Bayesian inference of cosmic density fields from non-linear, scale-dependent, and stochastic biased tracers

Metin Ata,* Francisco-Shu Kitaura† and Volker Müller

Leibniz Institut für Astrophysik, 14482 Potsdam, Germany

ABSTRACT

We present a Bayesian reconstruction algorithm to generate unbiased samples of the underlying dark matter field from halo catalogues. Our new contribution consists of implementing a non-Poisson likelihood including a deterministic non-linear and scale-dependent bias. In particular we present the Hamiltonian equations of motions for the negative binomial (NB) probability distribution function. This permits us to efficiently sample the posterior distribution function of density fields given a sample of galaxies using the Hamiltonian Monte Carlo technique implemented in the ARGO code. We have tested our algorithm with the Bolshoi N-body simulation at redshift \( z = 0 \), inferring the underlying dark matter density field from subsamples of the halo catalogue with biases smaller and larger than one. Our method shows that we can draw closely unbiased samples (compatible within 1-σ) from the posterior distribution up to scales of about \( k \sim 1 \ h \text{Mpc}^{-1} \) in terms of power-spectra and cell-to-cell correlations. We find that a Poisson likelihood including a scale-dependent non-linear deterministic bias can yield reconstructions with power spectra deviating more than 10 per cent at \( k = 0.2 \ h \text{Mpc}^{-1} \). Our reconstruction algorithm is especially suited for emission line galaxy data for which a complex non-linear stochastic biasing treatment beyond Poissonity becomes indispensable.

Key words: catalogues – galaxies: statistics – cosmology: theory – large-scale structure of Universe.

1 INTRODUCTION

The large-scale structure encodes the key information to understand structure formation and the expansion of the Universe. However, the luminous objects, i.e. the galaxies tracing the large-scale structure, represent only a biased fraction of the total underlying matter governing the laws of gravity.

In the era of precision cosmology, the data analysis methods need to account for the non-linear, biased and discrete nature of the distribution of galaxies to accurately extract any valuable cosmological information. This becomes even more important with the advent of the new generation of galaxy surveys. Many of these surveys rely on emission line galaxies, see WiggleZ† (Drinkwater et al. 2010), VIPERS2 (Guzzo & The Vipers Team 2013), DESI3 (Schlegel et al. 2011), DES4 (Frieman & Dark Energy Survey Collaboration 2013), LSST5 (LSST Dark Energy Science Collaboration 2012), J-PAS6 (Benitez et al. 2014), 4MOST7 (de Jong et al. 2012) or Euclid8 (Cimatti et al. 2009; Laureijs 2009). These objects provide denser sampled volumes, deeply tracing the non-linear cosmic web structure. Moreover, they introduce a more complex biasing, covering a wider range of galaxy masses, as compared to, e.g., luminous red galaxies.

We present in this work a Bayesian approach designed to deal with non-linear stochastic biased tracers. We consider non-Poisson probability distribution functions (PDFs) for the likelihood modelling the distribution of galaxies. In this way we account for the over-dispersion (larger dispersion than Poisson) of galaxy counts. We model the expected galaxy number density relating it to the dark matter density through a non-linear scale-dependent expression extracted from N-body simulations (see Cen & Ostriker 1993; de la Torre & Peacock 2013; Ahn et al. 2014; Kitaura, Yepes & Prada 2014b; Neyrinck et al. 2014). In this way we extend the works based on the Poisson and linear bias models (Kitaura & Enßlin 2008; Kitaura, Jasche & Metcalf 2010; Jasche & Kitaura...
following the ideas presented in Kitaura (2012a). In particular, we implement these improvements in the ARGON Hamiltonian-sampling code, which is able to jointly infer density, peculiar velocity fields and power-spectra (Kitaura, Gallerani & Ferrara 2012a). For the prior distribution describing structure formation of the dark matter field we use the lognormal assumption (Coles & Jones 1991). We note, however, that this prior can be substituted by another one, e.g. based on Lagrangian perturbation theory (see Hell, Kitaura & Gottlöber 2013; Jasche & Wandelt 2013; Kitaura 2013; Wang et al. 2013). Alternatively, one can extend the lognormal assumption in an Edgeworth expansion to include higher order correlation functions (Colombi 1994; Kitaura 2012b). We show in this work that our likelihood model is able to yield unbiased dark matter field reconstructions on $\sim 6 h^{-1}$ Mpc scales based on $N$-body simulations.

This paper is structured as follows. In Section 2, we describe our statistical approach. Then we present our numerical tests (Section 3) and finally we present our conclusions (Section 4).

2 METHOD

To infer the dark matter density field from biased tracers such as galaxies or haloes, one has to define a target distribution, called posterior PDF. We use the Bayesian framework to express the posterior distribution based on a model PDF for the data, the likelihood, and a model PDF for the signal, the prior. We then recap the Hamiltonian sampling technique used in this work from such a PDF, and present the Hamiltonian equations of motions for our model.

2.1 Bayesian approach: the posterior distribution function

In this work we will restrict ourselves to the reconstruction of dark matter fields given a set of biased tracers in real-space. We note that redshift-space distortions can be corrected within a Gibbs-sampling scheme and leave this additional complication for a later work (see Kitaura & Enßlin 2008; Kitaura et al. 2012a).

