UCSB, Physics 129AL, Computational Physics: Problem Set 3

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GitHub Submission Guideline

We will use GitHub for problem set submissions. By the due date, you should have a single public repository on GitHub containing all the work you have done for this problem set. Finally, upload a screenshot or a .txt file to Canvas with your GitHub username and repository name so the TA knows who you are and which repository you are using for the problem set.

Remember: talk to your fellow students, work together, and use GPTs. You will find it much easier than working alone. Good luck! All work should be done in the Docker container, and don't forget to commit it to Git!

Question 1: Normal Distribution (Gaussian)

Normal distribution (Gaussian) is one of the most important distributions in physics. The normal distribution is given by,

$$p(\mu, \sigma) \sim \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right), \tag{1}$$

where μ, σ are the mean and standard deviation. The one-dimensional integral is given by the following,

$$\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right) dx = \sqrt{\frac{2\pi}{\sigma^2}}. \tag{2}$$

Let's consider the N-dimensional integral,

$$I = \int_{-\infty}^{\infty} d\mathbf{v} \exp\left(-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v} + \mathbf{v}^T\mathbf{w}\right) = \sqrt{(2\pi)^N \det\left(\mathbf{A}^{-1}\right)} \exp\left(\mathbf{w}^T\mathbf{A}^{-1}\mathbf{w}\right), \tag{3}$$

where $\mathbf{v} = (v_1, v_2, \ldots, v_N)$ and $\mathbf{w} = (w_1, w_2, \ldots, w_N)$ are N-dimensional vectors, and $\mathbf{A}$ is the symmetric positive-definite $(N \times N)$ matrix with components A_{ij}.

a) Numerical Verification

Write a Python function that numerically verify the following expression with an input matrix and two input vectors, A, w,

$$I = \int_{-\infty}^{\infty} (D\mathbf{v}) \exp\left(-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v} + \mathbf{v}^T\mathbf{w}\right) = \sqrt{(2\pi)^N \det(\mathbf{A}^{-1})} \exp\left(\frac{1}{2}\mathbf{w}^T\mathbf{A}^{-1}\mathbf{w}\right), \tag{4}$$

by calculating the integral on the left hand side, and the closed-form expression on the right hand side. Hint: In components, the above expression becomes,

$$I = \int_{-\infty}^{\infty} \left(\prod_{i=1}^{N} dv_i\right) \exp\left(-\frac{1}{2}\sum_{i,j=1}^{N} v_i A_{ij} v_j + \sum_{i=1}^{N} v_i w_i\right), \tag{5}$$

The above equation can be expressed in an index form,

$$I = \sqrt{(2\pi)^N \det(\mathbf{A}^{-1})} \exp\left(\frac{1}{2}\sum_{i,j=1}^{N} w_i A^{-1}_{ij} w_j\right). \tag{6}$$

Now, preform the integral on the left hand side and verify against the closed-expression on the right hand side.

Hint: One way to do this is using the following Scipy function from scipy.integrate module, e.g. *integral_value, _ = nquad(integrand, [(-np.inf, np.inf)] * N)*. It will calculate the muti-dimensional integral with respect to a given integrand. We will be looking at numerical quadrature techniques soon.

b) Test run

Use your Python function to verify the following two matrices A, A',

$$A = \begin{pmatrix} 4 & 2 & 1 \\ 2 & 5 & 3 \\ 1 & 3 & 6 \end{pmatrix}, \quad A' = \begin{pmatrix} 4 & 2 & 1 \\ 2 & 1 & 3 \\ 1 & 3 & 6 \end{pmatrix}, \quad \mathbf{w} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

Do you notice any difference between A and A'?

c) Correlation function and Moments of a multivariate normal distribution

What you just saw in the above is called multivariate normal distribution. Let's consider the general moment definition,

$$\langle v_1^{p_1} v_2^{p_2} \cdots v_N^{p_N} \rangle = \int_{-\infty}^{\infty} \prod_{i=1}^{N} dv_i \, v_1^{p_1} v_2^{p_2} \cdots v_N^{p_N} \exp\left(-\frac{1}{2}\sum_{i,j=1}^{N} v_i A_{ij} v_j + \sum_{i=1}^{N} v_i w_i\right),$$

where $p_i \in Z^+$ is the power at i. Use the following $A, \mathbf{x}$,

$$A = \begin{pmatrix} 4 & 2 & 1 \\ 2 & 5 & 3 \\ 1 & 3 & 6 \end{pmatrix}, \qquad \mathbf{w} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

