FA22 Algorithms for Bioinformatics, EN.605.620

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Strassen's Method versus Brute Force Multiplication - An Analysis

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1. **Introduction**
   As part of Programming Project 1, an analysis of results obtained through comparison of two related algorithms is presented. The first algorithm is a 'naive' or 'brute force' implementation for calculating the product of two square matrices. The second algorithm represents an enhancement to the first and is known as Strassen's algorithm.

2. **Description and Justification**
   Strassen's algorithm (named for Volker Strassen) is a well-known improvement to a 'naive' solution for matrix multiplication. While it is faster than the standard matrix multiplication algorithm for larger matrices, the 'naive' equivalent is often better suited for smaller matrices.[1]

   An important caveat regarding application of Strassen is that the input matrices must be square and their order must be a power of two. These restrictions allow for the matrices to be split recursively into halfs until a base case is reached.

   (a) **Data Structures**
   I have used standard Python data structures such as lists and dictionaries throughout my implementation. One advantage of Python in this context has been the use of list comprehensions for populating and iterating over a 2-dimensional data structure such as a matrix.

   (b) **Implementation**
   I tried to follow sound developmental practices in designing my code. In part, this meant separating out functionality into independent modules. I also make use of Python's notebook functionality to allow recreation of my plots using Google Colab. My implementation of Strassen's may be run as a separate script, to test it.

[1] See: "Strassen Algorithm". In Wikipedia, June 13, 2022.

i. Language
I was granted permission to implement this solution in Python.

ii. Modular Design
The module 'algorithms' implements Strassen's and the standard algorithm; 'analysis' contains a Python notebook for plots; 'data' holds the input data and facility to create new matrices; 'filehandler' handles file input and output.

3. **Efficiency**
We refer to matrix **order** when speaking of runtime efficiency related to a size of n. A 2-row by 2-column matrix has an order of 2 ($n = 4$) while a 256x256 has an order of 256. For the naive algorithm, the triple-nested **for** loop is inefficient as the matrix order grows larger. Consider the following where we assume we have input matrices A (n x m), B (m x p) of equal order, and a third empty matrix C (n x p) of appropriate size, then the 'naive' algorithm is:

```
1.    For i from 1 to n:
2.      For j from 1 to p:
3.        Let sum = 0
4.        For k from 1 to m:
5.          Set sum ← sum + A[i,k] × B[k,j]
6.          Set C[i,j] ← sum
7.    Return C
```

(a) Time Complexity
For the naive algorithm the time complexity relates to it's three nested loops (Lines 1,2,4). Each runs n times and does $O(1)$ work at each iteration, thus the complexity is $n * n * n * O(1) = O(n^3) * O(1) = O(n^3)$. Strassen does better, achieving subcubic time. The algorithm makes 7 recursive calls along with several additions and subtractions that together take cn^2 time. If we let $f(n)$ be the number of operations for a 2^nx2^n matrix then $f(n) = 7f(n-1) + l4^2$ where l depends on the number of additions and subtractions. We obtain the recurrence $T(n) \leq 7T(n/2) + cn^2$ where $T(1) = 1$. Strassen's runtime is $O(n^{2.8})$.

(b) Space Complexity
For Strassen, we start with $3n^2$ space required for the (2) input and (1) output matrices then must allocate $3(n/2)^2$ space for recursive calls. Both the naive and Strassen algorithms are on the order of n^2 space complexity. However, Strassen may require significantly more memory compared to the naive algorithm.