Let us divide the volume under consideration into a grid with $N_C$ cells. Our input data vector is given by the number counts of haloes or galaxies per cell $N_G$ and the desired signal is the dark matter density $\delta_M$. In addition, we need to assume some model for the dark matter distribution $\mathcal{M}(\delta_M)$ and for the bias relating the number counts of galaxies to the underlying dark matter distribution $\mathcal{B}(N_G|\delta_M)$, including the non-linear deterministic and stochastic parameters (see Sections 2.2 and 2.3). We will assume in this work that there is one population of tracers and that they can be described with a set of bias parameters. Nevertheless, we show in Appendix A that we could sub-divide the sample into various tracer types, each one with its own bias parameters, and combine them in a multi-tracer analysis in a straightforward way, within the methodology presented here. The posterior distribution function of dark matter fields given $N_G$, $\mathcal{M}(\delta_M)$, and $\mathcal{B}(N_G|\delta_M)$ can be expressed within the Bayesian framework as the product between the prior $\pi$ and the likelihood $\mathcal{L}$ up to a normalization

$$
\mathcal{P}(\delta_M|N_G, \mathcal{M}(\delta_M), \mathcal{B}(N_G|\delta_M)) \propto \pi(\delta_M|\mathcal{M}(\delta_M)) \times \mathcal{L}(N_G|\mathcal{B}(N_G|\delta_M)).
$$

2.2 The likelihood: stochastic bias

Let us start defining the likelihood, which models the statistical nature of the data. First we assume that the biasing relation is known and define the expected number count by $\lambda \equiv \langle N_G \rangle_G$, where $\langle \ldots \rangle_G \equiv \sum_{i=N_G}^{\infty} \mathcal{L}(N_G|\mathcal{B}(N_G|\delta_M)) \langle \ldots \rangle$ denotes the ensemble average over the halo or galaxy realization. At this point we need to introduce the stochastic biasing parameters $\{\lambda_{SB}\}$, necessary to model the deviation from the Poisson distribution $\mathcal{L}(N_G|\mathcal{B}(N_G|\delta_M)) = \mathcal{L}(N_G|\lambda_{SB})$. The positive (negative) correlation of haloes at sub-grid resolution introduces over- (under-) dispersed distributions depending on the halo population and density regime (see Somerville et al. 2001; Casas-Miranda et al. 2002; Neyrinck et al. 2014). This effect was already predicted by Peebles (1980). We focus on modelling over-dispersion, as under-dispersion is a sub-dominant effect, only present for very massive objects (see Baldauf et al. 2012, 2013). We note that stochastic bias has been studied in a number of works, more or less explicitly (see e.g. Press & Schechter 1974; Peacock & Heavens 1985; Bardeen et al. 1986; Fry & Gaztanaga 1993; Mo & White 1996; Dekel & Lahav 1999; Sheth & Lemson 1999; Seljak 2000; Berlind & Weinberg 2002; Smith, Scoccimarro & Sheth 2007; Desjacques et al. 2010; Beltrán Jiménez & Durrer 2011; Valageas & Nishimichi 2011; Elia, Ludlow & Porciani 2012; Chan, Scoccimarro & Sheth 2012; Baldauf et al. 2012, 2013).

For a given distribution function $f(\lambda, N, \{\lambda_{SB}\})$ with expectation value $\lambda$, observed number count $N_G$ and the set of stochastic bias parameters $\{\lambda_{SB}\}$, the likelihood can be written as follows:

$$
\mathcal{L}(N_G|\lambda, \{\lambda_{SB}\}) = \prod_{i=1}^{N_G} f(\lambda_i, N_i, \{\lambda_{SB}\}).
$$

The product is computed over the number of cells $N_C$, which corresponds to the number of dimensions of the problem.

Let us consider the negative binomial (NB) distribution and the gravitational thermodynamics (GT) distribution by Saslaw & Hamilton (1984) to describe the deviation from Poissonity, which requires a single stochastic bias parameter $\beta$ and $b$, respectively. The Poisson $f_P$, the NB $f_{NB}$ and the GT $f_{GT}$ distributions are written as

$$
f_P(\lambda, N) = \frac{e^{-\lambda} \lambda^N}{N!},
$$

$$
f_{NB}(\lambda, N, \beta) = \frac{\lambda^N \Gamma(\beta + N)}{N! \Gamma(\beta) (\beta + \lambda)^N} \left(1 + \frac{\lambda}{\beta}\right)^{-1},
$$

$$
f_{GT}(\lambda, N, b) = \frac{\lambda^N e^{-\lambda(1-b)}N! (1-b) [\lambda(1-b) + bN]^{N-1}}{N!},
$$

respectively. The parameters $\beta$ and $b$ are connected to the expectation value $\lambda$ and the variance $\sigma^2$ by $\beta = \lambda^2/(\sigma^2 + \lambda)$ and $b = 1 - \sqrt{\lambda}/\sigma$, respectively. This implies that the over-dispersion term shows a quadratic and a linear dependence on the expected halo number count $\lambda$ for the NB $\sigma^2_{SB} = \lambda + \lambda^2/\beta$ and the GT $\sigma^2_{GT} = \lambda/(1-b)^2 = \lambda + \lambda(2-b)/(1-b)^2$ case, respectively. To obtain a different dependence, one could take the NB expression and include a dependence of $\beta$ on $\lambda$. For $\beta \propto \lambda$ we find that the NB and the GT PDFs are equivalent in terms of over-dispersion. For this reason we will focus in the following on the NB PDF and leave a study on the $\lambda$ dependence for a later work. One could investigate these dependencies for different population of haloes by taking, for instance, ensembles of high-resolution simulations like those in Aragon-Calvo (2012).

