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Two-point statistics without bins: A continuous-function generalization of the correlation function estimator for large-scale structure

Kate Storey-Fisher[1] and David W. Hogg[1, 2, 3, 4]

[1] *Center for Cosmology and Particle Physics, Department of Physics, New York University*
[2] *Center for Data Science, New York University*
[3] *Max-Planck-Institut für Astronomie, Heidelberg*
[4] *Flatiron Institute, Simons Foundation*

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ABSTRACT

The two-point correlation function (2pcf) is the most important statistic in structure formation, used to measure the clustering of density field tracers (e.g. galaxies). Current estimators of the 2pcf, including the standard Landy-Szalay (LS) estimator, have significant limitations. In this work we address the issue that the LS estimator evaluates the 2pcf in bins of separation between objects, which results in a loss of information and a poor trade-off between bias and variance, given the inappropriateness of hard bin edges in most scientific contexts. Hogg says: The issue is NOT the bias–variance trade-off; that exists everywhere. It is that this trade-off is bad when the model is inappropriate. It is the inappropriateness that we are addressing. I still don't like this wording, but I tried. We present a new estimator for the 2pcf, *the Continuous-Function Estimator*, which generalizes LS to a continuous representation and obviates binning in separation or any other property. Our estimator replaces the binned pair counts of LS with a linear superposition of any set of basis functions, and outputs the best-fit linear combination of basis functions to describe the 2pcf. It is closely related to the information-theory optimal estimator used in linear least-squares fitting. The choice of basis can take into account the expected form of the 2pcf, as well as its dependence on other properties beyond separation. We show that the Continuous-Function Estimator can estimate the clustering of artificial data in representations that provide more accuracy with fewer basis functions than LS. Using a spline basis representation, we show that the Continuous-Function Estimator achieves lower bias and lower variance than LS. We also demonstrate how the estimator can be used to directly estimate the Baryon Acoustic Oscillation scale. Critically, these representations reduce the number of mock catalogs required for covariance estimation, a limiting factor in 2pcf measurements. We discuss other applications and limitations of the Continuous-Function Estimator for present and future studies of large-scale structure, including determining the dependence of clustering on galaxy

properties and potentially unifying real-space and Fourier-space approaches to clustering measurements.

Keywords: cosmology: large-scale structure — galaxies: statistics

1. INTRODUCTION

The large-scale structure (LSS) of the universe is a critical probe of fundamental cosmology. It encodes information about the physics of the early universe and the subsequent expansion history. In particular, the LSS provides a probe of the Baryon Acoustic Oscillations (BAO), density fluctuations resulting from baryon-photon coupling in the early universe. The distance traveled by these waves imprints a feature on the statistical description of the LSS, which can be used to determine the characteristic BAO length scale (Eisenstein & Hu 1997). The LSS also contains the signature of redshift-space distortions caused by the peculiar velocities of galaxies, which probe the growth rate of structure (Kaiser 2014). Additionally, the LSS can be used to constrain galaxy formation in conjunction with models of galaxy bias (e.g. Hamilton 1988). With current observations, the LSS is well-described by a cold dark matter model with a cosmological constant, the standard ΛCDM model. Upcoming galaxy surveys will observe larger volumes with improved measurements, allowing us to test ΛCDM to even higher precision. KSF says: Should I name-drop surveys, and their data volume / sky area? Hogg says: I don't think it is necessary; use your judgement.

We characterize the LSS by using luminous sources to trace the underlying matter density field. These tracers are often to taken to be galaxies, but can also be galaxy clusters, quasars and other sources. KSF says: should i say that hereafter we will take them to be galaxies? Hogg says: Yes. The clustering of these objects is measured with two-point statistics, namely the power spectrum $P(k)$ and the two-point correlation function (2pcf). These characterize the clustering in Fourier space and real space, respectively, with the 2pcf defined as the Fourier Transform of the power spectrum: KSF says: i'm not sure about my notation here with the vectors and d3k

$$\xi(\mathbf{r}) = \frac{1}{(2\pi)^3} \int P(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{k}. \tag{1}$$

If we assume isotropy, we find that the spherically averaged correlation function is

$$\xi(r) = \frac{1}{2\pi^2} \int_0^\infty P(k) \frac{\sin(kr)}{kr} k^2 dk. \tag{2}$$

In principle, the power spectrum and the two-point correlation function contain the same information. However, in practical applications the survey boundaries introduce nontrivial issues in computing these statistics, leading to diverging approaches to their computation with a significant difference in expense. The 2pcf requires more computational power and extra survey products, but it is an incredibly useful tool;

for instance, it well-suited to the analysis of the BAO feature which manifests at a single scale in real space.

The 2pcf measures the excess probability that any two galaxies are separated by a given distance, compared to a uniform distribution; effectively, it characterizes the strength of clustering at a given spatial scale. In calculating the 2pcf, the boundaries of the surveys prevent us from directly summing pair counts due to nontrivial edge effects. To account for the survey boundaries as well as corrupted regions due to issues such as bright foreground stars, a set of random points are Poisson-distributed within the acceptable survey window. The pairwise correlations of these unclustered points are used to normalize out the survey window when estimating the 2pcf of the clustered data. Typically, this requires random points on the order of 10-100 times the number of data points, making the random correlations the limiting factor in 2pcf computation.

The 2pcf is computed in bins of radial separation, meaning that in practice it measures the volume average of the 2pcf over the bin. This binning introduces inherent limitations. First, the choice of bins requires a trade-off between bias and variance: fewer bins may bias the result, while more bins increases the variance of measurement. Finite-width bins also result in a loss of information about the property in which one is binning. As we strive for extreme precision in large-scale structure analyses, we should be maximizing the information we extract from the data.

