying this equation.

The pair-pair covariance matrix $\mathcal{C}_{ijkl}$ can be regarded as an operator that acts on pair-functions $\Psi_{kl}$. It is helpful to think of $\Psi_{kl}$ as a 2-particle wavefunction (symmetric under pair exchange $k \leftrightarrow l$), and $\mathcal{C}_{ijkl}$ as a Hermitian operator that acts on the space of such wavefunctions. The pair-wavefunctions $\Psi_{kl}$ of interest in the present case have translation and rotation symmetry, which means that they have zero total momentum and zero total angular momentum. In the Fourier representation such wavefunctions $\Psi_{kl}$ can be expressed in the form

$$\Psi(k_k, k_l) = (2\pi)^3 \delta_{3D}(k_k + k_l) \psi(k_k)$$

(147)

where $\psi(k_k)$ is a function of the scalar $k_k \equiv |k_k|$. In a general representation, equation (147) is

$$\Psi_{kl} = D_{kl}^0 \psi_{\alpha}$$

(148)

where $D_{kl}^0$ is the operator introduced in 2.4 equations (28) and (29).

In the FKP approximation, the selection functions $\bar{n}_i$ and $\bar{n}_j$ upon which the pair-covariance $\mathcal{C}_{ijkl}$ depends, equations (48) and (29), are taken to be locally constant, so that $\mathcal{C}_{ijkl}$ also has translation and rotation symmetry, i.e. it commutes with the operators of total momentum and total angular momentum. Thus in the FKP approximation, $\mathcal{C}_{ijkl}$ acting on a wavefunction $D_{kl}^0 \psi_{\alpha}$ with zero momentum and angular momentum yields another wavefunction $D_{ij}^0 \chi_{\beta}$ with zero momentum and angular momentum

$$\mathcal{C}_{ijkl} D_{kl}^0 \psi_{\alpha} = D_{ij}^0 \chi_{\beta}$$.

(149)

Take $\psi_{\alpha}$ in equation (149) to be the elements of a complete orthonormal basis of functions. Then equation (149) implies that

$$\mathcal{C}_{ijkl} D_{kl}^0 = D_{ij}^0 \mathcal{C}_{\alpha\beta}$$

(150)

for some matrix $\mathcal{C}_{\alpha\beta}$. Equation (150) is the desired equation (11) that was to be justified (at least if the indices on $\mathcal{C}_{\alpha\beta}$ are swapped in eq. 151, which is fine because $\mathcal{C}_{\alpha\beta}$ is symmetric, as proven below). The wavefunctions $\psi_{\alpha}$ and $\chi_{\beta}$ in equation (149) are related by

$$\mathcal{C}_{\alpha\beta} \psi_{\alpha} = \chi_{\beta}$$

(151)

A wavefunction of the form $D_{ij}^0 \psi_{\alpha}$ is unnormalized – that is, $\psi_{\alpha} D_{ij}^0 D_{ij}^0 \psi_{\beta}$ diverges – as is usual in quantum mechanics for a wavefunction that has definite momentum, and must therefore be defined over infinite space. The divergence can be tamed by regarding the wavefunction as being defined instead over an extremely large but finite volume $V$. Then

$$D_{ij}^0 D_{ij}^0 = 1_{i\alpha\beta} V$$

(152)

which is most easily proven from the real space representation of $D_{ij}^0$, equation (28). Equation (152) should be interpreted with due care. For example, equation (152) should not be substituted into equation (45) for the Fisher matrix in the FKP approximation, because the matrix $\mathcal{C}^{-1\gamma\gamma}(\bar{n}_i, \bar{n}_j)$ on the right hand side of equation (45) varies with positions $i$ and $j$.