2.3 Link between prior and likelihood: deterministic bias

Let us now define the link between the likelihood and the desired signal, i.e. the dark matter density field. This is given by the

\[ \langle \ldots \rangle_G \equiv \sum_{i=N_G}^{\infty} \mathcal{L}(N_G|\mathcal{B}(N_G|\delta_M)) \langle \ldots \rangle \]

\[ \mathcal{L}(N_G|\lambda_{SB}) = \mathcal{L}(N_G|\lambda)|_{\lambda_{SB}}. \]

\[ \mathcal{L}(N_G|\lambda) = \frac{e^{-\lambda} \lambda^N}{N!}. \]

\[ f(\lambda_i, N_i, \{\lambda_{SB}\}) = \frac{\lambda_i^N \Gamma(\beta + N_i)}{N! \Gamma(\beta) (\beta + \lambda_i)^N} \left(1 + \frac{\lambda_i}{\beta}\right)^{-1}. \]

\[ f(\lambda, N) = \frac{e^{-\lambda} \lambda^N}{N!}. \]

\[ f_{NB}(\lambda, N, \beta) = \frac{\lambda^N \Gamma(\beta + N)}{N! \Gamma(\beta) (\beta + \lambda)^N} \left(1 + \frac{\lambda}{\beta}\right)^{-1}. \]

\[ f_{GT}(\lambda, N, b) = \frac{\lambda^N e^{-\lambda(1-b)}N! (1-b) [\lambda(1-b) + bN]^{N-1}}{N!}. \]

\[ \lambda \equiv \langle N_G \rangle_G, \]

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deterministic bias relating the expected number counts to the dark matter over-density field, which is in general non-linear, scale dependent and non-local. We note that non-locality introduces a scatter which can be absorbed in the stochastic bias (see discussion in Kitaura et al. 2014a).

One could expand the dark matter overdensity field \( \delta_M = \rho_M / \bar{\rho}_M - 1 \) (with \( \bar{\rho}_M \) being the mean dark matter density) in a Taylor series (Fry & Gaztanaga 1993). Alternatively one could follow Cen & Ostriker (1993) and expand the series based on the logarithm of the density field (avoiding in this way negative densities allowed in the previous expansion). This model to linear order, corresponding to a power law of the dark matter field, has been proposed for resolution augmentation of N-body simulations (see de la Torre & Peacock 2013). The power law can be interpreted as a linear bias factor in Lagrangian space which undergoes gravitational evolution within the lognormal approximation. It has recently been found that the bias is very well fit by a compact relation including an exponential cut-off: \( \rho_i \propto \rho_M^{\alpha} \exp\left(-\left(\frac{\delta_i}{\delta_0}\right)^\gamma\right) \) (see Neyrinck et al. 2014), which can be approximated by a Heaviside step-function \( \theta(\delta_M - \delta_0) = 0 \text{ if } \delta_M < \delta_0, \text{ else } = 1 \); see Kitaura et al. (2014b). This model is in concordance with the Press & Schechter (1974) and the peak background split formalism (see e.g. Kaiser 1984; Bardeen et al. 1986; Cole & Kaiser 1989; Mo & White 1996; Sheth, Mo & Tormen 2001), which permit the formation of haloes only above a certain density threshold. It has recently been shown to be a crucial ingredient in the halo three-point statistics (Kitaura et al. 2014a). The deterministic bias model including the density power law and the density cut-off is given by the following expression for the expected halo/galaxy density:

\[
\lambda_i \equiv \langle \rho_i \rangle_0 = f_N \bar{\rho}_M \rho_M^{\alpha} \theta(\delta_M - \delta_0),
\]

where \( w_i \) is the completeness at each cell \( i \). In this way our method is able to deal with incomplete data samples as well (see also Jasche & Kitaura 2010; Kitaura et al. 2010, 2012a). The normalization ensuring a particular mean number count \( N \) is given by

\[
f_N = \bar{N} \left( \frac{w_i \bar{\rho}_M \rho_M^{\alpha} \theta(\delta_M - \delta_0)}{\bar{\rho}_M^\alpha} \right),
\]

where \( \{ \ldots \}_{M} = \int d\delta_M \rho_M(\delta_M) M(\delta_M) \{ \ldots \} \) denotes the ensemble average over all possible dark matter realizations (cosmic variance).

2.4 The prior: statistics of dark matter fields

Let us define now the model describing the distribution of dark matter density fields \( M(\delta_M) \). The Gaussian assumption has since long been commonly used in the literature. This assumption is, for instance, present in the Wiener reconstruction method (see e.g. Zaroubi et al. 1995; Kitaura et al. 2009). Nevertheless, it is well known that gravity induces deviations from Gaussianity. For this reason a non-Gaussian model is essential to exploit the accuracy of our likelihood model. For the sake of simplicity we will restrict this work to the lognormal assumption (see Coles & Jones (1991), and its implementation within a Bayesian context; Kitaura et al. (2010)). We note, however, that any structure formation model can be implemented at this point as has been shown in a series of recent works (see Jasche & Wandelt 2013; Kitaura et al. 2013; Wang et al. 2013; Heß et al. 2013; Wang et al. 2014). Moreover, the lognormal assumption has recently been shown to satisfy sufficient statistics (Carron & Szapudi 2014), and thereby extract the maximal cosmological information. However, it is known that the lognormal approximation fails at modelling the large-scale structure in the low-density regime (see e.g. Colombi 1994). However, it has been shown to be a good approximation for the moderate-to-high-density regime (Kitaura 2012a). We leave an extension with more complex models like those including higher order statistics for later work (Kitaura 2012b).

