QUANTIFYING AND CONTROLLING BIASES IN ESTIMATES OF DARK MATTER HALO CONCENTRATION

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ABSTRACT

We use bootstrapping to estimate the bias on estimates of concentration of N-body dark matter (DM) halos as a function of particle number. We find that algorithms based on the maximum radial velocity and radial particle binning tend to overestimate the concentration by 15%–20% for halos sampled with 200 particles and by 7%–10% for halos sampled with 500 particles. To control this bias at low particle numbers we propose a new algorithm that estimates halo concentrations based on the integrated mass profile. The method uses the full particle information without any binning, making it reliable in cases when low numerical resolution becomes a limitation for other methods. This method reduces the bias to <3% for halos sampled with 200–500 particles. The methods based on velocity and density have to use halos with at least ~4000 particles in order to keep the biases down to the same low level. We also show that the mass–concentration relationship could be shallower than expected once the biases of the different concentration measurements are taken into account. These results show that bootstrapping and the estimates of concentration based on the integrated mass profile are valuable tools to probe the internal structure of DM halos in numerical simulations.

Key words: dark matter – galaxies: halos – methods: numerical

1. INTRODUCTION

In the current paradigm of structure formation the properties of galaxies are coupled to the evolution of their dark matter (DM)-hosting halo. In this paradigm the sizes and dynamics of galaxies are driven by the internal DM distribution of each halo.

The internal DM distribution in a halo is usually parameterized through the density profile. In a first approximation this profile is spherically symmetric; the density depends only on the radial coordinate. One of the most popular radial parameterizations is the Navarro–Frenk–White (NFW) profile (Navarro et al. 1997). This profile can be considered as universal (Navarro et al. 2010), assuming that one is not interested in the very central region where galaxy formation takes place, and where the effects of baryon physics on the DM distribution are still unknown. This profile is a double power law in radius, where the transition happens at the so-called scale radius, \( r_s \). The ratio between the scale radius and the halo virial radius \( R_v \) is known as the concentration \( c = R_v / r_s \).

The concentration of the NFW profile provides a conceptual framework to study simulated DM halos as a function of redshift and cosmological parameters. Numerical studies (Neto et al. 2007; Duffy et al. 2008; Macciò et al. 2008; Muñoz-Cuartas et al. 2011; Prada et al. 2012; Ludlow et al. 2014, 2016; Klypin et al. 2016) have summarized their results through the mass–concentration relationship; that is, the distribution of concentration values at a fixed halo mass and redshift. The success of such numerical experiments rests on a reliable algorithm for estimating the concentration. Such an algorithm should provide unbiased results and must be robust when applied at varying numerical resolution.

There are two established algorithms to estimate the concentration parameter. The first method takes the halo particles and bins them into logarithmic radii to estimate the density in each bin, then it proceeds to fit the density as a function of the radius. A second method uses an analytic property of the NFW profile that involves the maximum of the ratio of the circular velocity to the virial velocity, \( V_{circ} / V_{vir} \). The concentration can be then found as the root of an algebraic equation dependent on this maximum value.

The first method is straightforward to apply but has two disadvantages. First, it requires a large number of particles in order to have a proper estimate of density in each bin. This makes the method robust only for halos with at least \( 10^2 \) particles. The second problem is that there is no way to estimate the optimal radial bin size; different choices may produce different results for the concentration.

The second method solves the two problems mentioned above. It works with low particle numbers and does not involve data binning. However, it effectively takes into account only a single data point and discards the rest of the data. Small fluctuations on the maximum can yield large perturbations on the estimated concentration parameter.

In this article we use bootstrapping to estimate the bias and standard deviation on the estimates of concentration as a function of particle number. We show that the two standard methods to estimate concentrations have increasing biases for decreasing particle numbers.

This motivates us to present a third alternative based on fitting the integrated mass profile. This approach has two advantages over the methods mentioned above. It does not involve any data binning and does not throw away data points. This translates into a robust estimate even at low resolution/particle numbers. Furthermore, since the method does not require any binning, there is no need to tune numerical parameters. This is a new independent method to estimate the concentration parameter.

2. BASIC PROPERTIES OF THE NFW DENSITY PROFILE

Let us review first the basic properties of the NFW density profile. This will help us to define our notation.
2.1. Density Profile

The NFW density profile can be written as

$$\rho(r) = \frac{\rho_s \delta_c}{(r/r_s)(1 + r/r_s)^2},$$

(1)

where $\rho_s \equiv 3H^2/8\pi G$ is the critical density of the universe, $H$ is the Hubble constant, $G$ is the universal gravitational constant, $\delta_c$ is the dimensionless characteristic density of the halo, and $r_s$ is the scale radius. This radius marks the point where the logarithmic slope of the density profile is equal to $-2$, the transition between the power-law scaling $\rho \propto r^{-1}$ for $r < r_s$ and $\rho \propto r^{-3}$ for $r > r_s$.