More generally, binning adds arbitrary boundaries between continuous data; results should not depend on bin choice, yet they sometimes do. Lanzuisi et al. (2017) noted that the choice of binning axis impacts the detected correlation between the luminosity of active galactic nuclei and their host galaxies; Grimmett et al. (2020) devised a method to investigate this correlation in a continuous manner using a hierarchical Bayesian model, eliminating the need for binning. Bailoni et al. (2016) explored the dependence of clustering analyses on the number of redshift bins, finding a non-negligible difference in cosmological parameter uncertainties. The implications for BAO analyses were explored by (Percival et al. 2014), who found that there is an optimal bin width given the analysis method. This balances the increasing statistical error with small bins and the offset in the derived BAO peak location with large bins; the effects are small but non-negligible.

Estimators of the 2pcf have been studied extensively (Peebles & Hauser 1974; Davis & Peebles 1983; Hamilton 1993). The current standard estimator was proposed by Landy & Szalay (1993), hereafter LS. It is based on summing all data pairs DD with a given separation and using data-random pairs DR and random pairs RR to correct for the survey boundary. The correlation function $\xi_k(r)$ for the k^{th} separation bin is

$$\xi_k(r) = \frac{DD_k(r) - 2DR_k(r) + RR_k(r)}{RR_k(r)}, \tag{3}$$

where we assume the pair counts are normalized. Compared with other estimators based on simple combinations of DD, DR and RR, LS has been shown to have the

lowest bias and variance (Kerscher et al. 2000). Estimators of the 2pcf must also take into account the imperfect nature of the survey area that is in the window, including the target completeness and fiber collisions; typically each galaxy pair is assigned a weight based on these. Then, pair counts are replaced by the sum of pair weights.

Variations on the random catalog pair count method have been proposed in recent years. Demina et al. (2016) replaced the DR and RR terms with an integral over the probability map, reducing computation time and increasing precision. An estimator proposed by Vargas-Magaña et al. (2013) iterates over sets of mock catalogs to find an optimal linear combination of data and random pair counts, reducing the bias and variance. The marked correlation function (White & Padmanabhan 2009) sums weights based on properties of the galaxies one is interested in, such as the local density or galaxy luminosity, and avoids the use of a random catalog. The estimators described so far have all taken probabilistic approaches; others have taken a likelihood approach. Baxter & Rozo (2013) introduced a maximum likelihood estimator for the 2pcf, which achieves lower variance compared to the LS estimator, enabling finer binning and requiring a smaller random catalog for the same precision.

These estimators present improvements to LS, but they are still limited to estimates in separation bins. Some require additional computational costs or layers of complexity, so the standard formulation of LS continues to be the default estimator used in most analyses.

In this paper, we present a new estimator for the correlation function, the Continuous-Function Estimator, which generalizes the LS estimator to produce a continuous estimation of the 2pcf. The Continuous-Function Estimator projects the galaxy pairs onto a set of continuous basis functions and computes the best-fit linear combination of these functions. The basis representation can depend on the pair separation as well as other desired properties, and can also utilize the known form of the 2pcf. For top-hat basis functions, the Continuous-Function Estimator exactly reduces to the LS estimator. This estimator removes the need for binning and allows for the 2pcf to be represented by fewer basis functions, requiring fewer mock catalogs to compute the covariance matrix. It is particularly well-suited to the analysis of LSS features such as the BAO peak; we find that we can accurately locate the peak with fewer components.

This paper is organized as follows. In §2, we motivate our estimator and explain its formulation. We demonstrate its application on a simulated data set, including a toy BAO analysis, in §3. We discuss the implications and other possible applications in §4.

2. MOTIVATION AND FORMULATION

2.1. *Standard Clustering Estimation*

We assume we have a data catalog with N_D objects and a random catalog with N_R objects. The pair counts for LS and related estimators are then defined explicitly as

$$DD_k \equiv \frac{2}{N_D(N_D-1)} \sum_{nn'} i(g_k < |x_n - x_{n'}| < h_k) \tag{4}$$

$$DR_k \equiv \frac{1}{N_D N_R} \sum_{nm} i(g_k < |x_n - x_m| < h_k) \tag{5}$$

$$RR_k \equiv \frac{2}{N_R(N_R-1)} \sum_{mm'} i(g_k < |x_m - x_{m'}| < h_k), \tag{6}$$

where DD_k is the count of data–data tracer pairs in bin k (which has bin edges g_k and h_k), $i()$ is an indicator function KSF says: define? Hogg says: yes, x is the tracer position, the n and n' indices index data positions, the m and m' indices index random catalog positions, DR_k is the count of data–random pairs, and RR_k is the count of random–random pairs. KSF says: decide on these normalization terms - generalize to D1 D2? simpler, but then need RD term

The LS estimator has been analyzed extensively; it is shown to have the lowest bias and variance compared to other pair-count-based estimators (e.g. Kerscher et al. 2000). In the limit of unclustered data, for a data volume much larger than the scales of interest, and an infinitely large random catalog, the LS estimator is known to be optimal: it is unbiased and has minimum variance. In practice the latter two limits are sufficiently satisfied, but the data we are interested in is clustered. LS does show a bias on very large scales (>130 h^{-1}Mpc), but the bias is significantly smaller than that of most other estimators (Kerscher 1999, Vargas-Magaña et al. 2013). LS is also less sensitive to the number of random points than other estimators (Kerscher et al. 2000). Vargas-Magaña et al. (2013) show that for clustered data, the LS estimator has lower variance than other estimators, but does not reach the Poisson noise limit.

