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 Ω_τ and Ω_σ be two well-separated boxes with centers $\boldsymbol{c}_\tau$ and $\boldsymbol{c}_\sigma$. Let $\boldsymbol{y} \in \Omega_\sigma$ be a source point and let $\boldsymbol{x} \in \Omega_\tau$ be a target point. Consider the error function

$$e(P) = \sup\left\{\left|\log|\boldsymbol{x}-\boldsymbol{y}| - \mathbf{B}_P(\boldsymbol{x},\,\boldsymbol{c}_\tau)\,\mathbf{Z}_P(\boldsymbol{c}_\tau,\,\boldsymbol{c}_\sigma)\,\mathbf{C}_P(\boldsymbol{c}_\sigma,\,\boldsymbol{y})\right| \,:\, \boldsymbol{y}\in\Omega_\sigma\ \boldsymbol{x}\in\Omega_\tau\right\}$$

where P is the length of the multipole expansion, and where

$\mathbf{C}_P(\boldsymbol{c}_\sigma,\,\boldsymbol{y}) \in \mathbb{C}^{P\times 1}$	maps a source to an outgoing expansion
$\mathbf{Z}_P(\boldsymbol{c}_\tau,\,\boldsymbol{c}_\sigma) \in \mathbb{C}^{P\times P}$	maps an outgoing expansion to an incoming expansion
$\mathbf{B}_P(\boldsymbol{x},\,\boldsymbol{c}_\tau) \in \mathbb{C}^{1\times P}$	maps an incoming expansion to a target

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

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

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

(c) Is the supremum for a given P attained for any specific pair $\{\boldsymbol{x},\,\boldsymbol{y}\}$?
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 $\mathbf{T}^{(\text{ofo})}$, $\mathbf{T}^{(\text{ifo})}$, and $\mathbf{T}^{(\text{ifi})}$ (i.e. set `flag_precomp=0`).

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

$$N_{\text{tot}} = 1\,000,\ 2\,000,\ 4\,000,\ 8\,000,\ 16\,000,\ 32\,000,\ 64\,000.$$

Set `nmax=50`. Provide plots that track the following costs:

t_{tot}	total execution time, including initialization.
t_{init}	cost of initialization (computing the tree, the object `T_OPS`, etc.).
t_{ofs}	cost of applying $\mathbf{T}^{(\text{ofs})}$.
t_{ofo}	cost of applying $\mathbf{T}^{(\text{ofo})}$.
t_{ifo}	cost of applying $\mathbf{T}^{(\text{ifo})}$.
t_{ifi}	cost of applying $\mathbf{T}^{(\text{ifi})}$.
t_{tfi}	cost of applying $\mathbf{T}^{(\text{tfi})}$.
t_{close}	cost of directly evaluating close range interactions.

(b) Repeat exercise (a) but now for a few different choices of `nmax`. 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 $N_{\rm tot}$ of charges. Create a plot of the best possible time $t_{\rm optimal}$ for several $N_{\rm tot}$ and estimate the dependence of $t_{\rm optimal}$ on $N_{\rm tot}$. 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 $k < n$, $\mathbf{A}$ is an $N \times N$ invertible matrix, and $\mathbf{B} = \mathbf{A}^{-1}$. Let us further assume that every diagonal block of $\mathbf{A}$ is invertible.

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

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}, \qquad \text{and} \qquad \mathbf{B} = \begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix},$$

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

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

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

where each block is of size $n \times n$. Suppose further that $\mathbf{A}_{12}$, $\mathbf{A}_{21}$, $\mathbf{A}_{34}$, $\mathbf{A}_{43}$, $\begin{bmatrix} \mathbf{A}_{13} & \mathbf{A}_{14} \\ \mathbf{A}_{23} & \mathbf{A}_{24} \end{bmatrix}$, and $\begin{bmatrix} \mathbf{A}_{31} & \mathbf{A}_{32} \\ \mathbf{A}_{41} & \mathbf{A}_{42} \end{bmatrix}$ all have rank k. What is the highest possible value for the rank of $\mathbf{B}_{12}$?

(c) *[Optional:]* Consider the natural generalization to a matrix consisting of 8×8 blocks. What is the maximal rank of $\mathbf{B}_{12}$? 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 $\mathbf{D} \in \mathbb{R}^{n\times n}$, $\mathbf{U} \in \mathbb{R}^{n\times k}$, $\mathbf{V} \in \mathbb{R}^{n\times k}$, and $\tilde{\mathbf{A}} \in \mathbb{R}^{k\times k}$.

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

$$\mathbf{A}^{-1} = \mathbf{I} - \mathbf{U}\big(\mathbf{I} + \mathbf{V}^*\mathbf{U}\big)^{-1}\mathbf{V}^*.$$

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

$$\mathbf{A}^{-1} = \mathbf{D}^{-1} - \mathbf{D}^{-1}\mathbf{U}\big(\mathbf{I} + \tilde{\mathbf{A}}\mathbf{V}^*\mathbf{D}^{-1}\mathbf{U}\big)^{-1}\tilde{\mathbf{A}}\mathbf{V}^*\mathbf{D}^{-1}. \tag{1}$$

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

(c) As in (b), set $\mathbf{A} = \mathbf{D} + \mathbf{U}\tilde{\mathbf{A}}\mathbf{V}^*$, and assume that $\mathbf{D}$ and $\mathbf{I} + \tilde{\mathbf{A}}\mathbf{V}^*\mathbf{D}^{-1}\mathbf{U}$ are both invertible. Consider the linear system

$$\begin{bmatrix} \mathbf{D} & \mathbf{U}\tilde{\mathbf{A}} \\ -\mathbf{V}^* & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \tilde{\mathbf{x}} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}. \tag{2}$$

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

(d) Assume again that $\mathbf{D}$ is invertible. You can then perform one step of a block LDU factorization to obtain the equality

$$\begin{bmatrix} \mathbf{D} & \mathbf{U}\tilde{\mathbf{A}} \\ -\mathbf{V}^* & \mathbf{I} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{X} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{Y} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{Z} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \tag{3}$$

for some matrices $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$. Specify $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$

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

$$\mathbf{A}^{-1} = \mathbf{G} + \mathbf{E}\big(\hat{\mathbf{D}} + \tilde{\mathbf{A}}\big)^{-1}\mathbf{F}^*, \tag{4}$$

where

$$\begin{aligned} \hat{\mathbf{D}} &= \big(\mathbf{V}^*\mathbf{D}^{-1}\mathbf{U}\big)^{-1}, \\ \mathbf{E} &= \mathbf{D}^{-1}\mathbf{U}\hat{\mathbf{D}}, \\ \mathbf{F} &= (\hat{\mathbf{D}}\mathbf{V}^*\mathbf{D}^{-1})^*, \\ \mathbf{G} &= \mathbf{D}^{-1} - \mathbf{D}^{-1}\mathbf{U}\hat{\mathbf{D}}\mathbf{V}^*\mathbf{D}^{-1}. \end{aligned}$$

For (4) to hold, we need to assume that $\mathbf{V}^*\mathbf{D}^{-1}\mathbf{U}$ is non-singular. Observe that $\hat{\mathbf{D}}$, $\mathbf{E}$, $\mathbf{F}$, and $\mathbf{G}$ 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!!!