Let us define the signal distribution \( s \) as a logarithmic transformation of the matter density field

\[
s = \log(1 + \delta_M) - \mu,
\]

with the mean field \( \mu = \langle \log(1 + \delta_M) \rangle \), ensuring that the mean of \( s \) vanishes, \( \langle s \rangle = 0 \). The Gaussian prior for the logarithmically transformed density field is then given as

\[
\pi(s) = \frac{1}{\sqrt{(2\pi)^N \det(S)}} \exp\left(-\frac{1}{2} s^T S^{-1} s\right),
\]

where the covariance matrix \( S = \langle s s^T \rangle \) (or power spectrum in Fourier-space) depends on the set of cosmological parameters \( \{ p_C \} \), where \( \langle \ldots \rangle = \int ds \pi(s|S|\ldots) \) denotes the ensemble average over all possible lognormal fields. In practice, we assume a linear power spectrum and the corresponding covariance matrix.

2.5 Sampling from the posterior distribution function

To sample from the posterior distribution we rely on the Hamiltonian Monte Carlo (HMC) sampling technique, which is a hybrid Markov Chain Monte Carlo (MCMC) approach that uses physically motivated equations of motion to explore the phase space avoiding inefficient random walks. Let us recap here the basics of Hamiltonian sampling. For more details we refer to Duane et al. (1987), Neal (1993) and more recently Neal (2012)). For applications to astronomy we refer to e.g. Taylor, Ashdown & Hobson (2008), Jasche et al. (2010), and Kitaura et al. (2012b). Here we briefly point to the main features and also emphasize the modifications we implemented. The HMC approach treats the problem as a thermodynamical system. The contact with a heat bath moves the system into equilibrium, i.e. to the statistical space in which samples are drawn from the posterior distribution \( \mathcal{P}(x) \). The key idea of the HMC approach consists of moving the system by solving the Hamiltonian equations of motions, which involve a stochastic kinetic term. Let us define in this physical analogy the potential \( U \), kinetic \( K \) and Hamiltonian \( \mathcal{H} \) energy through the following relations

\[
U(x) = -\ln \mathcal{P}(x),
\]

\[
\mathcal{H}(x, p) = U(x) + K(p),
\]

where \( U(x) \) is the potential function at the coordinate vector \( x \) and \( K(p) \) is the kinetic term of the momentum \( p \) of the form \( \sum_{i,j} \frac{1}{2} p_i M_{ij}^{-1} p_j \). Combining equations (10) and (11), we see that the target distribution \( \mathcal{P}(x) \) can be inferred from

\[
\exp(-\mathcal{H}) = \mathcal{P}(x) \cdot \exp\left(-\sum_{i,j} \frac{1}{2} p_i M_{ij}^{-1} p_j \right).
\]

This equation shows that drawing samples from \( \exp(-\mathcal{H}) \) yields the desired distribution if one is withdrawing the kinetic term by marginalizing over the momenta. The momenta are drawn from a multivariate Gaussian distribution with covariance matrix \( M_j \). In order to explore the high-dimensional phase space we need to evolve the system. Therefore, we solve the Hamiltonian equations
of motion
\[ \frac{dx_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \]
\[ \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial x_i} = -\frac{\partial U}{\partial x_i}. \]
Having fully evolved the initial position \((x_0, p_0)\) of the system, we apply a criterion to accept or withdraw the new point in phase space \((x_1, p_1)\) that writes
\[ P_{\text{Accept}} = \min \left[ 1, \exp(-\mathcal{H}(x_1, p_1) + \mathcal{H}(x_0, p_0)) \right]. \]

2.6 Hamiltonian equations of motion

As shown in equations (10), (13), (14) and (15), we need to calculate the logarithm of the target distribution \(P(x)\) and its gradient term. Let us summarize below the potential energy terms and the corresponding analytic gradient expressions required in our work.

2.6.1 Gaussian prior

We calculate the negative logarithm of equation (9) as
\[ -\ln \pi = -\ln \left[ \frac{1}{\sqrt{(2\pi)^N \det(S)}} \exp \left( -\frac{1}{2} s^T S^{-1} s \right) \right] \]
\[ -\ln \pi = -\frac{1}{2} s^T S^{-1} s - c, \]
where \(c\) incorporates all constant terms of the normalization.

The derivative w.r.t. the signal \(s\) writes
\[ -\frac{\partial}{\partial s} \ln \pi = -\frac{\partial}{\partial s} \ln \left[ \frac{1}{\sqrt{(2\pi)^N \det(S)}} \exp \left( -\frac{1}{2} s^T S^{-1} s \right) \right] \]
\[ -\frac{\partial}{\partial s} \ln \pi = S^{-1} s. \]
Here we substituted the dummy variable \(x\) with the logarithmic signal variable \(s\) we want to evaluate. We note that more complex schemes connecting the initial conditions with the final gravitationally evolved density fields assume this prior for the primordial fluctuations, but include the Lagrangian to Eulerian mapping in the likelihood (see Heß et al. 2013; Jasche & Wandelt 2013; Kitaura 2013; Wang et al. 2013). We will show below the likelihood expressions for the lognormal case, but include more general expressions in Appendix B.