Operating on equation (150) with $D_{ij}^0$ implies, from equation (152), that $(\bar{n}_i, \bar{n}_j)$ here are being regarded formally as fixed constants in the huge volume $V$.

$$D_{ij}^0 \mathcal{C}_{ijkl} D_{kl}^0 = V \mathcal{C}_{\alpha\beta}$$

(153)

It is evident from this equation that the pair exchange symmetry $ij \leftrightarrow kl$ of $\mathcal{C}_{ijkl}$ implies that $\mathcal{C}_{\alpha\beta}$ is similarly symmetric

$$\mathcal{C}_{\alpha\beta} = \mathcal{C}_{\beta\alpha}$$

(154)

Equation (153) shows that, modulo the normalization factor $V$, the reduced matrix $\mathcal{C}_{\alpha\beta}$ can be regarded as the matrix elements of the operator $\mathcal{C}_{ijkl}$ restricted to the class of wavefunctions that have zero total momentum and zero total angular momentum.

APPENDIX B: FFTLOG

B.1 Introduction

FFTLog computes the fast Fourier or Hankel (= Fourier-Bessel) transform of a periodic sequence of logarithmically spaced points. FFTLog can be regarded as a natural analogue to the standard FFT, in the sense that, just as the normal FFT gives the exact (to machine precision) Fourier transform of a linearly spaced periodic sequence, so also FFTLog gives the exact Fourier or Hankel transform, of arbitrary order $\mu$, of a logarithmically spaced periodic sequence. FFTLog shares with the normal FFT the problems of ringing (response to sudden steps) and aliasing (periodic folding...
of frequencies), but under appropriate circumstances FFTLog may approximate the results of a continuous Fourier or Hankel transform.

The FFTLog algorithm was originally proposed by Talman (1978). However, it seems worthwhile here to present the algorithm in some detail.

The FFTLog code may be downloaded from http://casa.colorado.edu/~ash/FFTLog/.

Consider the continuous Hankel (= Fourier-Bessel) transform pair
\[ \tilde{a}(k) = \int_0^\infty a(r) (kr)^\mu J_\mu(kr) \, k \, dr \]  
(155)
\[ a(r) = \int_0^\infty \tilde{a}(k) (kr)^{-\mu} J_\mu(kr) \, r \, dk . \]  
(156)
If the substitution
\[ a(r) = A(r) r^{-\mu} \quad \text{and} \quad \tilde{a}(k) = \tilde{A}(k) k^\mu \]  
(157)
is made, then the Hankel transform pair (155), (156), becomes equivalent to the transform pair
\[ \tilde{A}(k) = \int_0^\infty A(r) J_\mu(kr) \, k \, dr \]  
(158)
\[ A(r) = \int_0^\infty \tilde{A}(k) J_\mu(kr) \, r \, dk . \]  
(159)
Although the Hankel transform (155) with a power law bias \((kr)^{\pm\mu}\) is thus equivalent in the continuous case to the unbiased Hankel transform (155), the transforms are different when they are discretized and made periodic; for if \(a(r)\) is periodic, then \(A(r) = a(r) r^{\mu}\) is not periodic. FFTLog evaluates discrete Hankel transforms (155) and (156) with arbitrary power law bias.

Fourier sine and cosine transforms can be regarded as special cases of Hankel transforms with \(\mu = \pm 1/2\), since
\[ J_{1/2}(x) = (2/\pi x)^{1/2} \sin(x) \quad \text{and} \quad J_{-1/2}(x) = (2/\pi x)^{1/2} \cos(x) . \]  
(160)
(161)
As first noted by Siegman (1977), if the product \(kr\) in the Hankel transform is written as \(e^{ink+\ln r}\), then the transform becomes a convolution integral in the integration variable \(\ln r\) or \(\ln k\). Convolution is equivalent to multiplication in the corresponding Fourier transform space. Thus the Hankel transform can be computed numerically by the algorithm: FFT \(\rightarrow\) multiply by a function \(\rightarrow\) FFT back. This is the idea behind a number of Fast Hankel Transform algorithms (Candel 1981; Anderson 1982; Hansen 1985; Fanning 1996) including FFTLog (Talman 1978).

An advantage of FFTLog, emphasized by Talman (1978), is that the order \(\mu\) of the Bessel function may be any arbitrary real number. In particular, FFTLog works for \(1/2\)-integral \(\mu\), so includes the cases of Fourier sine and cosine transforms, and spherical Hankel transforms involving the spherical Bessel functions \(j_\lambda(x) = (\pi/2x)^{1/2} J_{\lambda+1/2}(x)\).