KSF says: Figure demonstrating trade-off between bias and variance? or too simple Hogg says: Only if the point isn't clear without it.

KSF says: Should i explain / show some of the other estimators? –¿ now i do in the beyond LS section Hogg says: No; our job is not to work through all estimators. But we SHOULD note that our mod can be applied to almost any estimator that currently uses bins!

KSF says: Do i need to explain real space vs redshift space vs projected correlation function? Hogg says: No, but always be absolutely unambiguous about what space you are in. To the point that you might even want to use different symbols.

2.2. *Least Squares Fitting*

Estimating clustering is closely related to least-squares fitting. We are trying to find the best representation of spatial data in the space of two-point radial separation. Recall that the linear least-squares fit to a set of data

$$X = [A^{\mathsf{T}} C^{-1} A]^{-1} [A^{\mathsf{T}} C^{-1} Y] \tag{7}$$

where X is the vector of best-fit parameters, A is a matrix with zeroth and first order terms of x data, C is the covariance matrix, and Y is a column vector of y data. The second bracketed term contains the observed data; the first bracketed term weights the data by the errors. Naively, in the case of the 2pcf, the observed data is the pair counts at a given separation, and the weights are provided by the pair counts of the random catalog. Indeed, this is reminiscent of the so-called natural estimator of the 2pcf, $\xi_k = DD_k/RR_k - 1$ (e.g. Kerscher et al. 2000).

From this connection, we can infer the form of the estimator. KSF says: expand this section

2.3. *The Continuous-Function Estimator*

We generalize the LS estimator defined above to any set of K basis functions f of the pair, so we now have

$$DD \equiv \frac{2}{N_D(N_D-1)} \sum_{nn'} f(T_n, T_{n'}) \tag{8}$$

$$DR \equiv \frac{1}{N_D N_R} \sum_{nm} f(T_n, T_m) \tag{9}$$

$$RR \equiv \frac{2}{N_R(N_R-1)} \sum_{mm'} f(T_m, T_{m'}) \tag{10}$$

$$QQ \equiv \frac{2}{N_R(N_R-1)} \sum_{mm'} f(T_m, T_{m'}) \cdot f^{\mathsf{T}}(T_m, T_{m'}), \tag{11}$$

where DD, DR, and RR are now K-vectors, T refers to the data for the given tracer, and QQ is a K-by-K matrix defined as the outer product of basis function evaluations of the random–random pairs.

Then, we can compute the 2pcf as

$$a \equiv QQ^{-1} \cdot (DD + 2DR - RR) \tag{12}$$

$$\xi(T_l, T_{l'}) \equiv a^{\mathsf{T}} \cdot f(T_l, T_{l'}) \tag{13}$$

where T_l and $T_{l'}$ contain the data values at which to evaluate ξ, and a is a K-vector of the "amplitudes" of the basis functions. This generalized two-point estimator, or the Continuous-Function Estimator, removes the need for binning as the basis functions can be continuous. It is invariant under affine transformations; we show this in Appendix A.

In the case where the basis functions only depend on the pair separation, we have $f = f(|x_n - x_{n'}|)$ and $\xi = \xi(r)$, where r is the separation at which to evaluate the correlation function. Specifically, we can choose to define a set of basis functions f^T as,

$$f_k^T(|x_n - x'_n|) = i(g_k < |x_n - x_{n'}| < h_k) \tag{14}$$

where k denotes a particular bin in separation. In this case the DD, DR and RR vectors become binned pair counts and the QQ matrix becomes diagonal, with diagonal

elements equal to the RR vector elements. Then for this set of functions f^T, which is the definition of a top-hat (rectangular) function, the estimator is equivalent to that of Landy-Szalay.

KSF says: Worth giving analytic formulation of RR term? Or at least mentioning that there is one and we have derived it? Hogg says: Huh? We have one?

KSF says: Discuss the limit of infinitesimal bins? Do we know what this is? Hogg says: Yes, we should discuss this, and show how we are related to that.

We implement this estimator based on the correlation function package `Corrfunc` by Sinha & Garrison (2019). The code is open-source and available at `github.com/kstoreyf/Corrfunc`. KSF says: Should give any detail about implementation? Hogg says: Yes, we should summarize why this is a good package to build on.

KSF says: where to put this link? In a footnote? And is it ok to keep it as a fork? Hogg says: Put link here and in a note at the end of the acks at the end which says "all of the code is available open-source at...

3. APPLICATIONS

KSF says: Does this count as Applications if its on fake data? Better name? Hogg says: I say "Experiments and results" these days.

KSF says: Clearly describe real-space vs redshift-space! where tho? We demonstrate the application of the Continuous-Function Estimator on artifical data. We generate lognormal mock catalogs (Coles & Jones 1991) using the `nbodykit` package (Hand et al. 2018). We use an input power spectrum with the Planck cosmology KSF says: CITE. The true correlation function is then known: it is the Fourier transform of the input power spectrum, computed numerically. Our test catalogs have size $(750\ h^{-1}\mathrm{Mpc})^3$ and a galaxy number density of 3×10^{-4}, to match that of the Brightest Cluster Galaxies KSF says: CITE. We construct 100 realizations of this box. We also generate a uniformly sampled random catalog with 10 times the number of galaxies as in the data catalogs.

