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1. Compute the following matrix multiplications:

   a)

   $$\begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 2 & 3 \end{bmatrix} \tag{1}$$

   b)

   $$\begin{bmatrix} -1 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 1 & -1 \end{bmatrix} \tag{2}$$

   c) Write an equation for matrix multiplication using summation notation

   a)

   $$\begin{bmatrix} 4 & 5 \\ 1 & 1 \end{bmatrix} \tag{3}$$

   b)

   $$\begin{bmatrix} 1 & -3 \\ 2 & -2 \end{bmatrix} \tag{4}$$

   c) $(\mathbf{AB})_{ij} = \sum_k A_{ik} B_{kj}$

.

2. Determine if the following matrices commute:

   $$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 3 \\ 3 & 2 \end{bmatrix} \tag{5}$$

   $$\mathbf{AB} = \begin{bmatrix} 3 & 2 \\ 2 & 3 \end{bmatrix} \tag{6}$$

   $$\mathbf{BA} = \begin{bmatrix} 3 & 2 \\ 2 & 3 \end{bmatrix} \tag{7}$$

   Therefore, as $\mathbf{AB} = \mathbf{BA}$ the matrices commute.

3. Determine the inverse of the following matrices:

   a)

   $$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \tag{8}$$

b)

$$\begin{bmatrix} 0 & 1 \\ 1 & 2 \end{bmatrix} \tag{9}$$

a)

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}^{-1} = \frac{1}{1 \times 1 - 0 \times 1} \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}^T = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \tag{10}$$

b)

$$\begin{bmatrix} 0 & 1 \\ 1 & 2 \end{bmatrix}^{-1} = \frac{1}{0 \times 2 - 1 \times 1} \begin{bmatrix} 2 & -1 \\ -1 & 0 \end{bmatrix}^T = \begin{bmatrix} -2 & 1 \\ 1 & 0 \end{bmatrix} \tag{11}$$

.

4. Write an analytic form for the eigenvalues of a 2×2 matrix.

$$\begin{vmatrix} a - \lambda & b \\ c & d - \lambda \end{vmatrix} = (a - \lambda)(d - \lambda) - bc = 0 \tag{12}$$

$$\lambda^2 - \lambda(a + d) + (ad - bc) = 0 \tag{13}$$

$$\lambda = \frac{(a + d) \pm \sqrt{(-a - d)^2 - 4(ad - bc)}}{2} \tag{14}$$

$$\lambda = \frac{(a + d)}{2} \pm \frac{\sqrt{(a - d)^2 + 4bc}}{2} \tag{15}$$

5. Show that the eigenvalues of a Hermitian matrix are real.

$$\mathbf{A} = \mathbf{A}^\dagger \tag{16}$$

$$\langle i|\hat{A}|j\rangle = \langle j|\hat{A}|i\rangle^* \tag{17}$$

$$\langle i|\hat{A}|i\rangle = \langle i|\hat{A}|i\rangle^* \tag{18}$$

$$\langle i|a_i|i\rangle = \langle i|a_i^*|i\rangle \tag{19}$$

$$a_i\langle i|i\rangle = a_i^*\langle i|i\rangle \tag{20}$$

$$(a_i - a_i^*)\langle i|i\rangle = 0 \tag{21}$$

$$a_i = a_i^* \tag{22}$$

6. First we will use github to obtain a computational library (MQCPack) designed to facilitate the coding of computational methodologies:

1. Log into your account on the CRC that you set up last week and type "cd .ssh".

2. Type "ls" and if you do not have a file named "id_rsa.pub" type "ssh-keygen" and follow the instructions (empty an empty password).

3. Type "cat id_rsa.pub" and copy the output to the clipboard.

4. Go to www.github.com and make an account using "sign up".

5. Click on your user icon in the top right-hand corner and then select "settings" from the drop-down menu.

6. Click "SSH and GPG keys" on the left-hand side and then "New SSH key".

7. Type "CRC" in the title box and the information that you copied into the key box.

8. Go to "https://github.com/thompsonresearchgroup/mqcPack" and click "Fork" in the top right corner.

9. Click the green button that says "Code" and copy the url in the box (the ssh version) . You will need to paste the url later.

Now we will install MQCPack on your user account on the CRC:

1. In your home directory, type "mkdir gauopen" and then cd gauopen". Type "wget http://gaussian.com/g16/gauopen_v2.zip" and then type "unzip gauopen_v2.zip". Once everthing is unzipped, go back to your home directory "cd ".

2. Type "git clone <url copied from github>" where the url is the same as you copied previously.

3. Type "qsub -I -q dev -l nodes=1:ppn=1,walltime=24:00:00" and wait to log into an interactive node

4. Type "cd mqcPack" and then "module load gcc/9.2.0". Then type "./mqc_install". If you have an error "permission denied", type "chmod 755 mqc_install". The install script will ask several questions:

   (a) Do you want to use and test the MatrixFile interface to MQCPack? [y or n]: – Type "y"

   (b) Please select a compiler. – Type "G"

   (c) Please enter the desired Installation Directory – Type "/home/**change-this-text-your-crc-username**/mqc_install"

   (d) Please enter how you would link BLAS – Type "-lblas"

   (e) Please enter how you would link LAPACK – Type "-llapack"

   (f) Enter the path to the gauopen directory – Type "/home/**change-this-text-your-crc-username**/gauopen"

   (g) Do you want to execute the tests that run Gaussian calculations? [y or n]: – Type "n"

5. Back in your home directory (type "cd ") type "mkdir .vim" then "mkdir .vim/ftplugin" then "cd .vim/ftplugin" then "vi fortran.vim". When vi opens press the "i" key and an insert indicator should appear at the bottom of the page. Copy the lines in the box below and then use Ctrl-v to paste. Once you have pasted the lines, press "Esc" and then type"wq" to write the modifications to the file and quit.

```
let s:extfname = expand("%:e")
if s:extfname ==? "f90"
let fortran_free_source=1
unlet! fortran_fixed_source
elseif s:extfname ==? "f03"
let fortran_free_source=1
unlet! fortran_fixed_source
else
let fortran_fixed_source=1
unlet! fortran_free_source
endif

let fortran_do_enddo=1

" Turn on line numbers and row/column numbers.
setlocal nu
setlocal ruler

" Make vim echo commands as they are being entered.
setlocal showcmd

" Set tabstops to two spaces and ensure tab characters are expanded into spaces.
setlocal smarttab
setlocal expandtab
setlocal smartindent
setlocal autoindent
setlocal tabstop=2
setlocal shiftwidth=2

" Fix backspace key.
setlocal bs=2

setlocal ignorecase
```