Optimal Smoothing for \textit{N}-Body Codes

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ABSTRACT

In any collisionless \textit{N}-body code, there is an optimal choice for the smoothing parameter that minimizes the average error in the force evaluations. We show how to compute the optimal softening length in a direct-summation code and demonstrate that it varies roughly as \(N^{-1/3}\).

1. Introduction

The role of smoothing in an \textit{N}-body code depends on the nature of the system being modelled. When simulating a system containing a modest number of point masses, like an open star cluster, the goal is to reproduce the exact level of graininess that exists in the real cluster. Ideally no softening would be used, but a nonzero softening length is usually included to eliminate the divergent forces that would result from a close encounter between two “stars.” When modelling globular clusters, the softening length may be increased to reduce the graininess of the potential to the level expected in a system containing a larger number of particles than can easily be handled in the computer. When simulating a system containing finite-sized objects, such as a galaxy cluster, the softening length may be increased still more to approximate the physical size of a typical object.

But \textit{N}-body codes are often used to study the evolution of systems, like galaxies, that contain extremely large numbers of particles. A code designed for such problems is sometimes called “collisionless,” since the system being modelled has a two-body relaxation time that greatly exceeds the elapsed time of the simulation. In a collisionless \textit{N}-body code, the particles do not represent real objects; they are simply Monte-Carlo realizations of the underlying, smoother mass distribution. The purpose of the smoothing in a collisionless code is to generate from the \textit{N} particles an accurate estimate, at each time step, of the gravitational forces corresponding to the much smoother system being modelled.
Smoothing parameters in $N$-body codes are often chosen in an ad hoc way. Here we show that the softening length in a collisionless code can be chosen objectively, so as to minimize the average errors in the force determinations. Too small a value for the smoothing parameter yields an estimate that is overly noisy, reflecting finite-$N$ fluctuations in the forces. Too large a smoothing parameter reduces the noise but increases the error from the “bias,” i.e. the systematic misrepresentation of the force due to the failure to resolve real features with scale lengths less than the softening length. In general, a unique value for the smoothing parameter may be found such that the combined error from these two sources is minimized.

The existence of an optimal softening length follows from the assumed smoothness of the underlying mass distribution; no such optimal degree of smoothing can be defined for a “collisional” code, where the accuracy of the force calculations can always be increased by decreasing the softening length.

Our analysis will focus on the simplest $N$-body algorithm, a direct-summation code in which the smoothing is imposed via a fixed softening length associated with each particle. But the general principles carry over without significant change to codes that implement the smoothing in very different ways, e.g. via a grid, or via expansion of the potential in a truncated basis set.

2. Definitions

The gravitational force on particle $i$, $1 \leq i \leq N$ in a direct-summation $N$-body code is given by

$$\mathbf{F}_i = Gm^2 \sum_{j=1}^{N} \frac{x_j - x_i}{(\epsilon^2 + |x_i - x_j|^2)^{3/2}},$$

where $\epsilon$, the softening length, determines the degree of smoothing. If the $N$ particles represent an underlying, smooth distribution of mass, there also exists a “true” value $\mathbf{F}_{\text{true}}(x_i)$ for the force on particle $i$. For instance, if the $N$ positions are generated from a Plummer density profile, $\mathbf{F}_{\text{true}}$ is the gravitational force corresponding to the Plummer mass distribution.

The optimal choice of $\epsilon$ may be defined as the value that minimizes the average deviation between $\mathbf{F}_i$ and $\mathbf{F}_{\text{true}}(x_i)$. There are many possible ways to define this average deviation; the simplest is the average square error, or

$$\text{ASE} = \frac{1}{N} \sum_{i=1}^{N} |\mathbf{F}_i - \mathbf{F}_{\text{true}}(x_i)|^2.$$
We may treat $\mathbf{F}$ as a continuous function, defined via Eq. (1) at any point $\mathbf{x}$. The continuous analog of the average square error is the integrated square error, or

$$\text{ISE} = \int \rho(\mathbf{x}) |\mathbf{F}(\mathbf{x}) - \mathbf{F}_{\text{true}}(\mathbf{x})|^2 d\mathbf{x} \quad (3)$$

with $\rho(\mathbf{x})$ the true density, normalized to unit total mass.

