Hello, welcome to Homework set 5 — MATH 397C — Spring 2022.

Due on Thursday May 5. Hand in solutions to problems 1, 2, 6, and 7.

Problem 1: The objective of this problem is to computationally investigate the error incurred by truncating multipole expansions. Consider the following geometry: Let \( \Omega_\tau \) and \( \Omega_\sigma \) be two well-separated boxes with centers \( c_\tau \) and \( c_\sigma \). Let \( y \in \Omega_\sigma \) be a source point and let \( x \in \Omega_\tau \) be a target point. Consider the error function

\[
e(P) = \sup_{x \in \Omega_\tau} \left| \log |x - y| - B_P(x, c_\tau) Z_P(c_\tau, c_\sigma) C_P(c_\sigma, y) \right| : y \in \Omega_\sigma \quad \text{where} \quad P \text{ is the length of the multipole expansion, and where}
\]

\[
C_P(c_\sigma, y) \in \mathbb{C}^{P \times 1} \quad \text{maps a source to an outgoing expansion}
\]

\[
Z_P(c_\tau, c_\sigma) \in \mathbb{C}^{P \times P} \quad \text{maps an outgoing expansion to an incoming expansion}
\]

\[
B_P(x, c_\tau) \in \mathbb{C}^{1 \times P} \quad \text{maps an incoming expansion to a target}
\]

(a) Estimate \( e(P) \) experimentally for the geometry:

\[
\Omega_\sigma = [-1, 1] \times [-1, 1], \quad \Omega_\tau = [3, 5] \times [-1, 1].
\]

(b) Fit the function you determined in (a) to a curve \( e(P) \sim c \cdot \alpha^P \). What is \( \alpha \)?

(c) Is the supremum for a given \( P \) attained for any specific pair \( \{x, y\} \)?

If so, find (experimentally) the pair. Does the choice depend on \( P \)?

(d) Repeat questions (a), (b), (c) for a different geometry of your choice. (Provide a picture.)

Hint: The provided file main_T_ops_are_fun.m might be useful.

Problem 2: The objective of this exercise is to familiarize yourself with the provided prototype FMM. The questions below refer to the basic FMM provided in the file main_fmm.m when executed on a uniform particle distribution. For this case, precompute only the translation operators \( T^{(ofo)} \), \( T^{(ifo)} \), and \( T^{(ifi)} \) (i.e. set flag_precomp=0).

(a) Estimate and plot the execution time of the FMM for the choices

\[
N_{\text{tot}} = 1000, 2000, 4000, 8000, 16000, 32000, 64000.
\]

Set \( n_{\text{max}} = 50 \). Provide plots that track the following costs:

\[
t_{\text{tot}} \quad \text{total execution time, including initialization.}
\]

\[
t_{\text{init}} \quad \text{cost of initialization (computing the tree, the object T,OPS, etc.).}
\]

\[
t_{\text{ofs}} \quad \text{cost of applying } T^{(ofo)}.
\]

\[
t_{\text{ofo}} \quad \text{cost of applying } T^{(ofo)}.
\]

\[
t_{\text{ifo}} \quad \text{cost of applying } T^{(ifo)}.
\]

\[
t_{\text{ifi}} \quad \text{cost of applying } T^{(ifi)}.
\]

\[
t_{\text{tfi}} \quad \text{cost of applying } T^{(tfi)}.
\]

\[
t_{\text{close}} \quad \text{cost of directly evaluating close range interactions.}
\]

(b) Repeat exercise (a) but now for a few different choices of \( n_{\text{max}} \). Which one is the best one? Provide a new plot of the times required for this optimal choice.
Problem 3: [Optional] Repeat Problem 3.2 but now use a non-uniform point distribution of your choice.

Problem 4: [Optional] Can you think of a better way of computing the interaction lists? Here “better” could mean either a cleaner code that executes in more or less the same time, or a code that executes significantly faster than the provided one. If your code is both cleaner and faster then so much the better!

Problem 5: [Optional] Code up the single-level Barnes-Hut method and investigate computationally how many boxes you should use for optimal performance for any given precision and given total number $N_{\text{tot}}$ of charges. Create a plot of the best possible time $t_{\text{optimal}}$ for several $N_{\text{tot}}$ and estimate the dependence of $t_{\text{optimal}}$ on $N_{\text{tot}}$. To keep things simple, consider only uniform particle distributions. You need only consider a fixed precision (say $P = 10$) but an ambitious solution should compute the optimal time for several different choices (say $P = 5, 10, 15, 20$).

Problem 6: In this problem, $n$ and $k$ are positive integers such that $k < n$, $A$ is an $N \times N$ invertible matrix, and $B = A^{-1}$. Let us further assume that every diagonal block of $A$ is invertible.