B.2 Normal discrete Fourier transform

First, recall the essential properties of the standard discrete Fourier transform of a periodic sequence of linearly spaced points. Suppose that \(a(r)\) is a continuous, in general complex-valued, function that is periodic with period \(R\),
\[ a(r + R) = a(r) . \]  
(162)
Without loss of generality, take the fundamental interval to be \([-R/2, R/2]\), centred at zero. Since \(a(r)\) is periodic, its continuous Fourier transform contains only discrete Fourier modes \(e^{2\pi imr/R}\) with integral wavenumbers \(m\). Suppose further that the function \(a(r)\) is ‘smooth’ in the specific sense that it is some linear combination only of the \(N\) lowest frequency Fourier modes, \(m = 0, \pm 1, \ldots \pm [N/2]\), where \([N/2]\) denotes the largest integer greater than or equal to \(N/2\),
\[ a(r) = \sum_m \tilde{c}_m e^{2\pi imr/R} \]  
(163)
the outermost Fourier coefficients being equal, \(\tilde{c}_{-N/2} = \tilde{c}_{N/2}\), in the case of even \(N\). The primed sum in equation (163) signifies a sum over integral \(m\) from \([-N/2]\) to \([N/2]\), with the proviso that for even \(N\) the outermost elements of the sum receive only half weight:
\[ \sum_n x_n \equiv \sum_{n=-[N/2]}^{[N/2]} \tilde{w}_n x_n \]  
(164)
with \(\tilde{w}_n = 1\) except that \(\tilde{w}_{-N/2} = \tilde{w}_{N/2} = 1/2\) if \(N\) is even.

The sampling theorem (e.g. Press et al. 1986 §12.1) asserts that, given a function \(a(r)\) satisfying equation (163), the Fourier coefficients \(\tilde{c}_m\) can be expressed in terms of the values \(a_n \equiv a(r_n)\) of the function \(a(r)\) at the \(N\) discrete points \(r_n = nR/N\) for \(n = 0, \pm 1, \ldots \pm [N/2]\). For even \(N\), the periodicity of \(a(r)\) ensures that \(a_{-N/2} = a_{N/2}\). Specifically, the sampling theorem asserts that the Fourier coefficients in the expansion (163) satisfy
\[ \tilde{c}_m = \frac{1}{N} \sum_n a_n e^{-2\pi imn/N} \]  
(165)
the discrete points \(a_n\) themselves satisfying
\[ a_n = \sum_m \tilde{c}_m e^{2\pi imn/N} \]  
(166)
in accordance with equation (163).

Equations (165) and (166) constitute a discrete Fourier transform pair relating two periodic, linearly spaced sequences \(a_n\) and \(\tilde{c}_m\) of length \(N\). The standard FFT evaluates the discrete Fourier transform exactly (that is, to machine precision).

B.3 Discrete Hankel transform

Now suppose that the function \(a(r)\), instead of being periodic in ordinary space \(r\), is periodic in logarithmic space \(\ln r\), with logarithmic period \(L\),
\[ a(re^{\ell}) = a(r) . \]  
(167)
Take the fundamental interval to be \([\ln r_0 - L/2, \ln r_0 + L/2]\), centred at \(\ln r_0\). As in §B.2, the periodicity of \(a(r)\) implies that its Fourier transform with respect to \(\ln r\) contains only discrete Fourier modes \(e^{2\pi im(\ln r/\ln r_0)}\) with integral wavenumbers \(m\). Suppose further, as in §B.2 eq. (163), that \(a(r)\) contains only the \(N\) lowest frequency Fourier modes
\[ a(r) = \sum_m \tilde{c}_m e^{2\pi im(\ln r/\ln r_0)} / L \]  
(168)
with $c_{-N/2} = c_{N/2}$ for even $N$. The sampling theorem asserts that the Fourier coefficients $c_m$ are given by

$$c_m = \frac{1}{N} \sum_n a_n e^{-2\pi i mn/N}$$

(169)

where $a_n \equiv a(r_n)$ are the values of the function $a(r)$ at the $N$ discrete points $r_n = r_0 e^{nL/2}$ for $n = 0, \pm 1, \ldots, \pm \lfloor N/2 \rfloor$, $a_n = \sum_m c_m e^{2\pi i mn/N}$.  