If we imagine generating many $N$-particle Monte-Carlo realizations of the same smooth model, we can define the expectation or mean value of the ISE as

$$\text{MISE} = \mathbb{E}(\text{ISE}) = \mathbb{E} \int \rho(\mathbf{x}) |\mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{x})_{\text{true}}|^2 d\mathbf{x}, \quad (4)$$

where $\mathbb{E}$ indicates an average over many realizations. It is easy to show that the MISE contains contributions from two terms, representing the bias and the variance of the force estimates. The bias is the mean deviation of the computed force at some point from the true force, $E\mathbf{F} - \mathbf{F}_{\text{true}}$; its integrated square value is

$$\text{ISB} = \int \rho(\mathbf{x}) |E\mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{x})_{\text{true}}|^2 d\mathbf{x}. \quad (5)$$

The variance is the mean square deviation of the force estimate from its mean value $E\mathbf{F}$; the integrated variance is $\text{IV} = \text{MISE} - \text{ISB}$.

The bias increases with the softening length while the variance falls off – a greater amount of smoothing produces smaller average fluctuations in the forces but also tends to smooth over real features of small scale. For $N$-particle realizations of a given model, therefore, there is an optimal choice of softening length $\epsilon_{\text{opt}}$ such that the sum $\text{ISB} + \text{IV}$ is minimized. One typically finds in problems of this sort (e.g. Scott 1992, p. 131) that the contribution to the total error from the bias and from the variance are of the same order when the smoothing length is optimized. Furthermore, the variance decreases with particle number while the bias is independent of $N$ (e.g. Silverman 1986, p. 39); thus as $N$ increases, one expects $\epsilon_{\text{opt}}$ to decrease.

3. Two Examples

We illustrate these ideas using $N$ equal-mass points generated from two simple models. The first is a spherical Plummer model of unit scale length:

$$\rho(r) = \frac{3}{4\pi}(1 + r^2)^{-5/2}. \quad (6)$$

The expectation value of the forces generated by a finite set of particles drawn from the density (6) will be spherically symmetric. We may therefore compute the terms in Eqs. (4)
and (5) on a linear grid in radius, taking averages over a large number of independent 3-D realizations of the particle distribution for any specified $N$. The number of Monte-Carlo realizations was taken to be $N_{MC} = 3 \times 10^6/N$, e.g. 1000 realizations for $N = 3000$.

Fig. 1 shows how the contribution to the force errors from the bias and variance depend on $\epsilon$ for $N = 1000$. As expected, the bias increases with $\epsilon$ while the variance decreases, producing an optimal value of $\epsilon$ for which the MISE is minimized, $\epsilon_{opt} \approx 0.16$. At $\epsilon = \epsilon_{opt}$, roughly 60% of the total error comes from the variance and the remainder from the bias.

Fig. 2 shows how the MISE vs. $\epsilon$ curve changes with $N$. As $N$ increases at fixed $\epsilon$, the variance decreases, roughly as $N^{-1}$. The result is an optimal $\epsilon$ that decreases with $N$. Fig. 3 presents $\epsilon_{opt}$ and MISE($\epsilon_{opt}$) as functions of $N$. The two quantities vary roughly as power-laws in $N$, with

$$
\epsilon_{opt} \approx 1.1 \times N^{-0.28}, \quad \text{MISE}_{opt} \approx 0.21 \times N^{-0.66}.
$$

(7)

Our second example is based on a spherical model with the density law

$$
\rho(r) = \frac{1}{2\pi}r^{-1}(1 + r)^{-3}
$$

(8)

which is a good approximation to the light distribution in early-type galaxies (Hernquist 1990). Figure 3 shows $\epsilon_{opt}$ and MISE($\epsilon_{opt}$) as functions of $N$. The relations in this case can be approximated as

$$
\epsilon_{opt} \approx 1.5 \times N^{-0.44}, \quad \text{MISE}_{opt} \approx 0.39 \times N^{-0.58}.
$$

(9)

The variation of $\epsilon_{opt}$ with $N$ in both models is such that the number of particles within one softening volume is approximately independent of $N$. However in both cases the dependence seems to be significantly different than $N^{-1/3}$.