2.6.2 Poisson likelihood

The terms for the Poisson likelihood write as follows
\[ \mathcal{L}(N_G | \lambda) = \prod_i \frac{e^{-\lambda_i} \lambda_i^{N_i}}{N_i!}, \]
\[ -\ln \mathcal{L} = \sum_i (\lambda_i - N_i \ln \lambda_i - c). \]
Finally the derivative w.r.t. to signal variable \(s\) writes as
\[ -\frac{\partial \mathcal{L}}{\partial \lambda_i} = \alpha \lambda_i \left[ 1 - \frac{N_i}{\lambda_i} \right]. \]

2.6.3 Non-Poisson likelihood: negative binomial

We calculate the corresponding terms for the NB distribution:
\[ \mathcal{L}_{\text{NB}}(N_G | \lambda, \beta) = \prod_i \frac{\lambda_i^{N_i} \Gamma(\beta + N_i)}{N_i! \Gamma(\beta) \Gamma(\beta + \lambda_i) \left( 1 + \frac{\lambda_i}{\beta} \right)^\beta}, \]
\[ -\ln \mathcal{L}_{\text{NB}} = \sum_i (-N_i \ln \lambda_i + N_i \ln(\beta + \lambda_i)) + \beta \ln(1 + \lambda_i / \beta) - c. \]
Corresponding to equation (19) we can write the derivative of these likelihood functions as
\[ -\frac{\partial \mathcal{L}_{\text{NB}}}{\partial \lambda_i} = \alpha \lambda_i \left[ 1 - \frac{N_i}{\beta + \lambda_i} - \frac{N_i}{\lambda_i} \right]. \]

2.7 Leap frog scheme

To explore the phase space and solve iteratively the Hamiltonian equations of motion we use the leapfrog scheme
\[ p_i \left( t + \frac{\epsilon}{2} \right) = p_i(t) - \frac{\epsilon}{2} \frac{\partial U(x)}{\partial x_i}, \]
\[ x_i(t + \epsilon) = x_i(t) - \frac{\epsilon}{m_i} p_i \left( t + \frac{\epsilon}{2} \right), \]
\[ p_i \left( t + \frac{\epsilon}{2} \right) = p_i \left( t + \frac{\epsilon}{2} \right) - \frac{\epsilon}{2} \frac{\partial U(x)}{\partial x_i}. \]
with \(n\) being the number of steps, \(\epsilon\) the step size and the total pseudo-time given by \(\tau = ne\).

3 VALIDATION OF THE METHOD

To validate our algorithm we take the Bolshoi dark matter simulation (Klypin, Trujillo-Gomez & Primack 2011) at redshift \(z = 0\), which was created using the following cosmological parameters: \(\Omega_m = 0.73, \Omega_b = 0.047, \Omega_k = 0.27, \sigma_8 = 0.8, n_s = 0.95, H_0 = 100 h \text{ km s}^{-1} \text{ Mpc}^{-1}, h = 0.7\).

We consider two different subsamples of the halo catalogue, named \(S_1\) and \(S_2\), created with the bound-density-maxima (BDM) halo finder (Klypin & Holtzman 1997) as inputs to our method.

For \(S_1\) we randomly select \(2 \times 10^{15}\) haloes of the masses between \(10^9\) and \(10^{15} M_\odot\). These mass limits represent the total mass range of the Bolshoi simulation (see Appendix D) and yield a bias lower than one (see Fig. 2).

Additionally, we consider the subsample \(S_2\) with a mass cut of \(3 \times 10^{12} M_\odot\) (see Appendix D), resulting in \(3 \times 10^{14}\) haloes and yielding a bias larger than one (see Fig. 3). Subsample \(S_2\) permits us to test threshold bias described in equation (6), which is negligible for subsample \(S_1\). To technically overcome divergencies caused by the threshold bias we introduce a Gibbs sampling procedure, described in Appendix B3.

We use the nearest-grid-point (NGP) scheme to compute the number density for each cell on a mesh with \(128^3\) cells. We use the dark matter distribution from the Bolshoi simulation as a reference to estimate the accuracy of our reconstructions and define it as the true dark matter field.

To test the different models described in Section 2, we apply our novel ARG0 code running a series of Hamiltonian Markov chains with different likelihoods and bias assumptions.
Figure 1. Slices of the density field \((1 + \delta)\) with thickness \(\sim 10\, h^{-1}\) Mpc from a volume of \(250\, h^{-1}\) Mpc side for left panel: the dark matter field from the Bolshoi simulation (about \(9 \times 10^9\) dark matter tracers), middle panel, top: halo catalogue \(S_1\) from the Bolshoi simulation with \(2 \times 10^5\) matter tracers, middle panel, bottom: halo catalogue \(S_2\) from the Bolshoi simulation created from haloes of at least \(3 \times 10^{12}\) M\(_\odot\), resulting in \(3 \times 10^4\) matter tracers, right panel, top: the \textsc{argo} NB reconstruction of \(S_1\), and right panel, top: the \textsc{argo} NB reconstruction of \(S_2\). The \textsc{argo} reconstructions have been averaged over 10 000 Hamiltonian iterations. The colour code indicates the density \(1 + \delta\).

(i) Poisson likelihood and unity bias using subsample \(S_1\),
(ii) Poisson likelihood and power-law bias using subsample \(S_1\),
(iii) NB likelihood and power-law bias using subsample \(S_1\),
(iv) NB likelihood and power-law bias including thresholding using subsample \(S_2\).

We disregard the first 2000 iterations of the chains until the power spectra have converged and use a total of 10 000 iterations for our analysis. The convergence behaviour is estimated through the Gelman & Rubin (1992) test in Appendix C.