3.1. *Demonstration using Spline Basis Functions*

KSF says: Should i have a figure showing the basis functions? Hogg says: yes

A natural extension of tophat basis functions is the B-spline. B-splines of order n are piecewise polynomials of order $n-1$; they constitute the basis functions for spline interpolation KSF says: CITE. They have the nice property that the functions and their derivatives can be continuous, depending on the order. Further, B-splines are well-localized, which provides a more direct comparison to the typical tophat basis (which is entirely localized). For this demonstration we use fourth-order B-splines, which constitute the set of basis functions for a cubic spline, as they are the lowest-order spline to have a continuous first derivative. We compare this standard estimator, reformulated as continuous functions using a tophat basis. For the tophat basis we use 44 basis functions in the range $40 < r < 150\ h^{-1}\mathrm{Mpc}$, each with a width of 2.5

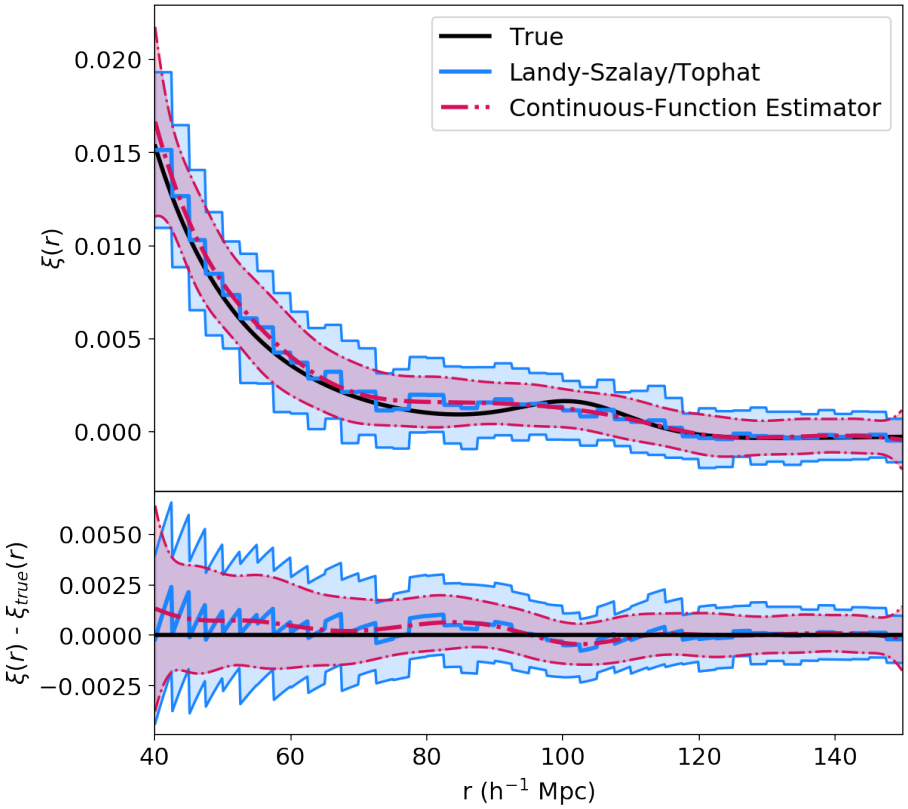

Figure 1. A comparison between the Continuous-Function Estimator with a cubic spline basis function (red dotted) and the standard tophat estimator (blue solid). The shaded region is the 1σ variation in the 100 mock catalogs. The cubic spline estimator has lower bias and lower variance with fewer bins. KSF says: quote rmse in caption? otherwise not clear from figure its less biased. Hogg says: yes KSF says: does tophat need to be a different linestyle?

KSF says: fix to dotted linestyle

h^{-1}Mpc. For the cubic spline basis, we use the same r range, but with only 11 basis functions, and knots chosen on a grid of 10 h^{-1}Mpc. KSF says: need to specify more about knots? is this accurate (not quite, the knots repeat values at the edge i think...) and should i mention control points?

The results are shown in Figure 3.1, compared to the true input 2pcf. The spline basis results in a 2pcf estimate that has a root mean square error (RMSE) with respect to the truth of 4.38×10^{-4}, compared to 5.31×10^{-4} for the tophat basis. This holds true when we average over the bin KSF says: need to do weighted average based on which r-values contribute? supposed to hear from tinker, as in standard practice, and then compute the RMSE. The spline basis also results in lower variance across the 100 mocks, compared to the tophat basis. Thus, the Continuous-Function Estimator allows for a more accurate and precise estimate of the 2pcf with fewer components.

We note that this is fundamentally different than a kernel-based estimator. In a kernel formulation, each data point is smoothed by a particular kernel, smoothing out features in the resulting function. With our estimator, the basis functions are

fixed and the data is projected onto them. This preserves the information in the data to the degree given by the chosen set of basis functions, which can in fact enhance features rather than smooth them. KSF says: please add/correct here

3.2. *BAO Scale Estimation Test*

Measurement of the BAO scale provides a good use case for our estimator. The BAO feature is a peak in clustering on large scales, ∼150 Mpc, making it less sensitive to small-scale astrophysical effects. It is one of the best tools for constraining cosmological models, in particular the distance-redshift relation (Kazin et al. 2010; Anderson et al. 2011, 2014; Alam et al. 2016).

KSF says: what else do I need to cite for BAO?

