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Polarization Measurements with Deep Learning Analysis of Nuclear Magnetic Resonance

Devin Seay,* **Ishara P. Fernando and Dustin Keller**

Department of Physics, University of Virginia, Charlottesville, Virginia, USA

E-mail: das5pzq@virginia.edu, ishara@virginia.edu, dustin@virginia.edu

Constant current continuous wave Nuclear Magnetic Resonance (NMR) has been an essential tool for polarized target experiments in Nuclear and High-energy physics. Q-meter based phase-sensitive detection can provide accurate monitoring of the polarization over the course of a scattering experiment with limitations due to some operational parameters. In this talk, we present recent studies of improved signal to noise in NMR-based Spin-1 polarization measurements as well as reliable measurements outside of the designated range of the Q-meter's operational parameters with the use of machine learning (ML). This approach will allow for real time online polarization monitoring and offline polarization data analysis for improved overall figure of merit for experiments using solid state polarized targets.

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1. Introduction

Nuclear Magnetic Resonance, or NMR, is the physical phenomenon that occurs when a constant magnetic field is applied to nuclei at resonance which is perturbed by a weak oscillating magnetic field, which causes the nuclei to respond by producing an electromagnetic signal with a frequency characteristic of the magnetic field of the nuclei. This technique allows us to access previously inaccessible energy states of target material, therefore making the separation between two energy levels more marked. In the Spinquest experiment at Fermilab, we are applying NMR techniques in our fixed-target experiment on Deuteron using Deuterated Solid Ammonia as the target material. Such techniques allow us to study the inner structure of Deuteron.

2. Methodology

The Liverpool Q-meter method is a technique that can be applied to measure Deuteron polarization in NMR. The method consists of using the Liverpool Q-meter, a device that is described in the literature in heavy detail about its application polarization [1, 2], to study Spin-1 material. In using this type of Q-meter, we are able to have a continuous wave signal to properly study the polarization of Deuterium. The Q-meter is used in tandem with a Nuclear Magnetic Resonance data acquisition system in order to plot the lineshape of Deuterium onto an oscilloscope and record data, being recorded in terms of frequency ω with respect to voltage V with a frequency range between 3 - 300 MHz. The Q-meter couples to the magnetic susceptibility of the target material. The signal passes from the Q-meter through a cable comprised of specific cable lengths that are called $\lambda/2$ lengths, where lambda is the wavelength of the target material at the Larmour frequency. The entire cable, which is made of copper, is comprised of an integer multiple of the $\lambda/2$ constant. Because the signal is sinusoidal, a precise measurement of the cable is necessary to insure that the lineshape is properly "tuned", i.e., the lineshape is symmetric and neither leaning to the left nor the right. In the case of a 5 Tesla magnetic field imposed on the material, each $\lambda/2$ cable length should be 358.0 cm. Under ideal conditions and within the Q-meter's operational parameters, we expect little relative error. However, because of the conditions set by our experiment, we wanted to develop a methodology that works outside of the Q-meter's operational parameters, with minimal systematic uncertainty in the method. Prior methods of determining Deuterium's polarization in experiments came with a relative error of approximately 4-6% [3]. The use of Neural Networks can improve the accuracy and precision of various measurements. Neural networks are capable of learning complex relationships between inputs and outputs. By incorporating neural networks into the measurement process, it is capable of facilitating a higher level of accuracy and precision compared to traditional methods. However, it is important to consider the quality and reliability of the training data and the suitability of the neural network architecture for the specific measurement task.

The Deuteron lineshape can be described by an analytical function. For the sake of brevity, the derivation and exact description will not be covered in this paper. For further information, The Spin Muon Collaboration delves deeply in the derivation of the function [4].

Training the model was performed with the Tensorflow package. We implemented a model that uses 'Adam' as an optimizer. Adam is a well-rounded optimizer that can be used in many different scenarios. The model was trained on 1 million sample data events, which simulated a Deuteron signal on a Q-curve for varying levels of polarization and noise. We also utilized KerasTuner, a function in the Keras package, to algorithmically optimize the architecture of the model. We measured the amount of noise in each event via the Signal-To-Noise (SNR) ratio, which gives an intuition as to how overpowering the noise is relative to the amplitude of the signal. We defined SNR as:

$$SNR = \frac{max(|Noise|)}{max(|Signal|)} \tag{1}$$

In this case, an SNR value of 1 indicates that the magnitude of the noise is the same magnitude of the lineshape. A value much greater than one indicates very little noise whereas a value much less than one indicates a very large amount of noise, all relative to the amplitude of the signal.