(170)

The continuous Hankel transform $\tilde{a}(k)$, equation (154), of a function $a(r)$ of the form (163) is

$$\tilde{a}(k) = \sum_m c_m \int_0^\infty e^{2\pi i m \ln(r/r_0)}/L \ (kr)^\mu J_\mu(kr) \ k \ dr.$$  

(171)

The integrals on the right hand side of equation (171) can be done analytically, in terms of

$$U_\mu(x) \equiv \int_0^\infty t^\mu J_\mu(t) \ dt = 2^{\mu+1} \frac{\Gamma(\mu+1)}{\Gamma(\mu+1-x/2)},$$  

(172)

where $\Gamma(z)$ is the usual Gamma function. Therefore, equation (171) reduces to

$$\tilde{a}(k) = \sum_m c_m u_m e^{-2\pi i m (k/k_0)}/L,$$  

(173)

where $u_m$ is

$$u_m(\mu, q) \equiv (k_0 r_0)^{-2\pi i m / k} U_\mu \left( q + \frac{2\pi i m}{L} \right).$$  

(174)

Notice that $u_m^\ast = u_{-m}$, which ensures that $\tilde{a}(k)$ is real if $a(r)$ is real. Equation (174) gives the (exact) continuous Hankel transform $\tilde{a}(k)$ of a function $a(r)$ of the form (163). Like $a(r)$, the Hankel transform $\tilde{a}(k)$ is periodic in logarithmic space $\ln k$, with period $L$. The fundamental interval is $[\ln k_0 - L/2, \ln k_0 + L/2]$, centred at $\ln k_0$, which may be chosen arbitrarily (but see §B.5 below).

The sampling theorem requires that $u_{-N/2} = u_{N/2}$ for even $N$, which is not necessarily satisfied by equation (174). However, at the discrete points $k_n = k_0 e^{nL/2}$ considered by the sampling theorem, the contributions at $m = \pm N/2$ to the sum on the right hand side of equation (174) are $(-1)^m c_{N/2}(u_{N/2} + u_{-N/2})/2$, whose imaginary part cancels out. Thus the equality (174) remains true at the discrete points $k_n$ if $u_{\pm N/2}$ are replaced by their real parts,

$$u_{\pm N/2} \rightarrow \text{Re} u_{N/2}.$$  

(175)

With the replacement (175), the sampling theorem asserts that the coefficients $c_m u_m$ in the sum (174) are determined by the values $a_n \equiv \tilde{a}(k_0)$ of the Hankel transform at the $N$ discrete points $k_0 = k_0 e^{nL/2}$ for $n = 0, \pm 1, \ldots, \pm \lfloor N/2 \rfloor$.

$$c_m u_m = \frac{1}{N} \sum_n a_n e^{2\pi i mn/N}$$  

(169)

$$\tilde{a}_n = \sum_m c_m u_m e^{-2\pi i mn/N}.$$  

(177)

Putting together equations (169), (174), (176) and (177), yields the discrete Hankel transform pair

$$\tilde{a}_n = \sum_m a_m v^+_m(\mu, q)$$  

(178)

in which the forward discrete mode $v^+_m(\mu, q)$ is the discrete Fourier transform of $u_m(\mu, q)$ given by equations (174) and (173).

$$v^+_m(\mu, q) = \frac{1}{N} \sum_n u_m(\mu, q) e^{-2\pi i mn/N}$$  

(179)

while the inverse discrete Hankel mode $v^-_m(\mu, q)$ is the discrete Fourier transform of the reciprocal $1/u_{-m}(\mu, q)$,

$$v^-_m(\mu, q) = \frac{1}{N} \sum_m \frac{1}{u_{-m}(\mu, q)} e^{-2\pi i mn/N}.$$  

