Business Application of RBM Based Tomography in Quantum Chemistry

Group 2 (Week 1)

July 2020

1. **Explain to a layperson the technical problem you solved in this exercise.**

In this project, we leverage the use of a technique from Machine Learning in order to better simulate the behaviour of certain molecules. Traditionally, these simulations take a lot of computational resources (such as time and memory) as the molecules of interest become more complex.

Using machine learning and some past data on the behaviour of these molecules, we can 'mimic' their behaviour in a way that would take fewer computational resources than the traditional way of simulating them.

The behaviour of these molecules is observed as binary data, which is fed into training a machine learning structure known as a Restricted Boltzmann Machine (RBM). Essentially, RBMs help extrapolate and represent a probability distribution of the binary states (which is essentially how likely a particular binary state "occurs") from the original limited observations.

RBMs are neural networks and are made up of neurons.

These neurons are divided into two groups with every neuron in one group connected to every neuron in the other group (but no inter group connections). There are numbers associated with each edge and neuron. Tweaking these numbers systematically is how we train the RBMs to extrapolate the distribution.

The quality of how well RBMs mimic the original molecule behaviour depends on many factors, some of them being: How much data did we use to train it (and how good is it)? How much time did we train it? How big is the RBM (in terms of neurons, the building block of RBMs) and many more?

This does not mean that machine learning is a panacea that solves the resource intensive nature of the problem entirely. But it helps alleviate it somewhat. Nonetheless, it is a valuable tool in our arsenal for understanding chemistry and physics.

2. **Explain or provide examples of the types of real-world problems this solution can solve.**

Calculating the potential energy stored in a molecule of Hydrogen can be useful to understand how to prepare a catalyst for example, which essentially is a chemical compound that is used in a chemical synthesis in order to speed up the reaction between two or more components involved.

The H2 molecule is often used in chemical synthesis called hydrogenations (1), or reductions.

Knowing the potential energy of the H2 molecule is important in order to produce the suitable catalyst that will interact with the Hydrogen molecule and so it is necessary to understand what sort of catalyst type and what conditions are required, e.g. temperature and pressure to break the Hydrogen bonds and allow the highly reactive Hydrogen atoms to react with the chemical compound.

3. **Identify at least one potential customer for this solution - ie: a business who has this problem and would consider paying to have this problem solved**

One potential customer that can benefit from the well detailed solution at point 2 could be for instance a petrochemical company like Shell that refines oil producing from its components many other products.

In fact, the use of the solution described at point 2, is helpful from a cost and environmental perspective because the company can study a new catalyst for hydrogenation reactions mentioned earlier, that works at lower temperature, allowing for example to save energy that is required to heat up the process and with the consequence of an impact on environment and company’s cost.

- References

(1) https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Map%3A_Organic_Chemistry_(McMurry)/08%3A_Alkenes-_Reactions_and_Synthesis/8.07%3A_Reduction_of_Alkenes_-_Hydrogenation