4. Discussion

Selection of the softening length in $N$-body codes is often made on the basis of the error due either to the bias or the variance of the force estimates. For instance, $\epsilon$ may be chosen to be small enough that some feature like the core is resolved (bias), or large enough that two-body relaxation is not a problem (variance). Our discussion shows that the total error in the estimated forces in a collisionless code is the sum of these two components, and that their contributions vary in opposite ways with $\epsilon$, leading to a formally optimal choice of $\epsilon$ for any $N$. 
The softening length in Eq. (1) may be interpreted as the window width of a kernel that is convolved with the density before computing the gravitational forces. Smoothing in collisionless $N$-body codes is usually carried out in other ways than via a kernel, e.g. on a grid. (Notable exceptions are the $N$-body studies of galaxies based on the GRAPE hardware, which incorporates Eq. (1) [Ebisuzaki et al. 1993].) However, any smoothing algorithm may be interpreted in terms of a generalized kernel whose shape and width varies with position (Scott 1992, p. 155); in this sense, the analysis given here is general. One could use similar arguments to compute the optimal cell size in a grid-based algorithm, or the optimal number of terms in a basis-function expansion.

It is well known that “collisionless” $N$-body codes often exhibit nearly as much relaxation as “collisional” codes (e.g. Hernquist & Barnes 1990). The reason is that the variance in the force estimates – which, crudely speaking, is responsible for the relaxation – cannot be arbitrarily reduced without introducing a bias, as shown by Fig. 1. The primary design goal for collisionless $N$-body experimenters (aside from speed) should be to smooth in such a way as to minimize the ISE of the force estimates at every time step, since by doing so they will have effectively minimized the variance.

One way to decrease the ISE is to vary the softening length with position (and hence with time). The optimal way of doing this is well known when the quantity to be estimated is the density itself (Abramson 1982), but apparently nothing is known about the best way to vary $\epsilon$ with position when estimating the gravitational forces. This would be a fruitful topic for further study.

One would like to be able to estimate the optimal smoothing parameter directly from the $N$ positions themselves, without having to know $F_{\text{true}}$. In a direct-summation code, automatic choice of $\epsilon$ would presumably have to be based on a time-intensive bootstrap algorithm. More rapid choice of the smoothing parameter could be made in a code that represents the forces via sums of terms like $R_{lm}(r)Y_{lm}(\theta, \phi)$, with $Y_{lm}$ an angular harmonic. The radial functions $R_{lm}$ may themselves be represented via basis-function expansions (e.g. Clutton-Brock 1973), but it seems to have escaped general notice that the job may be done more simply and efficiently using smoothing splines (Wahba 1990). Standard, and efficient, routines for computing the optimal degree of smoothing for such splines are widely available (e.g. Green & Silverman 1994). The result would be a code in which the radial dependence of the forces was computed with minimum ISE at every time step.

One sometimes sees implementations in which $N$ has been increased to very large values without corresponding adjustments in the degree of smoothing (e.g. Hernquist, Sigurdsson & Bryan 1995). Figure 2 shows that such a practice is likely to put the user far to the right of the minimum in the MISE curve.
Finally, we note that objective criteria for comparing the performance of different $N$-body codes are generally lacking. A natural criterion for collisionless codes would be the rate of decrease of the MISE with $N$. An optimal potential solver could be defined as one for which the MISE decreased most rapidly with $N$.

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Fig. 1.— Bias-variance tradeoff in the force evaluation errors for $N = 1000$ realizations of a spherical Plummer model.
Fig. 2.— MISE(ε) for $N = 30, 100, 300, 1000, 3000, 10000$ and 30000; $N$ increases downward.
Fig. 3.—Dependence of the optimal softening length $\epsilon_{\text{opt}}$, and the MISE at $\epsilon = \epsilon_{\text{opt}}$, on number of particles $N$ in two models: Eq. (6) (squares) and Eq. (8) (circles). The relations of Eqs. (7) and (9) are indicated by solid lines.