Polarized Target Nuclear Magnetic Resonance Measurements with Deep Learning

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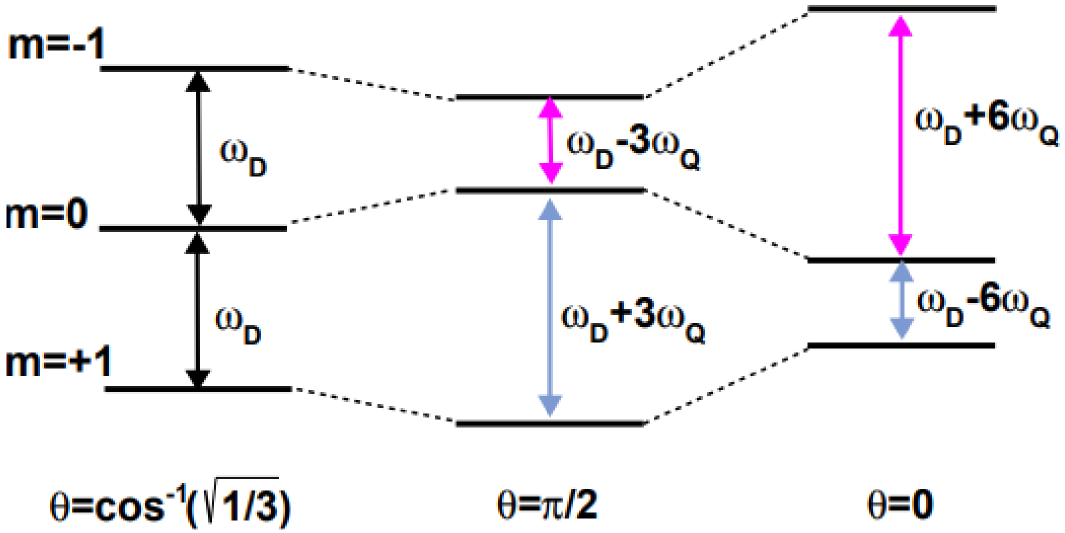
Outline

- NMR Measurements w/ (Liverpool) Q-Meter
- Simulations of ND3 and NH3 Lineshapes
- Neural Networks – **what are these? Why?!**
- Preliminary results
- Observations & Outlook

Nuclear Magnetic Resonance (NMR)

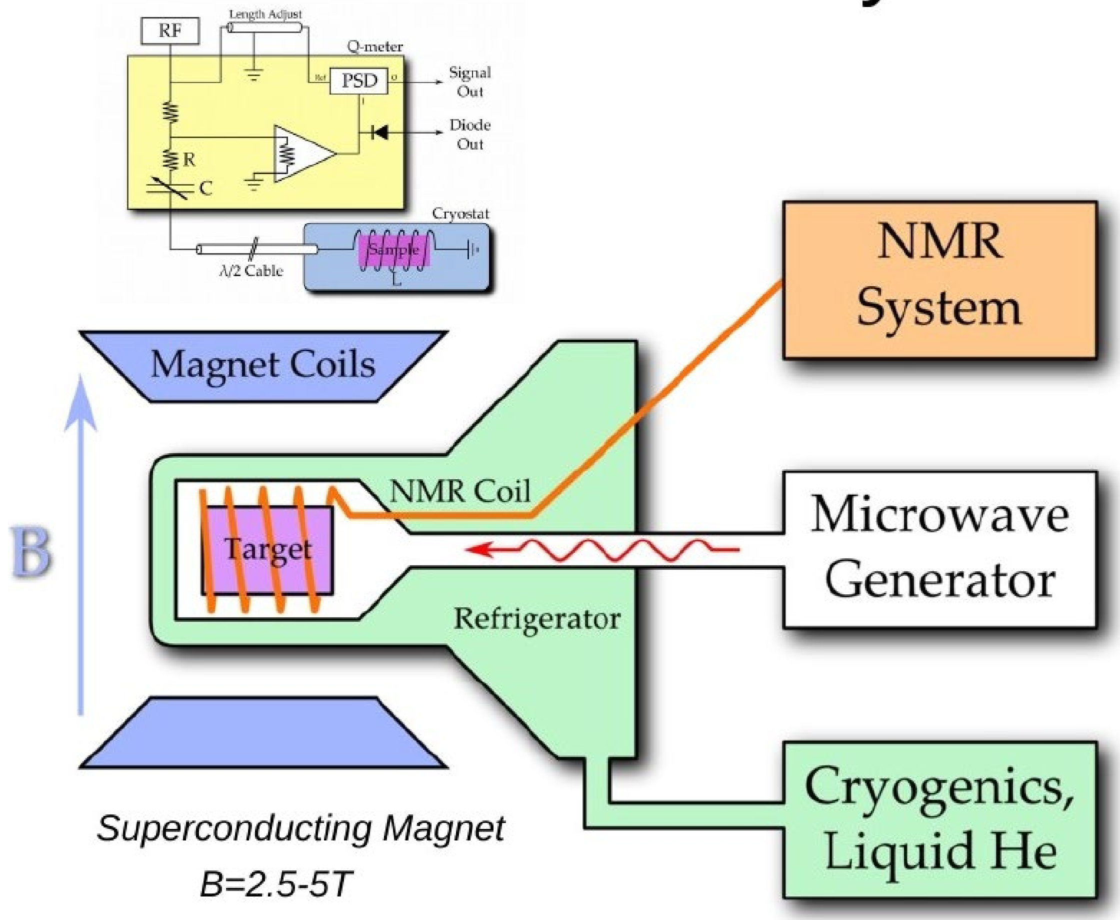
- Nuclear Magnetic Resonance, or NMR, is the physical phenomenon that occurs when a constant magnetic field is applied to nuclei at resonance which is perturbed by a weak oscillating magnetic field, which causes the nuclei to respond by producing an electromagnetic signal with a frequency characteristic of the magnetic field of the nuclei.
- NMR is being used to study the inner structure of various target material, e.g., ND3 and NH3