We define the virial radius of a halo, $r_v$, as the boundary of the spherical volume that encloses a density of $\Delta_0$ times the mean density of the universe. The corresponding mass $M_v$, the virial mass, can be written as $M_v = \frac{4\pi}{3}\rho_c r_v^3$. From these virial quantities we define new dimensionless variables for the radius and mass, $x \equiv r/r_v$ and $m \equiv M(<r)/M_v$.

In this article we use $\Delta_0 = 740$, a number roughly corresponding to 200 times the critical density at redshift $z = 0$.

2.2. Integrated Mass Profile

From these definitions we can compute the total mass enclosed inside a radius $r$:

$$M(<r) = 4\pi \rho_s \delta_c r_s^3 \left[ \ln\left(\frac{r_s + r}{r_s}\right) - \frac{r}{r_s + r} \right],$$

(2)

or in terms of the dimensionless variables for mass and radius,

$$m(<x) = \frac{1}{A} \left[ \ln(1 + xc) - \frac{xc}{xc + 1} \right],$$

(3)

where

$$A = \ln(1 + c) - \frac{c}{c + 1},$$

(4)

and the parameter $c$ corresponds to the concentration $c \equiv r_v/r_s$.

From this normalization and for later convenience we define the following function:

$$f(x) = \ln(1 + x) - \frac{x}{x + 1}.$$  

(5)

The most interesting feature of Equation (3) is that the concentration is the only free parameter to describe the integrated mass profile.

2.3. Circular Velocity Profile

It is also customary to express the mass of the halo in terms of the circular velocity $V_c = \sqrt{GM(<r)/r}$. From this we can define a new dimensionless circular velocity $v(<x) \equiv V_c(<r)/V_c(<r_s)$. Using the result in Equation (3), we have

$$v(<x) = \sqrt{A \left[ \frac{1}{x} \ln(1 + xc) - \frac{c}{xc + 1} \right]}.$$  

(6)

This normalized profile always shows a maximum provided that the concentration is larger than $c > 2$. It is possible to show that for the NFW profile the maximum is provided by

$$\max(v(<x)) = \frac{c}{\sqrt{\ln x_{\max} f(c)}},$$

(7)

where $x_{\max} = 2.163$ (Klypin et al. 2016) and the function $f(x)$ corresponds to the definition in Equation (5).

3. METHODS TO ESTIMATE THE CONCENTRATION FROM N-BODY SIMULATIONS

3.1. Estimates from the Density and Velocity Profiles

To date, there are two standard methods to estimate concentrations in DM halos extracted from N-body simulations. The first method takes all the particles in the halo and bins them by the logarithm of the radial coordinate from the center of the halo. Then, it estimates the density in each logarithmic bin. At this point is possible to make a direct fit to the density as a function of the radial coordinate. This method has been widely used for more than two decades to study the mass–concentration–redshift relation of DM halos. A second method uses the circular velocity profile. It finds the value of $x$ for which the normalized circular velocity $v(<x)$ shows a maximum. Using this value it solves numerically for the corresponding value of the concentration using Equation (7).

3.2. Estimate from the Integrated Mass Profile

Here we propose a new method to estimate the concentration. It uses the integrated mass profile defined in Equation (3). We build it from N-body data as follows. First, we define the center of the halo to be at the position of the particle with the lowest gravitational potential. Then we rank the particles by their increasing radial distance from the center. From this ranked list of $i = 1, N$ particles, the total mass at a radius $r_i$ is $M_i = i \times m_p$, where $r_i$ is the position of the $i$th particle and $m_p$ is the mass of a single computational particle. We then divide the enclosed mass $M_i$ and the radii $r_i$ by their virial values to finally obtain the dimensionless variables $m_i$ and $x_i$.

