A Universal Training Strategy and Resulting Universality for Machine Learning Phases
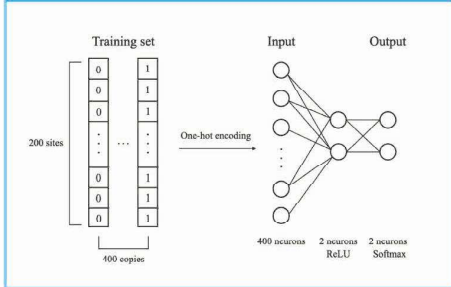
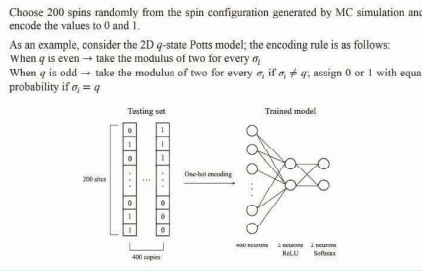國立臺灣師範大學 物理系 博士班五年級 曾元亨

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研究重點

The conventional training strategy requires substantial computing resources. It needs a large training set of observables to train a neural network (NN), and the NNs used in conventional training strategies are usually complicated. Therefore, one has to spend a considerable amount of time on training. In addition, the NN needs to be retrained if different system sizes and physical models are considered. However, our new training strategy is more efficient compared to the conventional one. The training set consists of two artificially created configurations on a one-dimensional lattice. The NN used for training has a simple structure: an input layer, a hidden layer with two neurons, and an output layer. Despite its simplicity, the NN only needs to be trained once to study the critical phenomena of various classical and quantum lattice models for different length scales. It seems like when machine learning is concerned, most phase transitions belong to a class with two elements, i.e., the Ising class.
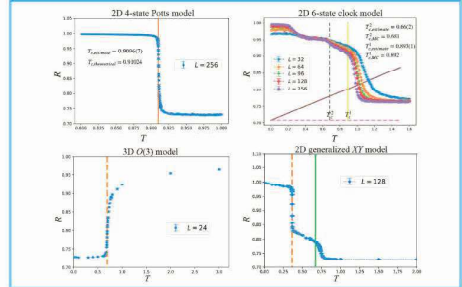
研究成果

Train the NN

Prepare the Testing Set

Choose 200 spins randomly from the spin configuration generated by MC simulation and encode the values to 0 and 1.

As an example, consider the 2D q-state Potts model; the encoding rule is as follows:
When q is even → take the modulus of two for every σ_i
When q is odd → take the modulus of two for every σ_i if $\sigma_i \neq q$; assign 0 or 1 with equal probability if $\sigma_i = q$
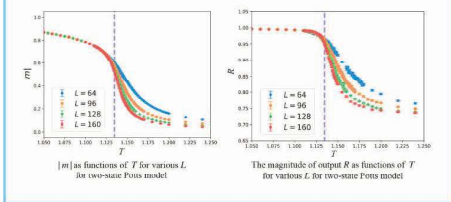

### Estimate the Critical Points

Meaning of NN's Output

The magnitude of NN's output, R, is similar to the order parameter, such as magnetization. The curves for different length scales converge to a single curve when $T < T_c$ and diverge around T_c. Finally, the curves reach their minimum value at high T.


Calculate the Critical Exponents

For a continuous phase transition, if the quantity Q is dimensionless, then a smooth data collapse curve should appear when plotting Q against $((T-T_c)/T_c)L^{1/\nu}$. By collapsing the curves for different length scales, we can determine the critical exponents.
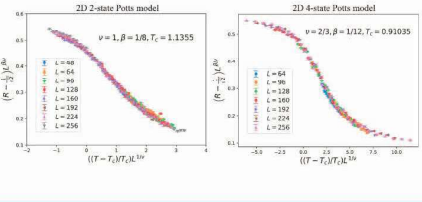
Study the Types of Transitions

The histogram of R is used to study the types of phase transitions. For a first-order phase transition, the histogram shows a distinct two-peak structure. In a first-order phase transition, the difference between the peaks and the valley increases with the system size, while in a second-order phase transition, this difference approaches a constant.
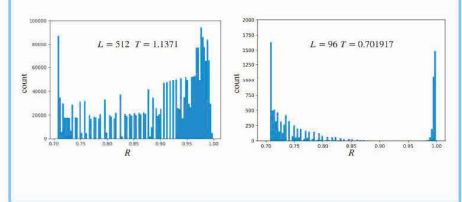
研究生活及心得

博士班是一條漫長且艱辛的道路，要從中找到方向並獲得成就感才能堅持下去。研究與生活要適當的平衡，路才能走得長遠。感謝江府峻老師的指導，讓我在自由開放的學術環境中成長，不斷讓我嘗試新的想法。感謝家人與朋友在背後的支持與鼓勵，讓我無後顧之憂地往前進。