18.336/6.335 Spring 2013
Fast Methods for Partial Differential and Integral Equations
Problem Set 2

Handed out: Mar. 12th, 2013,   Due Mar. 21st, 2013

The N-Body Problem

Problem Statement

The motion of more than two orbiting bodies is a challenging problem that had eluded mathematicians since Newton's time. In honour of his 60th birthday on January 21, 1889, Oscar II, King of Sweden and Norway, established a prize for anyone who could find the solution to the problem. The prize was awarded to Poincaré, even though he did not solve the original problem. Only a century later in 1990 was an analytical solution to the n-body problem finally found, in the form of a converging power series [1].

Fortunately, it is significantly easier to approximate the solution to this famous problem using low-rank numerical techniques. Newtonian gravitation is fully described by Poisson's equation:

$$\Delta\phi(\mathbf{x}) = -4\pi G\rho(\mathbf{x}),$$

where G is the universal Gravitational constant, and ρ is the volumetric mass density, comprising of n points (i.e stars), with each point j weighted by its own mass M_j:

$$\rho(\mathbf{x}) = \sum_{j=1}^{N} M_j \delta(\mathbf{x} - \mathbf{x_j}).$$

Once the gravitational potential ϕ is computed, the force field due to gravity $\boldsymbol{g}$ is readily obtained as the gradient of ϕ:

$$\boldsymbol{g} = -\nabla\phi.$$

Therefore, the trajectory $\mathbf{x_j}(t)$ of every particle $j = 1\ldots N$ with respect to time is simply the solution to the following ordinary differential equation:

$$M_j \frac{d^2}{dt^2}\mathbf{x_j} = \boldsymbol{g}(\mathbf{x_j}).$$

This deceptively simple ODE is greatly complicated by two considerations. Firstly, $\boldsymbol{g}$ is affected by the presence of all particles within the system, and computing the forces upon N particles due their interaction with N particles by direct summation is an $\mathcal{O}(N^2)$ operation. Secondly, the particles are mobile, and the forces upon the N particles must be repeatedly computed at each new time-step. Considering that galaxies are comprised of billions of stars, the complexity of computations quickly become prohibitive.

Fortunately, gravitation is a low-rank interaction, and fast algorithms have found great success in the simulation of the n-body problem. Recent simulations of galactic motion, such as the millenium simulation project by the Max Planck Institute for Astrophysics, have included over 300 billion particles simulated over the equivalent span of more than 13 billion years! In this problem set, we will study the low-rank nature of an interaction like gravity, and the numerical techniques used to cast the interactions to canonical form.

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[1] The paper is available at: http://adsabs.harvard.edu/abs/1991CeMDA..50...73W

Question 1 - Low-Rank Interactions

Before investigating methods used to resolve low-rank interactions, let us first investigate what exactly constitutes a "low-rank" interaction. In the following question, let us simplify all mass particles to point charges of unit mass. Label by $\mathbf{x_m}$: $m = 1 \ldots N$, N target points randomly located within a specified target square, and by $\mathbf{y_n}$, $n = 1 \ldots N$, N source point charges located randomly within the unit square $[0, 1]^2$.

1. Consider the Newtonial gravitational potential function ϕ as follows:

$$\phi(\mathbf{x}) = \frac{1}{|\mathbf{x}|}.$$

   The dense coefficient matrix G associated with the potential interaction between $\mathbf{x_m}$ and $\mathbf{y_n}$ under Newtonian gravity contains an element on the j-th row and k-th column equal to:

$$G_{m,n} = \frac{1}{\|\mathbf{x_m} - \mathbf{y_n}\|}.$$

   Compute the relative rank of this matrix, by performing a singular value decomposition $G \approx U\Sigma V^T$, so that the relative spectral error of the reconstruction $\|G - U\Sigma V^T\|_2/\|G\|_2 \leq \epsilon$, where $\epsilon = 10^{-5}$. The relative rank of the matrix is equal to the number of non-zero singular values with spectral norms $\geq \epsilon\|G\|_2$.

   (a) Use 20 source points in the unit square with lower left corner at the origin, and 20 test points in a target unit square. Produce a plot of the rank of the associated G matrix, as a function of the target square position. In particular, place the target square's bottom left corner at $[2, p]$ and the top right corner at $[3, p + 1]$. Vary p from 0 to 5 in steps of 0.5.

   (b) With the bottom left corner of the target square placed at $[2, 4]$ and the top right corner placed at $[3, 5]$. Vary the number of interacting points N from 20 to 200 in steps of 20. Does increasing the number of interactions and the size of the matrix G significantly affect its rank?

2. Suppose that Newtonian gravity were instead governed by the Helmholtz Green's function as follows:

$$\phi(\mathbf{x}) = \frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|}.$$

   The dense coefficient matrix G associated with the interaction between $\mathbf{x_m}$ and $\mathbf{y_n}$ associated with this new potential function contains an element on the m-th row and n-th column equal to:

$$G_{m,n} = \frac{e^{ik|\mathbf{x_m} - \mathbf{y_n}|}}{|\mathbf{x_m} - \mathbf{y_n}|},$$

   (a) Use 20 source points in the unit square with lower left corner at the origin, and 20 test points in a target unit square. Let $k = 10$, produce a plot of the rank of the associated G matrix, as a function of the target square position. In particular, place the target square's bottom left corner at $[2, p]$ and the top right corner at $[3, p + 1]$. Vary p from 0 to 5 in steps of 0.5.