Using bootstrapping data (Section 5.1), we find that at a given normalized radius, $x$, the logarithm of the normalized integrated mass, $m$, approximately follows a Gaussian distribution with variance

$$\sigma_x^2 = \frac{1}{x} \frac{1}{N}.$$  

(8)

If the integrated mass values at different radii were independent from each other we could write a likelihood distribution as $L(c|x_i) \propto \exp(-\chi^2(c, x_i)/2)$ with

$$\chi^2(c, x_i) = \sum_{i=2}^{N} \frac{[\log m_i - \log m(<x_i; c)]^2}{\sigma_i^2},$$

(9)

where $\sigma_i^2 = \sigma_x^2(x_i)$, $m(<x_i; c)$ corresponds to the values in Equation (3) at $x = x_i$ for a given value of the concentration parameter $c$, and the index $i$ sums over all the particles in the numerical profile. In this computation the particles $i = 1$ and $i = N$ are discarded to avoid divergent terms in the sum.

However, tests on the bootstrapping data show that using $\sigma_i^2 = \sigma_x^2(x_i)$, instead of the full inverse covariance matrix, grossly overestimates $\chi^2(c, x_i)$, providing small uncertainties around the best concentration value. To avoid the expensive
computation and inversion of a full covariance matrix we use the bootstrapping data to calibrate an effective $\sigma_{\text{eff}}^2 \approx \sigma_{\text{eff}}^2(x_i)$. We impose two conditions on the approximate $\sigma_{\text{eff}}^2$. It must keep the dependence on $x$ that we have discovered for the diagonal elements and it must give similar curves of $\chi^2(c, x_i)$ versus $c$ around the minimum to the full covariance matrix. We found that the effective $\sigma_{\text{eff}}^2$ can be approximated as

$$\sigma_{\text{eff}}^2 = \frac{1 - x}{x} \frac{N^{1.15}}{4.5 \times 10^3}. \quad (10)$$

We then use an affine-invariant Markov chain Monte Carlo (MCMC) method implemented in the Python module emcee (Foreman-Mackey et al. 2013) to sample the distribution of the likelihood function. From the $\chi^2$ distribution we find the optimal concentration value and its associated uncertainty. We stress that different choices for $\sigma_{\text{eff}}^2$ do not affect the optimal concentration value, only its uncertainty.

Run-time is roughly proportional to $N$. Using a single 2.3 GHz CPU core with two walkers over 500 steps takes ~0.5 ms per halo per particle in the halo, i.e., a halo with $N = 2 \times 10^5$ can be fit in one second.

4. NUMERICAL SIMULATIONS AND HALO SAMPLES

We use two different simulations to test our methods. The first is the Bolshoi run, a cosmological simulation that follows the nonlinear evolution of a DM density field sampled with 2048$^3$ particles over a cubic box of 250 $h^{-1}$ Mpc on a side. The cosmological parameters use a Hubble parameter $h = 0.73$, a matter density $\Omega_m = 0.3071$ and a normalization of the power spectrum $\sigma_8 = 0.82$. The data are publicly available at http://www.cosmosim.org/. Details about the structure of the database and the simulation can be found in Klypin et al. (2011) and Riebe et al. (2013).

We use the halos located in a cubic subvolume of 100 $h^{-1}$ Mpc on a side containing a total of 64,531 objects. From this sample we select all the halos at $z = 0$ detected with a friends-of-friends (FoF) algorithm with more than 300 particles, meaning that the masses are in the interval $4 \times 10^{10} \lesssim M_{\text{FoF}}/h^{-1} M_\odot \lesssim 10^{14}$. The FoF algorithm used a linking length of 0.17 times the mean interparticle distance. This choice translates into an overdensity $\Delta_h \approx 400$–700 dependent on the halo concentration (More et al. 2011).

From this set of particles we follow the procedure spelled out in Section 3 with $\Delta_h = 740$ to select a spherical region that we redefine to be our halo. This choice ensures that the overdensities are fully included inside the original FoF particle group. In the interests of providing a fair comparison against the density method we only report results from overdensities with at least 200 particles ($2.6 \times 10^{10} h^{-1} M_\odot$).

We also use public data from the Via Lactea simulation project (Diemand et al. 2008). This simulation contains a single isolated halo with a virial mass of the order of $10^{12} h^{-1} M_\odot$ simulated using the tree code PKDGRAV (Stadel 2001). The simulation had ~2 $\times 10^8$ particles to resolve this region. The cosmological parameters are different from those in the Bolshoi simulation, with a Hubble parameter $h = 0.73$, a matter density $\Omega_m = 0.238$, and a normalization of the power spectrum $\sigma_8 = 0.74$. The data available to the public correspond to a downscaled set of $10^7$ particles, which corresponds to a particle mass of $2.24 \times 10^7 h^{-1} M_\odot$.