(180)

The Hankel transform matrices $v^+_m(\mu, q)$ and $v^-_m(\mu, q)$ are mutually inverse

$$\sum_i v^+_i(\mu, q) v^-_{i+m}(\mu, q) = \delta_{mn}$$  

(182)

where $\delta_{mn}$ denotes the Kronecker delta. The forward and inverse Hankel modes have the interesting property of being self-similar; that is, Hankel modes $v^+_m(\mu, q)$ or $v^-_{-m}(\mu, q)$ with different indices $m$ consist of the same periodic sequence $v^+_n(\mu, q)$ or $v^-_n(\mu, q)$ cyclically shifted by $m$ notches.

FFTLog evaluates the forward and inverse discrete Hankel transforms given by equations (178), (179), exactly (to machine precision).

The reciprocal $1/u_{-m}(\mu, q)$ in equation (181) is equal to $u_{m}(\mu, -q)$, according to equations (174) and (177).

$$\frac{1}{u_{-m}(\mu, q)} = u_{m}(\mu, -q) \ (m \neq \pm N/2)$$  

(183)

except in the case $m = \pm N/2$ for even $N$, when the replacement (173) generally invalidates equation (183). However, in the special case where $u_{\pm N/2}$ are already real, then equation (175) leaves $u_{\pm N/2}$ unchanged, and equation (183) remains valid also at $m = \pm N/2$. This special case is of particular interest, and is discussed further in §B.5 below.

In the continuous case, the inverse Hankel transform is equal to the forward transform with $q \rightarrow -q$, equations (157) and (156). In the discrete case this remains true for odd $N$, but it is not generally true for even $N$ (the usual choice) except in the important special case discussed in §B.5.

In the general discrete case (i.e. if the condition $\lfloor N/2 \rfloor$ in §B.5 is not satisfied), the inverse discrete Hankel mode $v^-_n(\mu, q)$, equation (157), differs from the forward Hankel mode $v^+_n(\mu, -q)$, equation (180), only for even $N$ and only in the coefficient of the highest frequency Fourier component, $1/u_{-m}(\mu, q)$ versus $u_{m}(\mu, -q)$ for $m = \pm N/2$. To the extent that the highest frequency Fourier coefficient $c_{\pm N/2}$ of a sequence $a_n$ is small, the difference between its inverse discrete Hankel transform and its forward transform with $q \rightarrow -q$ should be small.

It is possible for the inverse discrete Hankel transform to be singular, if $u_{\pm N/2}$ is purely imaginary, so that its real part vanishes, making $v^-_n(\mu, q)$ singular. As discussed in §B.5, this singularity can be avoided by choosing a low-ringing value of $k_0 r_0$, equation (158).

The forward (inverse) discrete Hankel transforms are also singular at special values of $\mu$ and $q$, namely where $\mu + 1 + q$ (or $\mu + 1 - q$ in the inverse case) vanishes, because
$u_0(\mu, q) = U_n(q)$ is singular at these points. This singularity reflects a real singularity in the corresponding continuous Hankel transform (unlike the singularity of the previous paragraph, which is an avoidable artefact of discreteness). The singularity in $u_0$ leads to an additive infinite constant in the discrete Hankel transform. In physical problems this additive infinite constant may somehow cancel out (for example, in the difference between two Hankel transforms). FFTLog’s strategy in these singular cases is to evaluate the discrete Hankel transform with the infinite constant set to zero, and to issue a warning.

### B.4 FFTLog algorithm

The FFTLog algorithm for taking the discrete Hankel transform, equation (178), of a sequence $a_n$ of $N$ logarithmically spaced points is:

- **FFT** $a_n$ to obtain the Fourier coefficients $c_m$, equation (169);
- multiply by $u_m$ given by equations (174) and (177) to obtain $c_m u_m$;
- **FFT** $c_m u_m$ back to obtain the discrete Hankel transform $\tilde{a}_n$, equation (177).