We base our BAO estimation on the method of the BOSS DR10 and 11 analysis (Anderson et al. 2014). We measure the spherically averaged correlation function, $\xi(s)$, where s is the separation between pairs. In order to extract information about the baryon acoustic feature from galaxy clustering, we must choose a fiducial cosmological model to convert redshifts to distances. If we choose an incorrect model, the scales in the power spectrum will be dilated, so the oscillation wavelength—and thus the BAO peak position—will be shifted. We can model this shift as a scale dilation parameter, α, which is a function of the relevant distance scales in the true and fiducial cosmologies:

$$\alpha = \left(\frac{D_A(z)}{D_A^{\rm mod}(z)}\right)^{2/3}\left(\frac{H^{\rm mod}(z)}{H(z)}\right)^{1/3}\left(\frac{r_s^{\rm mod}}{r_s}\right), \tag{15}$$

where D_A is the angular diameter distance, H is the Hubble constant, r_s is the sound horizon scale at the drag epoch, and the superscript "mod" denotes the value for the fiducial model. Qualitatively, if the fit prefers $\alpha > 1$, this suggests the true position of the BAO peak is at a smaller scale than in the fiducial model, whereas if $\alpha < 1$, the peak is at a larger scale.

In standard practice, the fitting function used to determine the value of α is

$$\xi^{\rm fit}(s) = B^2\xi^{\rm mod}(\alpha s) + \frac{a_1}{s^2} + \frac{a_2}{s} + a_3 \tag{16}$$

where B is a constant that allows for a large-scale bias, and a_1, a_2, and a_3 are nuisance parameters to account for the broadband shape. A χ^2 fit is performed with five free parameters: α, B, a_1, a_2, and a_3. The resulting value for α is used to derive the actual values of the distance scales of interest. Typically, density-field reconstruction is performed before applying the estimator to correct for nonlinear growth around the BAO scale (Eisenstein et al. 2007); for our toy example, we will omit this step.

The form of the standard fitting function is well-suited to our estimator, as it is a few-parameter model with a linear combination of terms. To use our estimator to estimate α, we take the numerical partial derivative of the model with respect to α, using a change in α of size $d\alpha$. Our fitting function is then

$$\xi^{fit}(s) = B^2\xi^{mod}(s) + Cd\alpha\frac{d\xi_{mod}(\alpha s)}{d\alpha} + \frac{a_1}{s^2} + \frac{a_2}{s} + a_3, \tag{17}$$

where C describes the contribution of α. We input these five terms (with arbitrary scaling) as the basis functions of our estimator. The estimator outputs an amplitude vector a as described in §2.3, which give the contribution of each term—precisely the values of B, C, a_1, a_2, and a_3. From the value of C, we can directly compute α, as $\alpha_{\rm recovered} = \alpha + Cd\alpha$ (where α is our initial guess, typically starting with α=1). That is, a value of $C = 0$ indicates that the model is the best fit to the data and no scale dilation is needed, while nonzero values give the magnitude and direction of the scale dilation parameter.

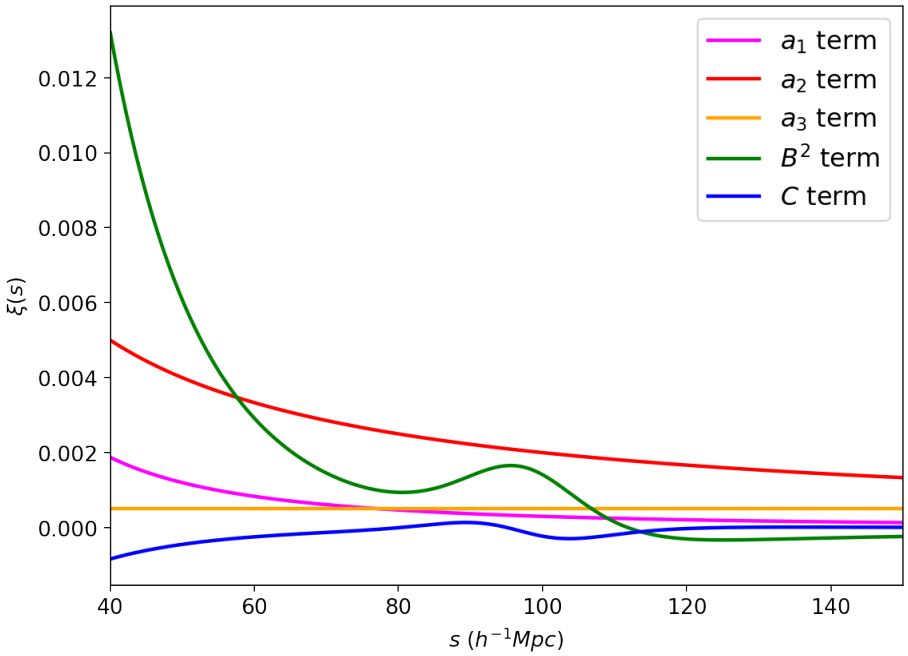

Figure 2. The set of basis functions used to fit for the BAO scale using our estimator. The B^2 term (green) is the fiducial model used to determine the scale dilation parameter α. The C term is the derivative of this model with respect to α, allowing for the estimation of this parameter. The a_1, a_2, and a_3 terms are nuisance parameters to fit the broadband shape. KSF says: Make colorblind friendly! and diff linewidths maybe

We demonstrate this method using the same set of lognormal mocks as in §3.1. We construct a recovery test following that in **?**. We assume the fiducial cosmological model used in **?**: $\Omega_{\rm m} = 0.31$, $h = 0.676$, $\Omega_{\rm b} = 0.04814$, $n_s = 0.97$. As we know the cosmology used for our mock catalogs, we can compute the true value of the scale dilation parameter, $\alpha_{\rm true} = 0.9574$ (a fairly extreme value but useful for testing purposes). With this fiducial model, we can construct the basis functions for our estimator; these are shown (with $\alpha = 1$ and the free parameters set to arbitrary values) in Figure 3.2.