   (b) Use 20 source points and 20 test points, and set the bottom left corner of the target square placed to $[2, 4]$ and the top right corner to $[3, 5]$. Produce a plot of the rank of the interaction as a function of k, varying from 1 to 100. What are the difficulties presented by having a high value of k?

Question 2 - Projection and Interpolation

All low-rank algorithms are fundamentally based on the concept of representing arbitrary interactions using a canonical representation. The process for embedding arbitrary interactions into a canonical representation is known as a projection operation, or a source-to-multipole (S2M) operation in multipole nomenclature.

Conversely, the process to translate a canonical representation of an interaction to the interaction itself is known as interpolation, or a local-to-target (L2T) operation.

In the following question, label by $\mathbf{x}_j$, $j = 1, 2, 3, 4$, the four corners of the square $[-1, 1]^2$, and by $\mathbf{y_k}$, $k = 1, 2, 3, 4$, the four corners of the square $[-5, 5]^2$. You may take the ordering to be the top-left, top-right, bottom-left, and bottom-right corners respectively, although any other choice is acceptable. Let us simplify the gravitational potential function ϕ to:

$$\phi(\mathbf{x}) = \frac{1}{|\mathbf{x}|}.$$

1. Consider a unit charge at $\mathbf{x}_0$, generating a potential $u(\mathbf{x}) = \phi(\mathbf{x} - \mathbf{x}_0)$. We say that canonical charges q_j placed at $\mathbf{x}_j$, $j = 1, 2, 3, 4$ are the *projections* by collocation of the unit charge at $\mathbf{x}_0$ if the combination $\sum_{j=1}^{4} q_j \phi(\mathbf{x} - \mathbf{x}_j)$ matches $\phi(\mathbf{x} - \mathbf{x}_0)$ at the four points $\mathbf{x} = \mathbf{y}_k$, $k = 1, 2, 3, 4$.

   (a) Find those four canonical charges q_j, $j = 1, 2, 3, 4$, in the case when $\mathbf{x}_0 = (0.1, 0.2)$.

2. (Interpolation via projection) We now reverse the roles of $\mathbf{x}_0$ and $\mathbf{y}_1$. Consider a unit charge at the point $\mathbf{y}_1$, generating a potential $v(\mathbf{x}) = \phi(\mathbf{x} - \mathbf{y}_1)$. Assume that you have at your disposal the evaluations of this potential at each of the four points $\mathbf{x} = \mathbf{x}_j$, $j = 1, 2, 3, 4$.

   (a) How can you use the knowledge of these four evaluations, and of the four canonical charges q_j of question 2.1, to perform *interpolation* to find an approximation of the value of the potential $v(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}_0$?

   (b) Find this numerical value in the case when $\mathbf{x}_0 = (0.1, 0.2)$, and compare it to the true value $v(\mathbf{x}_0)$. Justify your finding.

3. Consider again the function $v(\mathbf{x}) = \phi(\mathbf{x} - \mathbf{y}_1)$. We say that weights w_j placed at nodes $\mathbf{x}_j$, $j = 1, 2, 3, 4$, define an *interpolation* scheme for $v(\mathbf{x})$ if the combination $\sum_{j=1}^{4} w_j v(\mathbf{x}_j)$ is a good approximation of $v(\mathbf{x})$ for $\mathbf{x}$ in a neighborhood of the $\mathbf{x}_j$.

   (a) Find those four weights w_j in the case of bilinear interpolation at $\mathbf{x} = \mathbf{x}_0 = (0.1, 0.2)$.

   (b) Find the numerical value of the bilinear interpolant of $v(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}_0$, and compare it to the true value $v(\mathbf{x}_0)$.

4. (Projection via interpolation) We now revert the roles of $\mathbf{x}_0$ and $\mathbf{y}_1$ to what they were in question 2.1. Consider a unit charge at $\mathbf{x}_0$ generating a potential $u(\mathbf{x}) = \phi(\mathbf{x} - \mathbf{x}_0)$.

   (a) How can you use the knowledge of the bilinear interpolation weights w_j of question 2.3, to find the *projections* of the unit charge at $\mathbf{x}_0$ as canonical charges $\tilde{q}_j$ at each of the four points $\mathbf{x} = \mathbf{x}_j$, $j = 1, 2, 3, 4$?

   (b) Find the numerical values of these canonical charges when $\mathbf{x}_0 = (0.1, 0.2)$, and check their accuracy by comparing the true potential $u(\mathbf{x})$ to its approximation $\tilde{u}(\mathbf{x}) = \sum_{j=1}^{4} \tilde{q}_j \phi(\mathbf{x} - \mathbf{x}_j)$, when $\mathbf{x} = \mathbf{y}_1$. Argue the expected accuracy of this projection scheme.

The projection / interpolation operations are building blocks to fast algorithms for low-rank interactions. Once projected onto a canonical representation, the potentials can be quickly evaluated by computing the cyclic convolution using the FFT. Alternatively, a hierarchy of canonical representations can be constructed, and the projection / interpolation process can be recursively performed and evaluated.