(a) Suppose that $N = 2n$, and that we can write $A$ and $B$ as

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \quad \text{and} \quad B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix},$$

where each block is of size $n \times n$. Suppose further that $A_{12}$ and $A_{21}$ have rank $k$. What is the highest possible value for the rank of $B_{12}$?

(b) Suppose that $N = 4n$, and that we can write $A$ and $B$ as

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix}, \quad \text{and} \quad B = \begin{bmatrix} B_{11} & B_{12} & B_{13} & B_{14} \\ B_{21} & B_{22} & B_{23} & B_{24} \\ B_{31} & B_{32} & B_{33} & B_{34} \\ B_{41} & B_{42} & B_{43} & B_{44} \end{bmatrix},$$

where each block is of size $n \times n$. Suppose further that $A_{12}, A_{21}, A_{34}, A_{43}$, $A_{13} A_{14}$, $A_{23} A_{24}$, $A_{31} A_{32}$ all have rank $k$. What is the highest possible value for the rank of $B_{12}$?

(c) [Optional:] Consider the natural generalization to a matrix consisting of $8 \times 8$ blocks. What is the maximal rank of $B_{12}$? What about a matrix with $2^p \times 2^p$ blocks?

Please motivate your answers. If you rely on any formula for the inverse of a blocked matrix, then you may freely assume that any inverse that appears actually exists.
Problem 7: In this problem, let \( k \) and \( n \) be integers such that \( 0 < k < n \). Further, let \( D \in \mathbb{R}^{n \times n} \), \( U \in \mathbb{R}^{n \times k} \), \( V \in \mathbb{R}^{n \times k} \), and \( \tilde{A} \in \mathbb{R}^{k \times k} \).

(a) Set \( A = I + UV^* \). Prove that if \( I + V^*U \) is non-singular, then
\[
A^{-1} = I - U(I + V^*U)^{-1}V^*.
\]

(b) Set \( A = D + U\tilde{A}V^* \). Prove that if \( D \) and \( I + \tilde{A}V^*D^{-1}U \) are both invertible, then
\[
A^{-1} = D^{-1} - D^{-1}U(I + \tilde{A}V^*D^{-1}U)^{-1}\tilde{A}V^*D^{-1}.
\]  

Hint: You could write \( A = D(I + (D^{-1}U)(\tilde{A}V^*)) \) and apply (a).

(c) As in (b), set \( A = D + U\tilde{A}V^* \), and assume that \( D \) and \( I + \tilde{A}V^*D^{-1}U \) are both invertible. Consider the linear system
\[
\begin{bmatrix}
  D & U\tilde{A} \\
  -V^* & I
\end{bmatrix}
\begin{bmatrix}
  x \\
  \tilde{x}
\end{bmatrix} =
\begin{bmatrix}
  b \\
  0
\end{bmatrix}.
\]  

Prove that if \( \begin{bmatrix} x \\ \tilde{x} \end{bmatrix} \) solves (2), then \( x \) solves \( Ax = b \).

(d) Assume again that \( D \) is invertible. You can then perform one step of a block LDU factorization to obtain the equality
\[
\begin{bmatrix}
  D & U\tilde{A} \\
  -V^* & I
\end{bmatrix} =
\begin{bmatrix}
  I & 0 \\
  X & I
\end{bmatrix}
\begin{bmatrix}
  D & 0 \\
  0 & Y
\end{bmatrix}
\begin{bmatrix}
  I & Z \\
  0 & I
\end{bmatrix}
\]  

for some matrices \( X \), \( Y \), and \( Z \). Specify \( X \), \( Y \), and \( Z \).

(e) [Optional:] Observe that the formula (1) is not ideal for inverting a block separable matrix. The reason is that neither \( \tilde{A} \) nor \((I + \tilde{A}V^*D^{-1}U)^{-1}\) is block diagonal, so multiplying them together would be costly. In class, we instead used
\[
A^{-1} = G + E(\hat{D} + \tilde{A})^{-1}F^*,
\]  

where
\[
\hat{D} = (V^*D^{-1}U)^{-1},
\]
\[
E = D^{-1}UD,
\]
\[
F = (\hat{D}V^*D^{-1})^*,
\]
\[
G = D^{-1} - D^{-1}UDV^*D^{-1}.
\]

For (4) to hold, we need to assume that \( V^*D^{-1}U \) is non-singular. Observe that \( \hat{D} \), \( E \), \( F \), and \( G \) are all block diagonal. Prove (4). Hint: Huge bonus points if someone can think of a clean and elegant proof. I do not particularly like any that I have thought of, personally.

Note: Be on high alert for typos in this problem!!!