A variant of the algorithm is to sandwich the above operations with power law biasing and unbiasing operations. For example, one way to take the unbiased continuous Hankel transform $\tilde{A}(k)$ of a function $A(r)$, equation (158), is to bias $A(r)$ and $\tilde{A}(k)$ with power laws, equation (159), and take a biased Hankel transform, equation (153). The discrete equivalent of this is:

- Bias $A_n$ with a power law to obtain $a_n = A_n r_{\mu}^{-q}$, equation (157);
- **FFT** $a_n$ to obtain the Fourier coefficients $c_m$, equation (169);
- multiply by $u_m$ given by equations (174) and (177) to obtain $c_m u_m$;
- **FFT** $c_m u_m$ back to obtain the discrete Hankel transform $\tilde{a}_n$, equation (177).
- Unbias $\tilde{a}_n$ with a power law to obtain $\tilde{A}_n = \tilde{a}_n k_{\mu}^{-q}$, equation (153).

Although in the continuous limit the result would be identical to an unbiased Hankel transform, in the discrete case the result differs. With a simple unbiased discrete Hankel transform, it is the sequence $A_n$ that is taken to be periodic, whereas in the algorithm above it is not $A_n$ but rather $a_n$ that is periodic.

The inverse discrete Hankel transform is accomplished by the same series of steps, except that $c_m$ is divided instead of multiplied by $u_m$.

The FFTLog code is built on top of the NCAR suite of FFT routines (Swarztrauber 1979), and a modified version of an implementation of the complex Gamma-function from the gamef package by Ooura (1996).

FFTLog includes driver routines for the specific cases of the Fourier sine and cosine transforms.

### B.5 Low-ringing condition on $k_0 r_0$

The central values $\ln r_0$ and $\ln k_0$ of the periodic intervals in $\ln r$ and $\ln k$ may be chosen arbitrarily. However, ringing of the discrete Hankel transform may be reduced, for either even or odd $N$, if the product $k_0 r_0$ is chosen in such a way that the boundary points of the sequence $u_m$, equation (174), are equal

$$u_{-N/2} = u_{N/2}. \quad (184)$$

Recall that the general procedure, for even $N$, was to replace $u_{\pm N/2}$ by their real part, equation (176). The condition (184) requires that $u_{\pm N/2}$ are already real. The condition (184) reduces ringing because it makes the periodic sequence $u_m$ fold smoothly across the period boundary at $m = \pm N/2$.

In addition to reducing ringing, the condition (184) means that equation (183) remains true also at $m = \pm N/2$, so is true for all $m$. In this case the inverse Hankel mode $v_n^-(\mu, q)$, equation (183), is equal to the forward Hankel mode $v_n^+(\mu, q)$ with $q$ of the opposite sign

$$v_n^-(\mu, q) = v_n^+(\mu, q) = \frac{1}{N} \sum_m u_m (\mu, -q) e^{-2\pi i mn/N}. \quad (185)$$

In other words, if condition (184) is satisfied, then the inverse discrete Hankel transform equals the forward discrete Hankel transform with $q \rightarrow -q$. This is like the continuous Hankel transform, equations (155), (156), where the inverse transform equals the forward transform with $q \rightarrow -q$.

The periodicity condition (184) on $u_{\pm N/2}$ translates, for real $\mu$ and $q$, into a condition on $k_0 r_0$

$$\ln(k_0 r_0) = \frac{L}{N} \left\{ \frac{1}{\pi} \text{Arg} \left[ U_\mu \left( q + \pi i N/L \right) \right] + \text{integer} \right\} \quad (186)$$

where Arg$z \equiv \text{Im ln } z$ denotes the argument of a complex number, and integer is any integer. In other words, to reduce ringing, it may help to choose $k_0 r_0$ so as to satisfy the condition (186). This is not too much of a restriction, since $L/N$ is the logarithmic spacing between points (± one notch), so the low-ringing condition (186) allows $k_0 r_0$ to be chosen to lie within half a notch [≈ $L/(2N)$] of whatever number one chooses, for example within half a notch of $k_0 r_0 = 1$.

