Lagrangian Perturbation Theory from Direct Force Calculations

Daniel Eisenstein, July 31, 2015

1. Introduction

Taking $\mathbf{r}$ and $\mathbf{v}$ to be the comoving position and velocity, respectively, the equations of motion are

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \tag{1}$$

$$\frac{d\mathbf{v}}{dt} + 2H\mathbf{v} = \mathbf{g} \tag{2}$$

$$\nabla_r \cdot \mathbf{g} = -4\pi G \rho_{comoving} a^{-3} \delta \tag{3}$$

In other words, $\mathbf{g}$ is a^{-3} times the acceleration that one would derive from the inverse square law computed with comoving (not proper) separations.

We define $\mathbf{r} = \mathbf{x} + \mathbf{q}$ where $\mathbf{x}$ is the initial grid and $\mathbf{q}$ is the comoving Lagrangian displacement.

In linear theory, $\mathbf{g} = (3/2)\Omega_m H^2 \mathbf{q}$. This gives rise to the equation of motion

$$\frac{d^2\mathbf{q}}{dt^2} + 2H\frac{d\mathbf{q}}{dt} = \frac{3\Omega_m H^2}{2}\mathbf{q} \tag{4}$$

For $\Omega_m = 1$, we have $a \propto t^{2/3}$ and $H = 2/3t$. This gives the growing mode solution $\mathbf{q} \propto t^{2/3} \propto a$.

2. Perturbation Theory

Let's now write

$$\mathbf{q} = \epsilon d_1(t)\mathbf{q}_1 + \epsilon^2 d_2(t)\mathbf{q}_2 + \epsilon^3 d_3(t)\mathbf{q}_3 + O(\epsilon^4) \tag{5}$$

This particle distribution produces a gravitational force at the location of the particles that we can write

$$\mathbf{g} = \frac{3\Omega_m H^2}{2}\left[\epsilon d_1(t)\mathbf{g}_1 + \epsilon^2 d_2(t)\mathbf{g}_2 + \epsilon^3 d_3(t)\mathbf{g}_3 + O(\epsilon^4)\right] \tag{6}$$

From linear theory, we know that $\mathbf{g}_1 = \mathbf{q}_1$. At this point, these time dependences are just hypotheses; we'll see that they hold in $\Omega_m = 1$, but not in other cases.

2.1. Second order

In particular, for the case of $\mathbf{q} = \epsilon d_1(t)\mathbf{q}_1$, we must have a force series of the form

$$\mathbf{g} = \frac{3\Omega_m H^2}{2}\left[\epsilon d_1(t)\mathbf{q}_1 + \epsilon^2 d_1^2(t)\mathbf{S}(\mathbf{q}_1) + O(\epsilon^3)\right] \tag{7}$$

where the $\mathbf{S}$ function is some complicated mode-coupled thing that is second order in $\mathbf{q}$.

Considering $\mathbf{q}$ to second-order, we must have

$$\mathbf{g} = \frac{3\Omega_m H^2}{2}\left[\epsilon d_1(t)\mathbf{q}_1 + \epsilon^2 d_2(t)\mathbf{q}_2 + \epsilon^2 d_1^2(t)\mathbf{S}(\mathbf{q}_1) + O(\epsilon^3)\right] \tag{8}$$

Inserting this into the equation of motion, we have

$$(\partial_t^2 + 2H\partial_t)(\epsilon d_1\mathbf{q}_1 + \epsilon^2 d_2\mathbf{q}_2) = \frac{3\Omega_m H^2}{2}(\epsilon d_1\mathbf{q}_1 + \epsilon^2 d_2\mathbf{q}_2 + \epsilon^2 d_1^2\mathbf{S}(\mathbf{q}_1) \tag{9}$$

where ∂_t indicates a derivative with respect to time. Separating by orders, we recover the linear growth equation

$$(\partial_t^2 + 2H\partial_t - \frac{3\Omega_m H^2}{2})d_1\mathbf{q}_1 = 0 \tag{10}$$

For $\Omega_m = 1$, this has the solution $d_1 \propto t^{2/3}$. The next order is

$$(\partial_t^2 + 2H\partial_t - \frac{3\Omega_m H^2}{2})d_2\mathbf{q}_2 = \frac{3\Omega_m H^2}{2}d_1^2\mathbf{S}(\mathbf{q}_1) \tag{11}$$

Hence $\mathbf{q}_2 = \mathbf{S}(\mathbf{q}_1)$, and we have a simple ODE for $d_2(t)$. For $\Omega_m = 1$, the power-law ansatz works and we find $d_2(t) = (3/7)d_1^2(t)$, a familiar result.