We perform an iterative procedure to estimate α. After the first estimation with the $\alpha = 1$, model, we use the value of C to compute the recovered α, as described above. We then take that value as the new α, and re-run the estimator. (In practice, this often jumps over the true value, so we tune the choice of the next α with a

parameter η, as $\alpha_{\rm recovered} = \alpha + \eta C d\alpha$, where η is typically 0.1-0.5.) We stop when the percent change between α and $\alpha_{\rm recovered}$ is less than 0.1%; it typically takes fewer than 10 iterations to converge. KSF says: update this with true values We apply this procedure to each of the 100 mocks; the resulting estimate for the correlation function is shown in Figure 2. The mean BAO estimate is shown in orange, and the mean tophat estimate is in blue; the truth is in black. Our estimator clearly better represents the shape of the known 2pcf. The mean value of the final recovered scale dilation parameter is $\alpha = 0.9572 \pm 0.0315$, very close to the true value $\alpha_{\rm true} = 0.9574$.

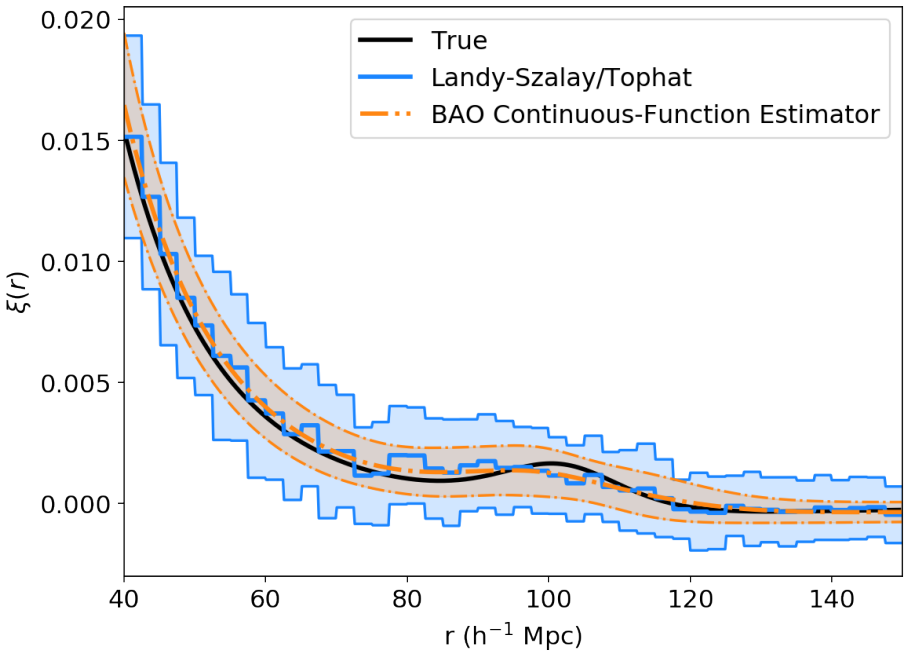

Figure 3. Estimation of the correlation function using our estimator with basis functions based on the BAO fitting function (orange dot-dashed). The line is the mean of the final estimate from the iteration procedure for 100 mocks, and the shaded region is the 1σ variation. We also show the standard Landy-Szalay estimator, displayed as a tophat function (blue), as well as the true input correlation function (black). KSF says: This is for the 1e-4 box, need to run bigger box. KSF says: Should this and the basis set figure be a single figure with two panels? KSF says: Should i have a figure showing the sum of the basis functions and how that gets you the final cf?

We note that these basis functions are significantly different than the tophat or B-spline bases previously explored, mainly because they are not localized. This means that data at all scales could contribute to all basis functions. It is then critical to ensure that the final parameter estimate does not rely on the range of scales chosen. We have confirmed that in this application, the result is robust to the chosen range as long as the scales cover the range $40 < r < 200\ h^{-1}$Mpc, the typical range used in BAO analyses. KSF says: Actually have to check this and update numbers!

4. DISCUSSION

4.1. *Beyond the Landy-Szalay Estimator*

While we have formulated our estimator as a generalization of LS, as it is the standard used in 2pcf analyses and has optimal properties under certain conditions, we can also reformulate it for other estimators. The formulation currently requires a normalization term (i.e. denominator) of the RR counts, as we replace this with our QQ term. This is the case for the Peebles & Hauser (1974) estimator and the Hewett (1982) estimator:

$$\xi_{PH}(r) = \frac{DD - RR}{RR} \tag{18}$$

$$\xi_{Hew}(r) = \frac{DD - DR}{RR}. \tag{19}$$

KSF says: dropped k and (r) notation here, do i need? We could also generalize estimators which have a DR term as the denominator, such as the Davis & Peebles (1983) estimator,

$$\xi_{DP}(r) = \frac{DD - DR}{DR} \tag{20}$$

by defining

$$DQ = \frac{2}{N_D N_R} \sum_{nm} f(T_n, T_m) \cdot f^{\mathsf{T}}(T_n, T_m). \tag{21}$$

This could be extended to almost any linear combination of pair counts. The estimator of Vargas-Magaña et al. (2013) selects the optimal combination of pair counts; our estimators could be combined to create an even more generalized estimator. KSF says: some of the terms in V-M include DD in the denom - need to mention this?

KSF says: Mention other work with Barnett about LS estimator?

4.2. *Computational Performance*

The computational scaling is by definition the same compared to traditional estimators due to the limiting factor of pair-finding. The Continuous-Function Estimator has the additional need for evaluating the function f for each pair of galaxies. For simple basis functions like splines, this will only marginally decrease performance. For more complicated functions such as evaluating a cosmological model, the Continuous-Function Estimator may incur extra computational expense. Basis functions can also be input on a grid and then interpolated; the performance is then the same for all functions, but the interpolation for each function for each pair does somewhat decrease the performance.

