

Due Wednesday November 18th, 2020.

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## 1. The unix/linux command line

- (a) Explain what the following commands do. (Hint: look up ‘piping’.)
- (i) `ps -f | grep firef`
  - (ii) `grep includegraphics manuscript.tex | wc`
- (b) You can look at file permissions using “ls -l”. You find out that one of your files has permissions

```
rwxr-xr--
```

Explain what this means.

- (c) What command would I use to change permissions on a file so that only I can read it?

## 2. Newton’s method for finding a minimum

- (a) Consider the single-variable function

$$f(x) = 1 + x^{4/3}$$

which has a single minimum at  $x = 0$ . Write down the iteration equation for Newton’ method.

The iterations do not converge. By sketching the derivative  $f'(x)$ , explain graphically why.

- (b) We want to find the location of the minimum of the function of 2 variables

$$f(x, y) = x^2 + xy + y^2 + 3x$$

using Newton’s method. Set up the iteration equations. You will have to invert a  $2 \times 2$  matrix.

Because the function is quadratic, the iteration should converge in a single step. Starting from any initial point (you can choose), show that the iteration converges in a single step.

- (c) I have a multidimensional minimization problem and calculating the inverse of the Hessian ( $\mathbb{H}^{-1}$ ) is too hard for me. As a very crude approximation, I replace  $\mathbb{H}^{-1}$  by  $\lambda\mathbb{I}$ , where  $\lambda$  is a small number and  $\mathbb{I}$  is the unit matrix. The resulting algorithm is then equivalent to a widely used algorithm. Which one?

### 3. Statistical Mechanics

*Note:* Some of the following is worked out in the student projects linked to on the webpage, under “Ising model”.

Remember  $Z = \sum_{\alpha} e^{-\beta E_{\alpha}}$ , where  $E_{\alpha}$  is the energy of the configuration  $\alpha$ . At thermal equilibrium, each configuration appears with probability  $P_{\alpha} = \frac{1}{Z} e^{-\beta E_{\alpha}}$ .

- (a) Show that the system energy and its square has expectation values

$$\langle E \rangle = \frac{1}{Z} \frac{\partial Z}{\partial \beta} = \frac{\partial}{\partial \beta} \ln Z \quad \text{and} \quad \langle E^2 \rangle = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2}$$

- (b) Hence show that the specific heat

$$C_v = \frac{\partial \langle E \rangle}{\partial T}$$

can be written as  $C_v = \beta^2 (\langle E^2 \rangle - \langle E \rangle^2)$ . I am probably setting the Boltzmann constant to unity here.

- (c) Perform the corresponding derivation for the magnetic susceptibility. You might have to remember that the configuration energy contains a term  $-BM_{\alpha}$ , where  $B$  is the magnetic field (often written as  $H$ ) and  $M_{\alpha}$  is the total magnetization of configuration  $\alpha$ .