5. RESULTS

5.1. Bootstrapping to Estimate Biases

We take halos with at least $10^7$ particles and subsample them by factors of 2 up to $10^3$. We measure the concentration at every resampling. We use a two-sample Kolmogorov–Smirnov test to compare the list of radial distances from each subsample against that of its parent halo. We find that the resulting $p$-value distribution is flat. This confirms that the radial particle distribution in the bootstrapped halo is consistent with coming from the distribution given by the parent halo. Why not use different simulations with the same initial conditions and lower resolutions (i.e., Springel et al. 2008)? Because we want to be sure that we are measuring only the bias of a given method as a function of particle number for statistically identical halos, and not a possible simulation artifact that changes the halo’s structure.

For every subsample we keep fixed the virial radius and the center found for the high-resolution halo. Leaving the virial radius and center free in each bootstrapping iteration has an effect on the concentration of less than 1%. In the Bolshoi simulation we select 14 massive halos and create 700 subsamples for each one. For the Via Lactea simulation the same halo is subsampled 10,000 times.

The average concentration value for the largest number of particles, $c_{\text{max}}$, provides a baseline from which to compare all the other results. We use the following statistic:

$$f_{\text{off}} = c_{\text{off}}/c_{\text{max}} - 1, \quad (11)$$

to account for the offset between the concentration at a given downsampled particle number $c_{\text{off}}$ and the baseline $c_{\text{max}}$.

Figure 1 summarizes our results. The plot on the left shows the average value of $f_{\text{off}}$ as a function of particle number. This can be interpreted as the statistical bias on the estimate of concentration. For large enough particle numbers, $N_p > 4 \times 10^4$, the results of the three algorithms show a bias below the 1% level. For a lower number of particles the results start to deviate. At 200 particles the velocity method overestimates the concentration by a factor 14% while the density method overestimates it by 20%. Around the same sampling scale, the new algorithm shows a more stable behavior, underestimating the concentration by only a factor of 1%–3%.

The thin lines on the same panel show a fit to the function

$$f_{\text{off}} = A \left(1 + \log_{10} N_p \right)^B, \quad (12)$$

with $A = 2842 \pm 1900$, $B = 7.96 \pm 0.54$; $A = 239 \pm 131$, $B = 6.23 \pm 0.43$; and $A = -0.46 \pm 3.49$, $B = 0.79 \pm 1.31$ for the methods based on density, velocity, and mass, respectively.

The right panel in Figure 1 shows different uncertainty results. The lines show the difference between 14% and 86% of the $f_{\text{off}}$ distribution at fixed mass. The three lines correspond to the three different methods for estimating the concentration applied to both simulations. This shows that the bootstrapping technique can help us to assign a 1σ uncertainty to the concentration values at a fixed $N_p$ as

$$\sigma_c = \frac{0.40}{\sqrt{N_p/200}}. \quad (13)$$
The circles in the same figure show the $1\sigma$ uncertainty on all the relaxed halos in the Bolshoi (Via Lactea) simulation. The density method noticeably overestimates the concentration up to a factor of 20%, while the new method only underestimates the concentrations by less than 3%. Right panel: $1\sigma$ uncertainties on the bootstrapped halos (lines) and the MCMC uncertainties on the estimates of concentration for each halo using the integrated mass method (circles). Lines show the width between 14% and 86% of the $f_{\text{off}}$ distribution at fixed particle number. The lines include the results for the three methods using Bolshoi data. To allow a fair comparison against $f_{\text{off}}$, the MCMC uncertainty has been normalized by the preferred concentration value for each halo.

Figure 1. Left panel: bias estimated via bootstrapping on the concentration as a function of particle number. Thick (thin) lines correspond to massive halos in the Bolshoi (Via Lactea) simulation. The density method noticeably overestimates the concentration up to a factor of 20%, while the new method only underestimates the concentrations by less than 3%. Right panel: $1\sigma$ uncertainties on the bootstrapped halos (lines) and the MCMC uncertainties on the estimates of concentration for each halo using the integrated mass method (circles). Lines show the width between 14% and 86% of the $f_{\text{off}}$ distribution at fixed particle number. The lines include the results for the three methods using Bolshoi data. To allow a fair comparison against $f_{\text{off}}$, the MCMC uncertainty has been normalized by the preferred concentration value for each halo.

Figure 2. Mass–concentration relationship for the three different methods on the Bolshoi data using only relaxed halos. The lines correspond to the median concentration values in each mass bin. The shaded region presents the 10%–90% spread. The three methods have a similar spread but for clarity we show only the spread for the new method. The dotted line corresponds to fits reported by Prada et al. (2012). The left panel shows the raw results coming from each algorithm. The right panel introduces a correction following the results on the bias as a function of particle number.

