Exercise Sheet 10

Due: 02.07.24 14h00

Fred Hamprecht
Christof Gehrig, Gerrit Gerhartz

General Regulations.

- Please hand in your solutions in groups of up to two people.
- Your solutions to theoretical exercises can be either handwritten notes (scanned), or typeset using LaTeX. In case you hand in handwritten notes, please make sure that they are legible and not too blurred or low resolution.
- For the practical exercises, always provide the (commented) code as well as the output, and don't forget to explain/interpret the latter. Please hand in an exported PDF of your notebook.
- Submit all your files in the Übungsgruppenverwaltung, only once for your group.

0 Evaluation

If you haven't already, please evaluate the lecture via `https://uni-heidelberg.evasys.de/evasys/online.php?pswd=HG8WV`.

1 Paper reading

- KineticNet [1]: You already finished this paper last week.
- M-OFDFT [2]: Please read the subsection "Geometric invariance" in "Methods" and appendix A.3.

Please compare how the machine learning models of KineticNet and M-OFDFT guarantee equivariance. (3 pts)

2 Representation theory

(a) Give the definition of a representation. What are irreducible representations? (2 pts)

(b) A matrix A transforms as RAR^{-1} under a rotation R. Decompose A into irreducible representations of the rotation group. (3 pts)

(c) Given a function $f\colon \mathcal{X} \to \mathcal{Y}$ and two representations $\rho_{\mathcal{X}}$ and $\rho_{\mathcal{Y}}$, the condition for the equivariance of f is

$$f(\rho_{\mathcal{X}}(g)x) = \rho_{\mathcal{Y}}(g)f(x) \quad \forall g \in G, x \in \mathcal{X}.$$

Why does it make sense to look at irreducible representations? (2 pts)

3 Tensor product

In this exercise, we want to use the package `e3nn` to investigate the irreducible representations of rotations.

(a) Write down the tensor product of an l_1-tensor and an l_2-tensor in components. Which l-values are allowed in the result? (2 pts)

(b) The package `e3nn` uses the class `e3nn.o3.Irreps` to represent irreducible representations. Create a tensor product of ten scalars and five vectors with `0e+1o+2e` irreps. Visualize the tensor product with the `visualize` method. Use the `FullyConnectedTensorProduct` to obtain 20 scalars and ten vectors. Explain how you can calculate the number of weights in this product. (4 pts)

(c) Compute spherical harmonics up to order five and check the equivariance. You can generate a random rotation matrix and use the Wigner D-matrix with the method `D_from_matrix`. (2 pts)

(d) Compute the Wigner D-matrix for the irreps `5x0e+3x1o+2x2e` for a random rotation and plot it. Explain the structure you observe. (2 pts)

(e) Choose a radial function with more than one zero crossing, multiply it with a spherical harmonic, and plot the resulting kernel. (**Bonus:** 3 pts)

References

[1] Roman Remme et al. "KineticNet: Deep learning a transferable kinetic energy functional for orbital-free density functional theory". In: *The Journal of Chemical Physics* 159.14 (Oct. 2023). ISSN: 0021-9606, 1089-7690. URL: https://pubs.aip.org/jcp/article/159/14/144113/2916356/KineticNet-Deep-learning-a-transferable-kinetic.

[2] He Zhang et al. "Overcoming the barrier of orbital-free density functional theory for molecular systems using deep learning". In: *Nature Computational Science* 4.3 (Mar. 2024), pp. 210–223. ISSN: 2662-8457. DOI: 10.1038/s43588-024-00605-8. URL: https://uebungen.physik.uni-heidelberg.de/c/image/d/vorlesung/20241/1883/material/zhang_24_overcoming.pdf.