KSF says: Is there a need to say much more? If not, maybe doesn't deserve its own section - could this go in the implementation section? Or maybe tacked onto another small section if we have one that makes sense

4.3. *Effect on Covariance Matrix Estimation*

We have shown that the Continuous-Function Estimator results in 2pcf estimates that are just as accurate with fewer components. This is critical when estimating the covariance matrix, which is necessary for parameter inference. The covariance matrix is difficult to compute theoretically;instead, it is usually estimated by evaluating the 2pcf on a large number of mock catalogs and computing the covariance between the bins (e.g. Reid et al. 2010; Anderson et al. 2014). The unbiased estimator for the sample covariance matrix is (e.g. Anderson 2003)

$$\hat{C}_{ij}^{ML} = \frac{1}{N_{mocks}-1}\sum_{k=1}^{N_{mocks}}\Big(x_i^k - \bar{x}_i\Big)\Big(x_j^k - \bar{x}_j\Big), \tag{22}$$

where k denotes the index of the mock, i and j denote the index of the bin or component, x denotes the estimate in that bin for that mock, and $\bar{x}$ denotes the mean value of the estimate in that bin across the mocks. To get an unbiased estimate of the inverse covariance matrix, we require a correction factor, as the inverse of an unbiased estimator is not necessarily unbiased. The unbiased estimator for the sample inverse covariance matrix can be shown to be (Hartlap et al. 2007)

$$\hat{C}^{-1} = \frac{N_{mocks}-N_{bins}-2}{N_{mocks}-1}\Big(\hat{C}^{ML}\Big)^{-1}. \tag{23}$$

The variance in the elements of this estimator then have a dependence on N_{mocks} and N_{bins}. This propagates to the derived cosmological parameters, resulting in an overestimation of the error bars (Hartlap et al. 2007; Dodelson & Schneider 2013 Percival et al. 2014; Taylor & Joachimi 2014). Assuming that $N_{mocks} >> N_{bins}$ (and both much larger than the number of parameters to be estimated), and that the measurements are Gaussian distribued, the error bars are inflated by a factor of $(1 + N_{bins}/N_{mocks})$ (i.e., the true constraints are tighter than the derived ones). This factor becomes critical at the precision of cosmological parameter estimation (Percival et al. 2014).

Typically, this is dealt with by generating a very large number of mocks. For the Baryon Oscillation Spectroscopic Survey (BOSS, Dawson et al. 2013), ∼600 mocks were needed and the analysis used 41 bins (Sánchez et al. 2012). Future surveys will have more costly requirements on mock catalogs, with larger simulations necessary to cover the larger survey volumes.

An alternative to increasing N_{mocks} is decreasing N_{bins} to achieve the same error on precision. In the standard method, this is shown to *increase* the statistical error, albeit only slightly Percival et al. (2014). A substantial increase in bin width would prevent capturing information in finer clustering features; even the relatively broad BAO peak requires a bin size on the order of its width of $\sim 10h^{-1}$Mpc. In fact, in the standard method more bins would be desireable, but the number is limited by the available number of mocks due to the error discussed above.

With our estimator, we have shown that we can reduce the variance by using fewer components, without sacrificing accuracy. This means that we can safely reduce N_{bins},

or in our replacement of bins with continuous functions, the number of basis functions K. The covariance matrix will be the covariance between these basis functions. KSF says: worth noting that the structure of this covmat will be significantly different, esp if non-orthogonal? To then achieve the same precision on the error on the cosmological parameters, a lower value of N_{mocks} becomes possible. This will significantly reduce requirements on mocks, which will be particularly important for upcoming large surveys.

KSF says: I think the result of discussions was that there wasn't a good way of showing this without propagating all the way to cosmological parameters. Would love a figure showing lower covariance errors but not sure how without full propagation

4.4. *Further Applications*

The formulation of the Continuous-Function Estimator opens up many possibilities for extracting information from the correlation function. The most straightforward applications are standard basis functions or linearizeable astrophysical models, as we have shown here. Other applications for the direct estimation of cosmological parameters could include the growth rate of cosmic structure f (Satpathy et al. 2016; Reid et al. 2018) and primordial non-Gaussianity in the local density field f_{NL}^{local} (Karagiannis et al. 2014). KSF says: mention idea of doing full cosmo model analysis by taking derivs wrt cosmological params? cool but less connected to citeable papers perhaps

We can take our estimator a step further by choosing basis functions that depend not only on the separation between tracer pairs, but also on the properties of the tracers themselves. One such application is the redshift dependence of the Alcock-Paczynski effect Alcock & Paczynski (1979), which can be used to constrain the matter density Ω_m and the dark energy equation of state parameter w (Li et al. 2016). The basis functions f in this case would take the form

$$f_k(T_n, T_m) = f_k(r_{nm}, z_n, z_m), \tag{24}$$

where z is the redshift of tracer n or m. Another potential use case is the luminosity and color dependence of galaxy clustering, which can be used to probe galaxy formation (Zehavi et al. 2011). This could be extended to other galaxy properties.

The estimator gives us the opportunity to investigate more subtle or exotic signals which are anomalous with respect to our conventional models. Anomalies could appear as inhomogeneities or anisotropies in the data. For example, cosmological parameters could vary across the sky, which has previously investigated in patches across the Cosmic Microwave Background (Mukherjee & Wandelt 2018). Another possibility is anisotropy in the cosmic acceleration, which could appear in various probes including the BAO peak (Faltenbacher et al. 2012) and Type Ia supernovae (Colin et al. 2019). With our estimator, we could introduce a dependence on location or direction into our basis functions, and constrain the potential deviation from homogeneity or isotropy. While these effects would be highly degenerate with systematics, our estimator com-

bined with robust systematics mitigation allows us to investigate the possibility of new physics.