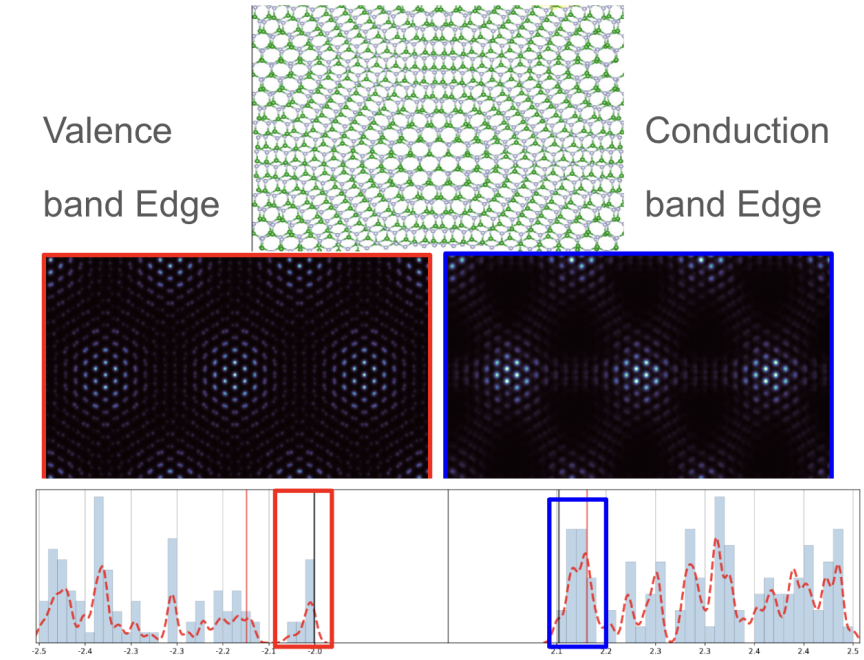
, numerically calculate the following moments and find a closed form for each expression,

- $\langle v_1 \rangle, \langle v_2 \rangle, \langle v_3 \rangle$,
- $\langle v_1 v_2 \rangle, \langle v_2 v_3 \rangle, \langle v_1 v_3 \rangle$,
- $\langle v_1^2 v_2 \rangle, \langle v_2 v_3^2 \rangle$,
- $\langle v_1^2 v_2^2 \rangle, \langle v_2^2 v_3^2 \rangle$.

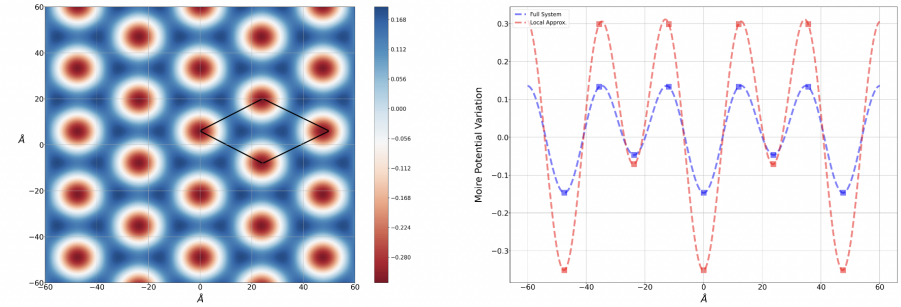
Express those closed-forms in terms of $A, \mathbf{w}$, and verify with numerically.

Question 2: Local Density of States for Electrons

The Local Density of States (LDOS), in the context of electronic structure and solid-state physics, is a fundamental concept used to describe the density of available electronic states for electrons at a specific position in a material or a solid. It is a crucial quantity in understanding the electronic properties of materials, particularly in the study of electronic band structures, energy levels, and electron behavior. In this problem, you will be looking at the local density of states for a material near the conduction and valance band edge. The files and figures provided below are the world first large-scale many-body ab initio calculations on a 2D-Moire system using density functional theory beyond local approximations.



We want to establish a physical model that describes the localization of electrons in a material. For example, the local density of states mentioned above can be understood as a measure of potential energy strength (Figure below).



Each file inside the directory 'Local_density_of_states_near_band_edge' contains the local density of states of a 2-dimensional material at a specific energy level. You want to understand the correlation between energies and the patterns of local density of states.

a)

For each text file in the directory, generate a 2-dimensional heatmap depicting the local electron density. Include a color legend to indicate the intensity. Label each heatmap with the same file index and save the images in a your own directory named 'local_density_of_states_heatmap' within 'Local_density_of_states_near_band_edge'.

b)

For each text file in the directory, create a 2-dimensional surface plot where the height profile represents the local density of states. Label each height profile with the same file index and save the image in a new directory named 'local_density_of_states_height' within 'Local_density_of_states_near_band_edge'.

c)

Select a local sub-region and quantitatively illustrate the changes while offering some physical speculations. For instance, the basic analysis you should present involves calculating the average local density of states within a predefined subregion for each file and plotting these changes across all indices. Feel free to explore different analyses, but ensure that their complexity is comparable to the example provided above.