

# CS 3824

## Homework Assignment 3

**Given:** February 17, 2010

**Due:** February 23, 2010

**General directions.** The point value of each problem is shown in [ ]. Each solution must include all details and an explanation of why the given solution is correct. In particular, write complete sentences. A correct answer without an explanation is worth no credit. The completed assignment must be placed inside the box labeled “CS 3824” outside 2160J Torgersen by 4:00 PM EST on February 23, 2010. **No late homework will be accepted.**

**Digital preparation of your solutions is mandatory.** Use of  $\LaTeX$  is optional, but encouraged. No matter how you prepare your homework, **please include your name.**

**Use of  $\LaTeX$  (optional, but encouraged).**

- Retrieve this  $\LaTeX$  source file, named `homework3.tex`, from the course web site.
  - Rename the file `<Your VT PID>_solvehw3.tex`, For example, for the instructor, the file name would be `heath_solvehw3.tex`.
  - Use a **text editor** (such as `vi`, `emacs`, or `pico`) to accomplish the next three steps.
  - Uncomment the line  

```
% \setboolean{solutions}{True}
```

in the document preamble by deleting the %.
  - Find the line  

```
\renewcommand{\author}{Lenwood S. Heath}
```

and replace the instructor’s name with your name.
  - Enter your solutions where you find the  $\LaTeX$  comments  

```
% PUT YOUR SOLUTION HERE
```
  - Print out and submit your solutions by 4:00 PM on February 23, 2010.
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For a protein with  $n$  residues, you can define its residue-residue “contact map”, which is simply an  $n \times n$  matrix  $A = (a_{ij})$  such that  $a_{ij} = 1$  if residues (amino acids)  $i$  and  $j$  touch each other and 0, otherwise. Naturally, you assume that amino acids are labeled sequentially in the polypeptide chain.

[15] 1. Is it likely for a functional enzyme protein in its working state to have  $A = (a_{ij})$  such that  $a_{ij} = 1$  if and only if  $|i - j| = 0$  or 1? Explain.

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[25] 2. A  $100 \times 100$  matrix  $A = (a_{ij})$  is defined as  $a_{ij} = 1$  if  $|i - j| < 6$  OR if  $i = 25$ ;  $a_{ij} = 0$ , otherwise. Can this be the contact matrix (map) of a real protein? Explain.

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**NOTE:** No rigorous proofs required, just good logic.

If you want to know more about contact maps and are curious about what a contact map of a real protein from the protein data-bank (PDB) site<sup>1</sup> might look like, you may download the Macromolecular Contact tool<sup>2</sup> and play with it. It is Java-based, and should be pretty much plug-and-play. However, this is absolutely not necessary to correctly answer the questions above.

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<sup>1</sup><http://www.rcsb.org/>

<sup>2</sup><http://people.cs.vt.edu/~onufriev/software.php>