FFTLog can be set to use automatically the low-ringing value of $k_0 r_0$ nearest to any input value of $k_0 r_0$.

How else does the choice of $k_0 r_0$ affect the Hankel transform? Increasing the value of $\ln(k_0 r_0)$ by one notch $L/N$ cyclically shifts the discrete Hankel transform $\tilde{a}_n$, equation (174), by one notch to the left, $\tilde{a}_n \rightarrow \tilde{a}_{n-1}$. In other words, changing $\ln(k_0 r_0)$ by an integral number of notches shifts the origin of the transform, but leaves the transform otherwise unchanged, as might have been expected.

In practice, since in most cases one is probably using the discrete Hankel transform as an approximation to the continuous transform, one would probably want to use $k_0 r_0 \approx 1$ (or 2, or $\pi$, according to taste).

### B.6 Unitary Hankel transform

The discrete Hankel transform with both low-ringing $k_0 r_0$ and no power law bias, $q = 0$, is of particular interest because it is unitary, like the Fourier transform. Indeed, being also real, the low-ringing unbiased Hankel transform is orthogonal, i.e. self-inverse, like the Fourier sine and cosine transforms. This is like the continuous unbiased ($q = 0$) Hankel transform, equations (159), (160), which is self-inverse.

The discrete Hankel modes $v_m(\mu, 0) = v_m^-(\mu, 0) =$
\( v_m(\mu, 0) \) in the low-ringing unbiased \((q = 0)\) case are periodic, orthonormal, and self-similar, equation \((182)\):

\[
\sum_l v_{m+l}(\mu, 0) v_{l+n}(\mu, 0) = \delta_{mn}.
\]

Like any orthogonal transformation, the low-ringing unbiased \((q = 0)\) Hankel transform commutes with the operations of matrix multiplication, inversion, and diagonalization (for non-low-ringing or biased Hankel transforms, \(q \neq 0\), the operations do not commute). That is, the Hankel transform of the product of two matrices is equal to the product of their Hankel transforms, and so on.

All else being equal (which it may not be), given a choice between applying an unbiased \((q = 0)\) or biased \((q \neq 0)\) Hankel transform, and between a low-ringing \(k_0\omega_0\), equation \((186)\), or otherwise, one would be inclined to choose the low-ringing unbiased transform, because of its orthogonality property.

### B.7 Example

Figure 12 shows the correlation function \(\xi(r)\) computed by FFTLog for the nonlinear CDM power spectrum of Eisenstein \& Hu (1998) shown in Figure 10. Two different resolutions are plotted on top of each other, a low resolution case with 96 points over the range \(r = 10^{-3}\) to \(10^3 h^{-1}\)Mpc, and a high resolution case with 768 points over the range \(r = 10^{-6}\) to \(10^6 h^{-1}\)Mpc. Both cases used an unbiased \((q = 0)\) transform and a low-ringing value of \(k_0\omega_0\) (actually the choice of \(k_0\omega_0\) made little difference here).

The low and high resolution correlation functions shown in Figure 12 agree well except near the edges \(r \approx 10^{-3}\) and \(10^3 h^{-1}\)Mpc; in particular, the low resolution correlation function tends to a positive constant \(\approx 10^{-5}\) at \(r \to 10^3 h^{-1}\)Mpc, whereas the high resolution correlation function is negative and declining as a power law \(\propto r^{-4}\) at large \(r\). The disagreement is caused by aliasing (see §B.8) of small and large separations in the low resolution case. Aliasing is almost eliminated in the high resolution case because the range \(r = 10^{-6}\) to \(10^6 h^{-1}\)Mpc over which the transform was computed is much broader than the range plotted.

The bottom panel of Figure 12 shows the ratio \(\xi_{\text{FFT}}/\xi_{\text{FFTLog}}\) of the correlation function \(\xi_{\text{FFT}}\) computed with a normal FFT (sine transform) with 1023 points over the range \(r = 0.125\) to \(128 h^{-1}\)Mpc, to the (high resolution) correlation function \(\xi_{\text{FFTLog}}\) computed with FFTLog. Even with 1023 points, the FFT’d correlation function rings noticeably, with an amplitude of about \(\pm 5\) percent.