Finally, our estimator can be directly related to a power spectrum analysis. We could use a Fourier basis as our set of continuous functions. This would allow us to directly project the data onto Fourier modes. This represents a step towards unifying the correlation function and the power spectrum. KSF says: there's more to say here but I'm not sure what

5. SUMMARY

We did cool science!

KSF says: Do we want a summary? Think it might be useful for this particular paper, but def repetitive

It is a pleasure to thank...

APPENDIX

A. AFFINE INVARIANCE

The estimator is invariant under an affine transformation. We represent this by a matrix M, such that

$$f' \leftarrow Mf \tag{A1}$$

Then in the primed basis, the pair counts become

$$DD' = \sum_{nn'} M f_{nn'} = M\,DD \tag{A2}$$

$$DR' = \sum_{nm} M f_{nm} = M\,DR \tag{A3}$$

$$RR' = \sum_{mm'} M f_{mm'} = M\,RR \tag{A4}$$

where $f_{nn'} = f_k(T_n, T_{n'})$. We have factored M out of the summation. For the QQ matrix we have

$$QQ' = \sum_{mm'} (M f_{mm'}) \cdot (M f_{mm'})^{\mathsf{T}} \tag{A5}$$

$$= M \left[\sum_{mm'} f_{mm'} \cdot f_{mm'}^{\mathsf{T}} \right] M^{\mathsf{T}} \tag{A6}$$

$$= MQQM^{\mathsf{T}} \tag{A7}$$

Then the amplitudes in the primed basis become

$$a' = [MQQM^{\mathsf{T}}]^{-1} \cdot [MDD - 2\,MDR + MRR] \tag{A8}$$

$$= (M^{\mathsf{T}})^{-1} QQ^{-1} \cdot [DD - 2\,DR + RR] \tag{A9}$$

$$= (M^{\mathsf{T}})^{-1} a \tag{A10}$$

and the estimator in the primed basis is

$$\xi' = [(M^{\mathsf{T}})^{-1}a]^{\mathsf{T}} \cdot (Mf) \tag{A11}$$
$$= a^{\mathsf{T}}[(M^{-1})^{\mathsf{T}}]^{\mathsf{T}} \cdot (Mf) \tag{A12}$$
$$= a^{\mathsf{T}}M^{-1} \cdot Mf \tag{A13}$$
$$= a^{\mathsf{T}} \cdot f = \xi. \tag{A14}$$

Thus after an affine transformation of the basis function, the resulting estimator is equivalent to the estimator in the original basis.

We note that this requires M be invertible. However, any two equivalent bases must be related by the inverse of a transformation matrix, so this requirement is already satisfied.

B. COMPUTING RR AND QQ ANALYTICALLY

The autocorrelation of the random catalog is meant to approximate the window function. When we have a periodic cube, we can compute this RR term analytically. Here we derive this, and then derive the equivalent for our continuous-basis RR and QQ terms.

We consider an annulus around a single galaxy. This annulus has a volume V_{ann}. Taking the box to have average number density $\bar{n}$, the number of galaxies expected in the annulus is $N_{ann} = A\bar{n}$, and thus this galaxy is part of N_{ann} pairs. We do this for each of the $N_D - 1$ other galaxies, and find a total of $(N_D - 1)N_{annulus} = \frac{1}{2}(N_D - 1)V_{ann}\bar{n}$ pairs, where the factor of $\frac{1}{2}$ accounts for the fact that this double-counts pairs. For a cube, $\bar{n} = \frac{N_D}{L^3}$, so we finally count $\frac{1}{2}\frac{N_D}{L^3}(N-1)V_{ann}$ pairs.

For hard-edged radial bins, we can compute A simply as the difference between spherical volumes. We can also represent this as an integral:

$$V_{ann} = \int_{b_1}^{b_2} dV = 4\pi \int_{b_1}^{b_2} r^2 dr \tag{B15}$$

We can generalize this to any basis function $f(r)$ that is a function of r:

$$V_{ann} = 4\pi \int_{b_1}^{b_2} f^2(r) r^2 dr \tag{B16}$$

which we can see reduces to Equation B15 when $f(r)$ is the tophat function (returning 1 or 0 depending on whether r is between b_1 and b_2).

This gives us our full generalized analytic RR term, which has elements

$$RR_{i,\mathrm{ana}} = \frac{1}{2}\frac{N_D}{L^3}(N_D - 1)4\pi \int_0^{r_{\max}} f_i(r) r^2 dr \tag{B17}$$

where i is the index of the basis function vector. Based on the definition of QQ in Equation 11 as the outer product of the basis function vector and its transpose, we can see that the elements analytic QQ term are:

$$QQ_{ij,\mathrm{ana}} = \frac{1}{2}\frac{N_D}{L^3}(N_D - 1)4\pi \int_0^{r_{\max}} f_i(r) f_j(r) r^2 dr \tag{B18}$$

This could be further generalized to account for basis functions that take other properties as input.

When considering a periodic box, the naive estimator is no longer biased, so we can also avoid computing the DR term and calculate the amplitudes as

$$a_{\rm ana} = QQ_{\rm ana}^{-1} \cdot DD. \tag{B19}$$

Looking back, it might have seemed strange that we use N_D in calculating the analytical RR term, but we now see that this normalization prefactor cancels out with that of the DD term. Finally, we can compute the correlation function as before in Equation 13.

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