The circles in the same figure show the $1\sigma$ uncertainty on all the relaxed halos in the Bolshoi simulation sample using the MCMC results. To allow for a fair comparison with the bootstrapping results, this uncertainty is normalized to the concentration value. The uncertainty from the bootstrapping experiment provides an upper bound to the uncertainty on the estimate of concentration for individual halos.

5.2. Impact on the Mass–Concentration Relationship

We now inspect the mass–concentration relationship resulting from the three different algorithms. This can help us to identify possible consequences of the biases detected through the bootstrapping experiments.

Figure 2 shows the mass–concentration relationship for the methods based on density, velocity, and integrated mass. The left panel shows the results as they are produced by each of the algorithms. The thin dashed line marks the trend reported by Prada et al. (2012) using the velocity method, showing that our implementation of the velocity method can reproduce their results.

The results from the new algorithm follow the velocity algorithm very closely at high masses ($M_\bullet > 10^{12} h^{-1} M_\odot$ or equivalently for $>4 \times 10^3$ particles). For lower masses there is...
a difference between the medians of the two methods, but they are still consistent within the statistical uncertainties.

We hypothesize that the increase in the results for the methods based on velocity and density below $4 \times 10^3$ particles comes from the systematic bias described in the previous section. To test the general consistency of this hypothesis, we correct the concentration values in the methods based on velocity and integrated mass by a factor of $1/(1 + f_{\text{off}})$, using the definition in Equation (11) and the parameters obtained from the data presented in Figure 1. The correction brings the results from the velocity/density methods and those from the new algorithm into good agreement.

We also notice that the results from the density method have a systematic 15% offset from those from the velocity method. This offset was already presented by Prada et al. (2012) for low concentrations ($c < 6$) and high halo masses ($M_h > 10^{12} h^{-1} M_\odot$). Recently, Klypin et al. (2016) summarized results for the mass–concentration relationship coming from different methods and data sets to show that similar systematic offsets are present. Dutton & Macciò (2014) studied the mass–concentration relationship using the methods based on maximum velocity and density and did not report any significant difference. However, they implemented a modified version of the velocity algorithm that bins the particle data, which might explain why no offset was not reported.

How do these results impact the most recent mass–concentration estimates? Ludlow et al. (2016) and Klypin et al. (2016) estimated the mass–concentration relation over different suites of cosmological $N$-body simulations using the methods based on density and velocity, respectively. Both used halos with at least $5 \times 10^3$ particles. This imposes a lower limit on halo mass of $\sim 10^{12} h^{-1} M_\odot$ (Figure 8 in Ludlow et al. (2016), Figure 17 in Klypin et al. (2016)) to have robust estimates. This means that their results for individual halos should not be affected by the bias we report here. This also leaves open the question about what other methods can robustly say about the flattening we report below $10^{12} M_\odot$ using the new method. However, there are other results at lower masses and higher redshifts (i.e., Prada et al. 2012) that should be reconfirmed using higher-resolution simulations because they use halos with only 500 particles.

6. CONCLUSIONS

In this article we used bootstrapping to quantify the biases on estimates of concentration. We found that methods commonly used in the literature can overestimate the concentrations by factors of 15%–20% for halos with 200 particles, or 7%–10% for halos with 500 particles. This procedure provides a robust technique to quantify the bias in estimates of concentration with the advantage that it works without having to run new simulations.

These results motivated us to introduce a new method based on the integrated mass profile that show a robust performance at low particle numbers. The new algorithm showed a bias of <3% for halos with 200 particles and less than 1% for halos with 500 particles or more. To keep the bias of the methods based on velocity and density below 2%, only halos with at least $\sim 4000$ particles should be considered.

The three methods are in broad agreement, within the statistical uncertainties, concerning their estimates of the mass–concentration relationship. Some noticeable differences include concentrations that are systematically 15% higher in the density method than in the velocity method. This systematic offset has been reported before with the same data set (Prada et al. 2012) and with different simulations (Klypin et al. 2016) without any conclusive explanation for its origin. Another difference is that the methods based on velocity and integrated mass start to differ for masses below $10^{12} h^{-1} M_\odot$ ($\sim 4000$ particles). We found that correcting the mean concentration by the mean bias factor found through bootstrapping brings these two techniques into agreement.

These results show that using the integrated mass profile to estimate the DM halo concentrations is a tool deserving deeper scrutiny. Further tests with larger simulated volumes, varying numerical resolution, higher redshifts, stacked data, and different density profiles are the next natural step to explore the full potential of this new method.

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