How to find $\mathbf{S}(\mathbf{q}_1)$? If we write the force from $\mathbf{r} = \mathbf{x} + d_1\mathbf{q}_1$ as $\mathbf{g}[d_1\mathbf{q}_1]$, then quick inspection of (8) says that we must have

$$d_2\mathbf{q}_2 = \frac{3}{7}d_1^2\mathbf{S}(\mathbf{q}_1) = \frac{3}{7}\frac{2}{3\Omega_m H^2}\frac{1}{2}\left(\mathbf{g}[d_1\mathbf{q}_1] + \mathbf{g}[-d_1\mathbf{q}_1]\right) \tag{12}$$

This sum cancels out the $O(\epsilon^3)$ terms. Hence, two force calculations with opposing first-order displacements isolates second-order displacement to third-order accuracy.

2.2. Third order

Let's continue to third order. Using the third order $\mathbf{q}$, we must have

$$\mathbf{g} = \frac{3\Omega_m H^2}{2}\left[\epsilon d_1(t)\mathbf{q}_1 + \epsilon^2 d_2(t)\mathbf{q}_2 + \epsilon^3 d_3(t)\mathbf{q}_3 + \epsilon^2 d_1^2(t)\mathbf{S}(\mathbf{q}_1) + \epsilon^3 d_1^3(t)\mathbf{T}_{111}(\mathbf{q}_1) + \epsilon^3 d_1(t)d_2(t)\mathbf{T}_{12}(\mathbf{q}_1) + O(\epsilon^4)\right] \tag{13}$$

For the case of $\Omega_m = 1$, we have $d_2 \propto d_1^2$, so these two third order terms have the same time dependence and we can combine the two vectors into a single vector $\mathbf{T}(\mathbf{q}_1)$. Note that this mode-coupling does depend on the second-order vector $\mathbf{S}$; we suppress this dependence because we assume that we are using the $\mathbf{S}$ that comes from $\mathbf{q}_1$.

Inserting into the equation of motion, we have the third-order terms

$$(\partial_t^2 + 2H\partial_t - \frac{3\Omega_m H^2}{2})d_3\mathbf{q}_3 = \frac{3\Omega_m H^2}{2}d_1^3\mathbf{T}(\mathbf{q}_1) \tag{14}$$

As before, we find $\mathbf{q}_3 = \mathbf{T}(\mathbf{q}_1)$ and an ODE for $d_3(t)$. For $\Omega_m = 1$, we find $d_3 = (1/6)d_1^3(t)$.

To find $\mathbf{T}$, we use

$$\mathbf{g}[d_1\mathbf{q}_1 + d_2\mathbf{q}_2] = \frac{3\Omega_m H^2}{2}\left[d_1\mathbf{q}_1 + d_2\mathbf{q}_2 + d_1^2\mathbf{S}(\mathbf{q}_1) + d_1^3\mathbf{T}(\mathbf{q}_1)\right] \tag{15}$$

So we have

$$d_3\mathbf{q}_3 = \frac{1}{6}d_1^3\mathbf{T}(\mathbf{q}_1) = \frac{1}{6}\left(\frac{2}{3\Omega_m H^2}\mathbf{g}[d_1\mathbf{q}_1 + d_2\mathbf{q}_2] - d_1\mathbf{q}_1 - (10/3)d_2\mathbf{q}_2\right) \tag{16}$$

This difference has errors at $O(\epsilon^4)$, but it is not worth cancelling them out because we had these errors in our formula for $d_2\mathbf{q}_2$.

Note that we did use the $\Omega_m = 1$ assumption here. At second order for $\Omega_m \neq 1$, we would not have $d_2 \propto d_1^2$, but we could still solve the ODE for d_2 and proceed. But at third order, we needed to use $d_2 \propto d_1^2$ to combine two terms that would otherwise have different time dependences.

For our applications, Ω_m at high redshift is very close to 1, so that we are not making a big error. Still, we should assess the size of it. Bouchet et al. (1995) assert that the Ω dependence of d_2 is amazingly weak, $\Omega_m^{1/143}$, relative to the $(3/7)d_1^2$ factor. If so, then we are completely fine at high redshift and only 1% off even at $z = 0$! The behavior of d_3 is likely similar, but I haven't checked.

