GEORGIA INSTITUTE OF TECHNOLOGY
SCHOOL of ELECTRICAL and COMPUTER ENGINEERING

ECE 8803-GGDL Fall 2023
Problem Set #4

Assigned: 11 Nov
Due Date: 21 Nov

Please contact the TAs for clarification on the instructions in the homework assignments.

Problem 1: Score-based Diffusion Models (40 points). You are provided with a notebook to help you understand the core ideas behind Diffusion generative models, namely using the score to enable reversal of the diffusion process. You will work on the notebook `score-diff.ipynb`, in which part of the necessary code has already been filled out for you. Pay attention to the cells marked **YOUR CODE HERE**: these are the only cells you need to edit. For those using the PACE clusters, a conda environment has been provided for you with the necessary packages for this notebook: `hw4-p1`.

a. Setup: Run the setup cells to load the necesary libraries and utility functions.

b. Part 1: Score and diffusion.

   i. Run the cell illustrating the diffusion process. What role does lambda play in this type of process?

   ii. Run the cells corresponding to the score for Gaussian Mixtures exercise. What does the direction and magnitude of the score tell you? For a multi-modal distribution, how does the score of the individual mode relate to the overall score?

   iii. Run the cells corresponding to the reversal of the diffusion process, implementing the required functions. How well does the reverse diffusion capture the original distribution?

c. Part 2: Denoising. Implement the denoising scoe matching objective and test your implementation by running the remaining cells in the section. Recall your interpretation of the score for multi-modal distribution. How does that connect to the denoising objective? In principle, is there a way to optimize the score-matching objective to 0? Explain.

d. Part 3: Diffusion on MNIST.

   i. Implement the variance of the marginal distribution and the diffusion coefficient, and run the cells defining the network architecture. How is time modulation implemented in this model? How might the final normalization step help or harm the score learning?

   ii. Implement the loss function, train the model and visualize a few samples. Are you able to notice that the data is generated from a noise distribution?

Problem 2: Steerable CNNs (40 points). You are provided with a notebook to help you understand the core ideas behind representation and Fourier theory, leading into how these concepts are used to realize Steerable CNNs. You will work on the notebook `steerable-cnns.ipynb`, in which part of the necessary code has already been filled out for you. Pay attention to the cells marked **YOUR CODE HERE**: these are the only cells you need to edit. For those using the PACE clusters, a conda environment has been provided for you with the necessary packages for this notebook: `hw3-p2`.

a. Part 1: Representation Theory & Harmonic Analysis. Read through the section and run the corresponding cells, implementing the required Fourier transforms. What do you think happens when irreps have partially or completely redundant entries? How does this affect the resulting basis they constitute? What happens to the corresponding regular representation? *Hint: think about the case of the group of planar rotations* $SO(2)$

b. Part 2: Steerable CNNs. Read through the section and run the cells illustrating the framework of Steerable CNNs, implementing the requested model.

   - Does transforming an image with the group $G = C_4$ require any interpolation? Why or why not?
   - Is the model `equivariant_so2_model` perfectly equivariant? Why is this an expected behaviour?

c. Part 3: Build and Train Steerable CNNs. Read through and run the cells to evaluate a Steerable CNN on the MNIST dataset.

   - Is perfect invariance to $SO(2)$ achievable by any of the trained models? Which model is more stable over the rotations of the test set?
   - Are both models perfectly equivariant to rotations by multiples of $\pi/2$? Explain.

Problem 3: Sufficient condition for equivariance on graphs (10 points). Prove the conjecture regarding the equivariance of GNNs in slide 13 of lecture 21.

Problem 4: Different realization of graph neural networks (10 points). Do the exercise outlined in slide 43 of lecture 21.