Fig. 1 shows a slice through the volume of the Bolshoi simulation. This figure illustrates the problem, as the haloes (middle panel) represent in our case-study only \(4\) to \(5\) orders of magnitude less matter tracers than the dark matter particles used for the simulation (left panel). We have plotted the means of an ensemble of 10 000 reconstructions using the NB model including a power-law bias (upper right panel without and lower right panel with thresholding bias) and find that the relevant structures are in general terms very well recovered. The filaments in the low-density regions are less accurately reconstructed (see upper and lower right panels). This is expected from the low signal-to-noise ratio in those regions. Moreover, the models we are using for the low-density regime are not optimal. We lack a good description of the dark matter field in the low-density regime due to the lognormal approximation. We also find that the high-density peaks are less pronounced than in the true dark matter field. This is caused by the smoothing introduced from averaging the reconstructed samples, i.e. the mean estimator yields, as expected, a conservative reconstruction.

3.1 Two-point statistics: power spectra

Let us further investigate the two-point statistics of the reconstructed fields in Fourier space, i.e. the power spectrum. This is shown in Figs 2 and 3. In these plots we can clearly see the scale-dependent bias of the halo samples (solid green line) with respect to the dark matter field (solid black line). The power spectra of the halo fields have been corrected for the mass assignment kernel and shot-noise following Jing (2005). Therefore, the halo power spectra can be trusted up to approximately \(0.8\, h\, \text{Mpc}^{-1}\), which is about 50 per cent of the Nyquist frequency. In Fig. 2 the reconstruction using the Poisson likelihood with unity bias (dashed magenta line) is very close to the halo power spectrum, essentially confirming that the shot-noise correction follows a Poisson model, as the deterministic bias is neglected in this run. We find a considerable improvement by adjusting the power-law bias (dotted red line). Nevertheless, the power spectrum lacks power towards high \(k\); since the dispersion has been underestimated. We register \(> 10\) per cent deviation at \(k = 0.2\, h\, \text{Mpc}^{-1}\). Only when modelling also over-dispersion with the NB likelihood we find an excellent agreement with the dark
3.2 Cell-to-cell cross-correlation

To further assess the accuracy of our reconstructions, we compare them to the true dark matter field within a cell-to-cell correlation (see Fig. 4). To have a fair comparison we smooth each catalogue with a Gaussian kernel with smoothing length of $\sigma_R = 6 \, h^{-1} \text{Mpc}$ (see left panels in Fig. 4). This should compensate for the different number density of haloes and dark matter particles. For the $\text{ARGO}$ reconstructions the average over 10 000 samples is shown. We find that the haloes and the Poisson unity bias case show very similar cell-to-cell correlations, which are strongly biased towards high densities. This could have interesting applications to reconstruct the expected halo density field (see Appendix E, Fig. E1). In the low-density regime we can see that the reconstruction is more biased than the halo sample. This must be caused by the lognormal assumption, as the bias was set to one in this run. The NB reconstruction shows unbiased cell-to-cell correlations towards high densities, and the same bias at low densities. We can see that the scatter is larger for the NB than for the Poisson unity bias case or the halo distribution. This is expected from the stochasticity included in the model. Non-local contributions, which may be deterministic, are absorbed in our stochastic bias model, thereby possibly enhancing the scatter. Interestingly, we see in our run (iv), including the thresholding bias, that the biased low halo density (see lower left panel in Fig. 4) is corrected in the low-density region (see lower right panel in Fig. 4), achieving a similar accuracy to the run (iii) where haloes are included in the low-density regions (see upper right panel in Fig. 4). We also find in run (iv) using subsample $S_2$ (moderate massive objects of minimum mass of $3 \times 10^{12} \, M_\odot$) that the deviation from Poissonity is negligible. We expect an under-dispersed distribution for more massive haloes, clusters or quasars. The method presented in this work is therefore optimal for over-dispersed tracers like emission line galaxies.

4 CONCLUSIONS

We have presented a Bayesian reconstruction algorithm, which is able to produce unbiased samples of the underlying dark matter field from non-linear stochastic biased tracers.

We find in this study that an accurate reconstruction of the dark matter field requires both modelling of the stochastic and the deterministic bias. Our results using a power-law bias model and the NB distribution function are very encouraging, as they produce unbiased statistics over a wide range of scales and density regimes.

We have focused on the NB distribution function and discussed for which parameter dependencies it can be equivalent to the gravitational thermodynamics PDF. Furthermore, we model the deterministic bias relating the expected galaxy number density to the dark matter density through a non-linear scale-dependent expression.

We have presented the Hamiltonian equations of motions for our model and implemented them in the $\text{ARGO}$ code. We have shown that this permits us to efficiently sample the posterior distribution function of density fields given a set of biased tracers. We have also introduced a Gibbs-sampling scheme to deal with strongly biased objects tracing the high-density peaks.

In particular, we have tested our algorithm with the Bolshoi N-body simulation, inferring the underlying dark matter density field from a subsample of the corresponding halo catalogue. We found that a Poisson likelihood yields reconstructions with power spectra deviating more than 10 per cent at $k = 0.2 \, h \text{Mpc}^{-1}$. Our method shows that we can draw closely unbiased samples (compatible within 1 $\sigma$) from the posterior distribution up to scales of about...
Figure 4. Cell-to-cell density correlation after Gaussian smoothing with radius $\sigma_R = 6$ $h^{-1}$ Mpc between the dark matter density $1 + \delta_{\text{N_BODY}}^{\text{Haloes}}$ and top left panel: the halo field with $2 \times 10^5$ tracers, top right panel: the corresponding ARGO NB reconstruction, and bottom left panel: the halo field with $3 \times 10^4$ tracers and mass cut, bottom right panel: the corresponding ARGO reconstruction with density thresholding. The colour code indicates the number of cells. In Appendix E, we also show the cell-to-cell density correlation after applying a unity bias Poisson reconstruction.