In this particular instance, FFTLog outperforms the normal FFT on all counts: it is more accurate, with fewer points, over a larger range, and it shows no signs of ringing. This does not mean that FFTLog is always better than FFT. Rather, FFTLog is well matched to the problem at hand: the cosmological power spectrum extends over many orders of magnitude in wavenumber \(k\), and varies smoothly in \(\ln k\).

### B.8 Ringing and aliasing

FFTLog suffers from the same problems of ringing (response to sudden steps) and aliasing (periodic folding of frequencies) as the normal FFT.

Usually one is interested in the discrete Fourier or Hankel transform not for its own sake, but rather as an approximation to the continuous transform. The usual procedure would be to apply the discrete transform to a finite segment of the function \(a(r)\) to be transformed. For FFTLog, the procedure can be regarded as involving two steps: truncating the function to a finite logarithmic interval, which causes
ringing of the transform; followed by periodic replication of the function in logarithmic space, which causes aliasing.

Figure 13 illustrates these steps for the unbiased \((q = 0)\) Hankel transform, equation (155), of order \(\mu = -1/2\) of a function that is Gaussian in the log

\[
a(r) = \exp[-(\ln r)^2/2].
\]

(188)

Truncation of the function \(a(r)\) leads to ringing of its transform \(\tilde{a}(k)\) at high frequencies \(k\), as seen in the middle right panel of Figure 13. The oscillations at large \(k\) are actually uniformly spaced in \(k\), but appear bunched up because of the logarithmic plotting.

Periodic replication means taking a sum of copies shifted by integral periods. From the definition \((153)\) of the continuous Hankel transform, it can be seen that periodically replicating a function \(a(r)\) in logarithmic space \(\ln r\) and then taking its continuous Hankel transform is equivalent to Hankel transforming the function \(a(r)\) and then periodically replicating the transform \(\tilde{a}(k)\) in \(\ln k\). But truncating a function does not truncate its transform. So whereas a truncated, periodically replicated function \(a(r)\) contains contributions from only one period at each point \(r\), the periodically replicated transform contains overlapping contributions from many periods at each point \(k\). This is aliasing. In Figure 13 aliasing is visible as an enhancement of the periodically replicated transform \(\tilde{a}(k)\) on the high \(k\) side of the periodic interval.

Ringing and aliasing can be reduced by taking suitable precautions.

The ringing that results from taking the discrete transform of a finite segment of a function can be reduced by arranging that the function folds smoothly from large to small scales. It may help to bias the function with a power law before transforming it, as in the second algorithm in §B.4. It may also help to use a low-ringing value of \(k_0 r_0\), §B.5.

Aliasing can be reduced by enlarging the periodic interval. Aliasing can be eliminated (to machine precision) if the interval can be enlarged to the point where the transform \(\tilde{a}(k)\) goes sensibly to zero at the boundaries of the period. Note that it is not sufficient to enlarge the interval to the point where \(a(r)\) is sensibly zero at the period boundaries: what is important is that the transform \(\tilde{a}(k)\) goes to zero at the boundaries.

Figure 13. Illustrating the ringing and aliasing that occurs when the continuous Hankel transform of a function is approximated by the discrete Hankel transform of a finite segment of the function. Lines are dashed where values are negative. The function \(a(r)\) is shown to the left, and its corresponding Hankel transform \(\tilde{a}(k)\) to the right. The panels from top to bottom are: (top) the original function \(a(r)\) and its Hankel transform \(\tilde{a}(k)\); (middle) the truncated function \(a(r)\) and its Hankel transform \(\tilde{a}(k)\), which rings at high frequencies \(k\); and (bottom) the truncated, periodically replicated function \(a(r)\) and its corresponding periodically replicated Hankel transform \(\tilde{a}(k)\), which is aliased. Vertical lines in the bottom panels demarcate periodic intervals.