2.3. Velocities

Because our expansion for $\mathbf{q}$ has known time dependence, we can easily compute the comoving velocities from $\mathbf{v} = \partial_t\mathbf{r}$. We generally have

$$\partial_t d_j = d_j \frac{1}{d_j}\frac{d\,d_j}{da}\frac{da}{dt} = d_j H f_j \tag{17}$$

where f_j is the familiar $d\ln d_j/d\ln a$. For $\Omega_m = 1$, we have $d_1 \propto a$ and so $f_1 = 1$, $f_2 = 2$, $f_3 = 3$. For a comoving displacement $\mathbf{q} = \sum d_j\mathbf{q}_j$, we then have the comoving velocity $\mathbf{v} = \sum f_j H d_j \mathbf{q}_j$.

2.4. Implementation

One can implement this as follows.

1. Generate the initial Fourier modes and Fourier transform $i\mathbf{k}\hat{\delta}_{\mathbf{k}}$ to get the linear displacement field at the desired redshift. Apply to the positions.

2. Compute the force $\mathbf{g}[d_1\mathbf{q}_1]$. Store in the velocity. This is like a Kick.

3. Rearrange the positions to generate $\mathbf{r} = \mathbf{x} - d_1\mathbf{q}_1$. This can be done because we know the initial grid location (e.g., from the particle id number). This can be a surrogate Drift.

4. Compute the force $\mathbf{g}[-d_1\mathbf{q}_1]$. Add to the velocity. This is like a Kick.

5. Take the position (currently holding the displacement $-d_1\mathbf{q}_1$) and the velocity (currently holding $7H^2 d_2\mathbf{q}_2$) and manipulate to form the second-order position $\mathbf{x} + d_1\mathbf{q}_1 + d_2\mathbf{q}_2$ and second-order velocity $Hd_1\mathbf{q}_1 + 2Hd_2\mathbf{q}_2$. Store in the position and velocity. This can be a surrogate Drift.

6. Compute the force from the new position $\mathbf{g}[d_1\mathbf{q}_1 + d_2\mathbf{q}_2]$. Multiply by $2/3H^2$. Subtract the quantity $d_1\mathbf{q}_1 - (10/3)d_2\mathbf{q}_2$, which is currently encoded as $(7/3)\mathbf{v}/H - (4/3)\mathbf{q}$. Divide by 6 to get $d_3\mathbf{q}_3$. Add this to the position and 3 times this to the velocity.

The result is third-order Lagrangian perturbation theory for the cost of 3 force evaluations and memory requirements equal to the normal simulation code.

One should be wary, however, that third-order accuracy doesn't necessarily change the redshift where one can start by very much. If one wants 1allows one to advance by a factor of 10 in scale factor relative to Zel'dovich. 3LPT only gets another factor of 2.

What the accuracy actually is, i.e. what the small parameter of the perturbation expansion is, is not so clear. The Lagrangian displacement in CDM cosmologies is dominated by scales around 50 Mpc. So one can have displacements that are large compared to the grid spacing even though the overdensity is small. Putting this another way, nothing in the above formalism knows about the grid spacing. The breakdown in perturbation theory presumably occurs as we approach shell crossing, i.e., so that $\Delta q \sim \Delta x$. This also corresponds to overdensities of order unity.

Eisenstein, Seo, & White (2006) equation 9 gives a formula for the rms pairwise Lagrangian displacement as a function of separation. The result for the variance of the parallel displacement is

$$\frac{V(\Delta q)}{r_{12}^2} = \int \frac{k^2\,dk}{2\pi^2} P(k) f_{\|}(kr_{12}) \tag{18}$$

where

$$f_{\|}(x) = \frac{2}{x^2}\left(\frac{1}{3} - \frac{\sin x}{x} - \frac{2\cos x}{x^2} + \frac{2\sin x}{x^3}\right) \tag{19}$$

which converges to $1/5 - x^2/84$ at small x. I think that we want this variance to be small on the grid spacing, using the full power spectrum (just to be conservative). At $z = 0$ for $\sigma_8 = 0.8$, this value is about 1.7 Mpc/h for $r_{12} = 0.5$ Mpc/h, growing to 2.1 Mpc/h for 0.25 Mpc/h and dropping to 1.05 Mpc/h for 2 Mpc/h. To be conservative, we could use 2 Mpc/h as the rms displacement on the grid scale. We probably want this to be more like 10% of the grid spacing, which would be $z = 40$!

We'll need to test this in practice to see what comes out.