$k \sim 1$ $h$ Mpc$^{-1}$ in terms of power-spectra and cell-to-cell correlations with the NB PDF.

We have furthermore analytically shown that our method can deal with incomplete data and perform a multi-tracer analysis. Further investigation needs to be done here to demonstrate the level of accuracy of such approaches.

We will demonstrate in a forthcoming publication that we can also correct for redshift-space distortions in an iterative way. Our work represents the first attempt to deal with non-linear stochastic bias in a reconstruction algorithm and will contribute towards an optimal analysis of galaxy surveys.

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field only

\[ \mathcal{L}(N_{G1}, \ldots, N_{GN} | \delta_M, B(N_{G1}, \ldots, N_{GN} | \delta_M)) \]

\[ \propto \mathcal{L}(N_{G1} | \delta_M, B(N_{G1} | \delta_M), \ldots, \mathcal{L}(N_{GN} | \delta_M, B(N_{GN} | \delta_M)). \quad (A2) \]

Hence, we can write the posterior PDF as

\[ \mathcal{P}(\delta_M | N_{G1}, \ldots, N_{GN}, B(N_{G1} | \delta_M), \ldots, B(N_{GN} | \delta_M)) \]

\[ \propto \tau(\delta_M | \{pc\}) \times \mathcal{L}(N_{G1} | \delta_M, B(N_{G1} | \delta_M)) \]

\[ \ldots \mathcal{L}(N_{GN} | \delta_M, B(N_{GN} | \delta_M)). \quad (A3) \]

For the Hamiltonian sampler (see Section 2.6) we need to compute the potential energy, which is defined as

\[ -\ln \mathcal{P}(\delta_M | N_{G1}, \ldots, N_{GN}, B(N_{G1} | \delta_M), \ldots, B(N_{GN} | \delta_M)) \]

\[ = \text{const} - \ln \tau(\delta_M | \{pc\}) \]

\[ - \ln (\mathcal{L}(N_{G1} | \delta_M, B(N_{G1} | \delta_M))) \]

\[ \ldots \]

\[ - \ln (\mathcal{L}(N_{GN} | \delta_M, B(N_{GN} | \delta_M))). \quad (A4) \]

This expression permits us to incorporate any additional galaxy sample and combine different galaxy catalogues with the method presented in this work. The above calculations demonstrate that the dark matter field serves as a common denominator for different halo/galaxy samples and allows one to perform a multi-tracer analysis.

**APPENDIX B: GRADIENT CALCULATIONS**

Here we calculate the derivatives of the prior and the likelihood (see Section 2.5) separately with signal vector \( s \).

\[ \frac{\partial}{\partial s_i} \ln \mathcal{P}(\delta_M | \{pc\}) = - \frac{\partial}{\partial s_i} \ln \tau(\delta_M | \{pc\}) \]

\[ - \frac{\partial}{\partial s_i} \ln (\mathcal{L}(N_{G1} | \delta_M)). \quad (B1) \]

\[ - \frac{\partial}{\partial s_i} \ln (\mathcal{L}(N_{GN} | \delta_M)) \quad (B2) \]

**B1 Prior**

The derivative for the Gaussian prior for the linearized Gaussian field \( s = \ln(1 + \delta_M) - \mu \) writes as

\[ \frac{\partial}{\partial s_i} \ln \tau = - \frac{\partial}{\partial s_i} \ln \left[ \frac{1}{\sqrt{(2\pi)^N \det(S)}} \exp \left( -\frac{1}{2} s^T S^{-1} s \right) \right] \]

\[ = \frac{1}{2} \sum_{ij} (S^{-1})_{ij} \delta_{ij} \]

\[ = \frac{1}{2} \left[ \sum_{ij} (S^{-1})_{ij} + \sum_{i} (S_{ii}^{-1}) \right] \]

\[ - \frac{\partial}{\partial s_i} \ln \tau = S^{-1} s. \quad (B3) \]

**B2 Likelihood**

We calculate the gradient of the likelihood

\[ \mathcal{L}_{NB} = \prod_{i=1}^{N_C} \left[ \frac{\lambda_{i,1}^{N_i} \Gamma(\beta + N_i)}{N_i! \Gamma(\beta + \lambda_i)^{N_i}} \frac{1}{\left(1 + \frac{\lambda_i}{\beta}ight)^\beta} \right] \quad (B4) \]
as follows:

$$\frac{\partial}{\partial x_i} = \left( \frac{\partial L}{\partial \delta_j} \right)^{-1} \frac{\partial L}{\partial x_i} \frac{\partial}{\partial \delta_j}, \quad \text{(B5)}$$

$$\left( \frac{\partial s}{\partial \delta_j} \right)^{-1} = 1 + \delta_j, \quad \text{(B6)}$$

$$\frac{\partial \lambda_k}{\partial \delta_j} = \frac{\alpha \lambda_k}{1 + \delta_j}. \quad \text{(B7)}$$

We can now just calculate the derivative of the likelihood w.r.t. $\lambda$ and get the final result as

$$- \frac{\partial \ln L_{NB}}{\partial \lambda_k} = -\frac{N_k}{K_k} - \frac{N_k}{\beta + \lambda_k} + \frac{1}{1 + \frac{\lambda_k}{\beta}}. \quad \text{(B8)}$$

Taking this into account, the derivative of the Likelihood writes as

$$- \frac{\partial \ln L_{NB}}{\partial \delta_i} = \alpha \lambda_i \cdot \left[ -\frac{N}{\lambda_i} - \frac{N}{\beta + \lambda_i} + \frac{1}{1 + \frac{\lambda_i}{\beta}} \right]. \quad \text{(B9)}$$

We note that for $\lim_{\beta \to \infty} \left( \frac{N}{\lambda_i} - \frac{N}{\beta + \lambda_i} + \frac{1}{1 + \frac{\lambda_i}{\beta}} \right) = 1 - \frac{N}{\lambda_i}$, which is identical to the solution of the likelihood.