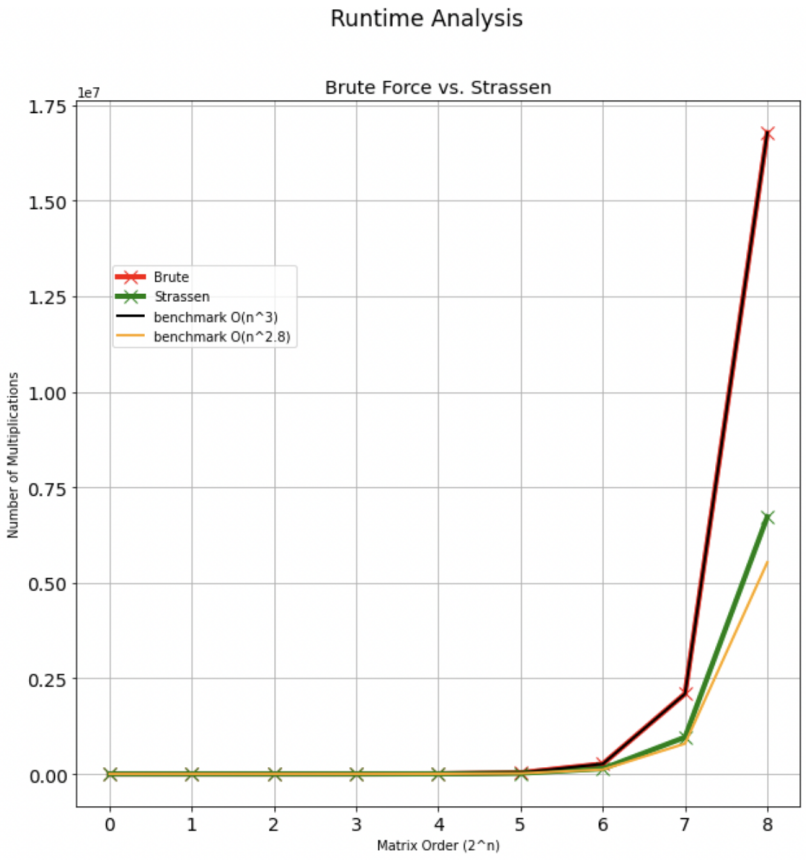
4. **Asymptotic Observation**
Table 1 and the plot that follows it (next page) show the relative performance of my implementations of the naive versus Strassen's algorithm. I gathered data were each square matrix's order was a power of two. Note that where $n = 0$ each matrix has a single element (the base case).

Where the matrix order grows to 256 ($n = 8$) the difference in the number of multiplications required for the naive algorithm is 2.5 times that of Strassen's.

In the plot below Table 1 are four different colored lines. The red is the naive or 'brute force' algorithm; the green is my Strassen's; the black is a benchmark function for n^3; and the yellow is a benchmark for the function $n^{2.8}$.

Matrix Order 2^n	Naive algorithm	Strassens's algorithm
1	1	0
2	8	7
4	64	56
8	512	399
16	4,096	2800
32	32,768	19,607
64	262,144	137,256
128	2,097,152	960,799
256	16,777,216	6,725,600

Table 1: Number of multiplications required in Naive versus Strassen algorithms.



Note that the black and red lines are exactly the same (one covers the other) meaning that the naive algorithm precisely mimics the benchmark function. For Strassen's algorithm the results diverge, with the benchmark $f(n^{2.8})$ (in yellow) rising slower compared with my implementation of the algorithm (in green).

5. **Observation versus Theory**
   It's not a surprise that the naive implementation performs exactly as one would expect relative the the benchmark. Whatever other runtime costs are associated with my implementation, the cubic component entirely obscures these. Both cubic and the less-than-cubic functions seem to do about the same until the order of the matrices reaches 64 ($n = 6$). At $n = 7$ my implementation's performance begins to rise relative to the benchmark. Two factors may account for this: 1) the benchmark function is rounded to a power of 2.8 where in reality it is slighty large than this; and 2) I am only counting multiplications, not additional costs of additions and subtractions.

6. **Lessons Learned**
   This was a challenging exercise that made me wonder how much more challenging will subsequent ones be as the semester progresses! I struggled with my implementation of Strassen's algorithm and ultimately relied on research done on Stack Overflow. This is noted in the code. I learned much about how to use the Python's command-line parser **argparse**. This is a valuable skill to have when developing command line applications for bioinformatics.

7. **Applicability to Bioinformatics**
   In general, bioinformatics applications are replete with examples where matrices are a key data structure: from differential expression (RNA-Seq) experiments to integrative 'omics' studies, to basic theoretical work on genetic control. As an example, expression quantitative trait loci (eQTL) analysis links variations in gene expression levels to genotypes. eQTL analysis is a computationally intensive task that generates large datasets; testing for association of billions of transcript-SNP (single-nucleotide polymorphism) pairs is a standard practice. Such pairs can be represented as large matrices and thus manipulating these structures efficiently is central to the task. [1]

   Independent Component Analysis (ICA) is another example, where matrix factorization methods are used for data dimension reduction. [2]

   The application of ICA (Independent Component Analysis) to multiple gene expression datasets has uncovered important insights about cancer biology. In such studies, large ICA-based meta-analyses of transcriptomic data are defined by sets of meta-genes that are associated with universal factors of cancer types. ICA application to transcriptomics data relies heavily on fast and efficient matrix manipulations.

References

[1] Andrey A. Shabalin. Matrix eqtl: Ultra fast eqtl analysis via large matrix operations. *Bioinformatics*, 28(10), 2012.

[2] Jane Merlevede Askhat Molkenov Ainur Seisenova Altynbek Zhubanchaliyev Petr V Nazarov Emmanuel Barillot Ulykbek Kairov Captier, Nicolas and Andrei Zinovyev. Biodica: A computational environment for independent component analysis of omics data. *Bioinformatics*, 38(10), 2022.