3. Preliminary Results

After training the model on 1 million sample data events, as well as tweaking the architecture of the model, we reached a steady state for the Neural Network's learning curve indicated by a plot of its loss function (mean squared error) over epochs.

We present sample plots of the Deuteron lineshape's actual polarization with that of the Neural Network's predicted polarization. Below are some sample plots.

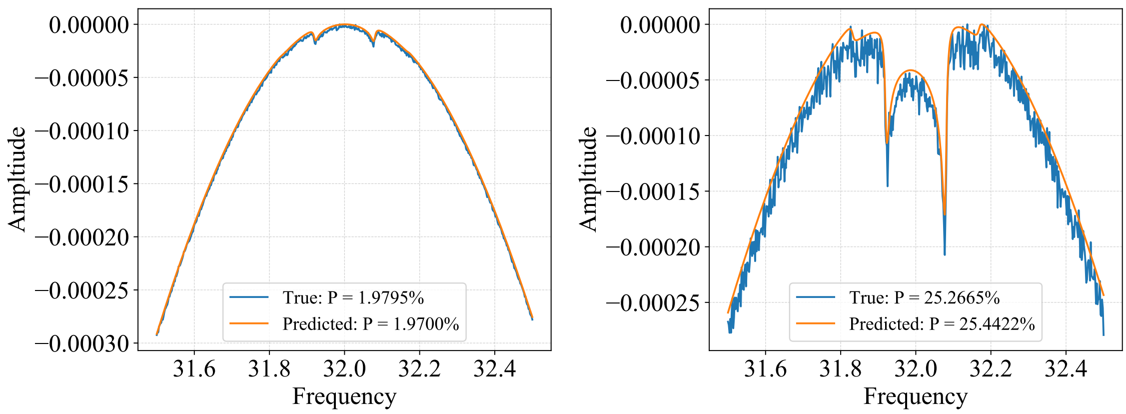

Figure 1: Simulated lineshapes plotted on a Q-Curve for sample data versus replotted lineshapes with predicted polarization. The lefthand figure has a relative uncertainty of ϵ = .48% with SNR = 2.4. The righthand figure has a relative uncertainty of ϵ = .69% with SNR = 1.83.

Preliminary results indicate a model accuracy of 99.97% and precision of 99.94% when trained for very low levels of polarization and 99.88% accuracy and 99.63% precision when trained for the entire range of polarization. Compared to results yielded by previous polarization extraction methods, the Neural Network approach yields better, more accurate, and more precise results.[3]

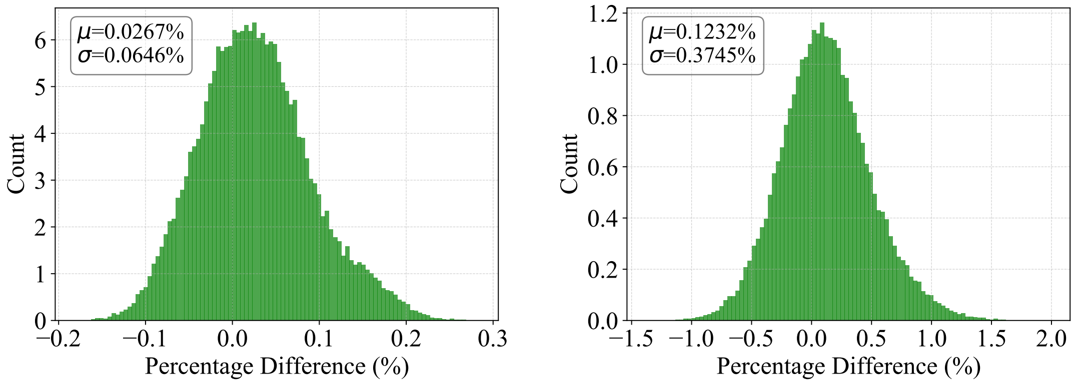

Figure 2: Histograms of the percentage difference between actual and predicted polarization. The figure on the left side is for sample data between 0% - 1% for a model trained within that range and the figure on the right side is for sample data of 0% - 100%, the entire range of possible polarization values also trained within that range. The percentage difference is defined as $\Delta P = P_{\text{true}} - P_{\text{predicted}}$. μ corresponds to the mean of the histogram while σ corresponds to its standard deviation.

4. Outlook

Further efforts in optimizing an architecture will improve future predictions made by a Neural Network model, increasing both accuracy and precision. In order to probe polarization around thermal equilibrium ($\sim$ 0.05%), the model must be as accurate and precise as possible. Future results of these efforts are on their way to be submitted for publication in the journal for Nuclear Instrumentation and Methods.

5. Acknowledgements

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