### B3 Gibbs sampling of the thresholding

The density cut-off bias component introduces a numerical instability, since the additional gradient terms diverge around the density threshold. Therefore we follow a Gibbs-sampling strategy by considering the $\theta(\delta_M - \delta_m)$ step-function to be constant with respect to the signal $\delta_M$. This permits us to neglect all the terms where gradients and logarithms of the step-function appear (see the previous section). The scheme can be described as follows:

$$\delta_M \sim P(\delta_M | \theta, N_G, \mathcal{M}(\delta_M), B(N_G | \delta_M)) \quad \text{(B10)}$$

$$\theta \sim P(\theta | \delta_M, \delta_m). \quad \text{(B11)}$$

We consider a vanishing uncertainty for the PDF of the step function given $\delta_M$ and $\delta_m$, which is equivalent to a Dirac delta density function. We have tested this scheme and found it very stable. Nevertheless, we consider investigating the introduction of some uncertainty in the PDF of the step function in future work. This may yield to an even better agreement in the power spectra.

### APPENDIX C: CONVERGENCE OF THE HAMILTONIAN SAMPLER WITH NON-LINEAR NON-POISSON LIKELIHOODS

There is no unique way to estimate the convergence of a Markov Chain nor a stopping criterion in literature. In principle, multiple chains are supposed to converge to the same stationary distribution and thus all samples should be consistent. Also within one running chain the drawn samples should be consistent after the burn-in phase. So comparing the means and variances within one converged chain to the samples of independently run chains will probe the convergence of the chains. This has been introduced by Gelman & Rubin (1992). The test can be applied to any parameter without loss of generality.

We assume $N_{\text{chains}}$ chains of length $N_{\text{length}}$. The output of the chain is denoted as $x_{c,s}$, with $c \in \{1, 2, \ldots, N_{\text{chains}}\}$ and $s \in \{1, 2, \ldots, N_{\text{length}}\}$. In our case $x$ would the multidimensional ensemble $\{\delta_i\}$ of the overdensity of cell $i$ in our reconstructed volume. For simplicity we show the calculations for a one-dimensional observable $x$. Starting from an identical proposal distribution we calculate as follows:

(i) Calculate each chain’s mean value

$$\bar{x}_c = \frac{1}{N_{\text{length}}} \sum_s x_{c,s}. \quad \text{(i)}$$

(ii) Calculate each chain’s variance

$$\sigma^2_c = \frac{1}{N_{\text{chains}} - 1} \sum_c (x_{c,s} - \bar{x}_s)^2. \quad \text{(ii)}$$

(iii) Calculate all chains’ mean

$$\bar{x} = \frac{1}{N_{\text{chains}}} \sum_c \frac{1}{N_{\text{length}}} \sum_s x_{c,s} = \frac{1}{N_{\text{chains}}} \sum_c \bar{x}_c. \quad \text{(iii)}$$

(iv) Calculate the weighted mean of each chain’s variance

$$B = \frac{N_{\text{length}}}{N_{\text{chains}} - 1} \sum_c (\bar{x}_c - \bar{x})^2. \quad \text{(iv)}$$

(v) Calculate the average variance within one chain

$$W = \frac{1}{N_{\text{chains}}} \sum_c \sigma^2_c. \quad \text{(v)}$$

(vi) The potential scale reduction factor (PSRF) then is defined as

$$\text{PSRF} = \sqrt{ \frac{N_{\text{length}} - 1}{N_{\text{length}}} + \frac{N_{\text{chains}} + 1}{N_{\text{chains}} N_{\text{length}}} \frac{B}{W} }. \quad \text{(vi)}$$

If all chains converge to the same target distribution, we expect the variance within one chain to be close to the variance between the $N_{\text{chains}}$ chains, so that the PSRF be close to one as can be seen in Fig. C1.

**Figure C1.** PSRF from the Gelman–Rubin test for the convergence of the Hamiltonian Markov Chain shown for the NB run including a power-law bias. Each point corresponds to one (out of 128$^3$) specific cell of the reconstructed volume of $\alpha$CO. The PSRF estimator on the y-axis should be around 1 to indicate that the chain is converged.
APPENDIX D: MASS RANGES OF THE BOLSHOI SIMULATION

In Fig. D1 we show the mass function of the Bolshoi simulation in a cumulative histogram. Our cut of $3 \times 10^{13} M_\odot$ creates a subsample with 13,000 tracers.

APPENDIX E: RECONSTRUCTION OF THE HALO DENSITY FIELD

We also run ARGO with a Poisson likelihood and unity bias. We can see in Fig. E1 that this model creates smoothed reconstructions of the biased halo field (compare Fig. 4). The averaged cell-to-cell correlation is in excellent agreement with the outcome of the halo field.