Q-Meter Based NMR

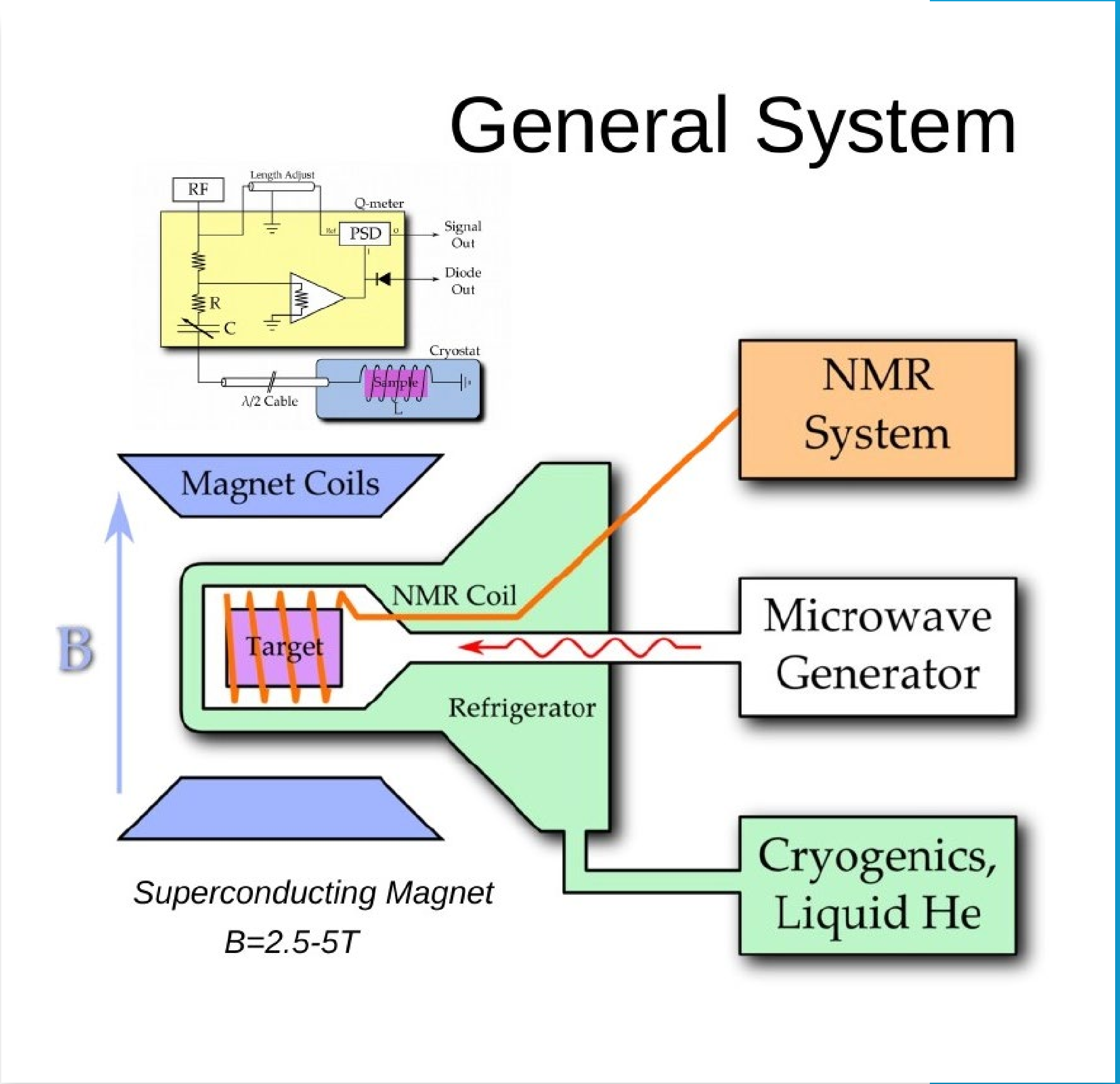
- Using a **non-destructive continuous** wave
  phase-sensitive detector
  (ex., a Q-meter), is required to
  make **accurate** measurements of
  polarization in scattering experiments

General System



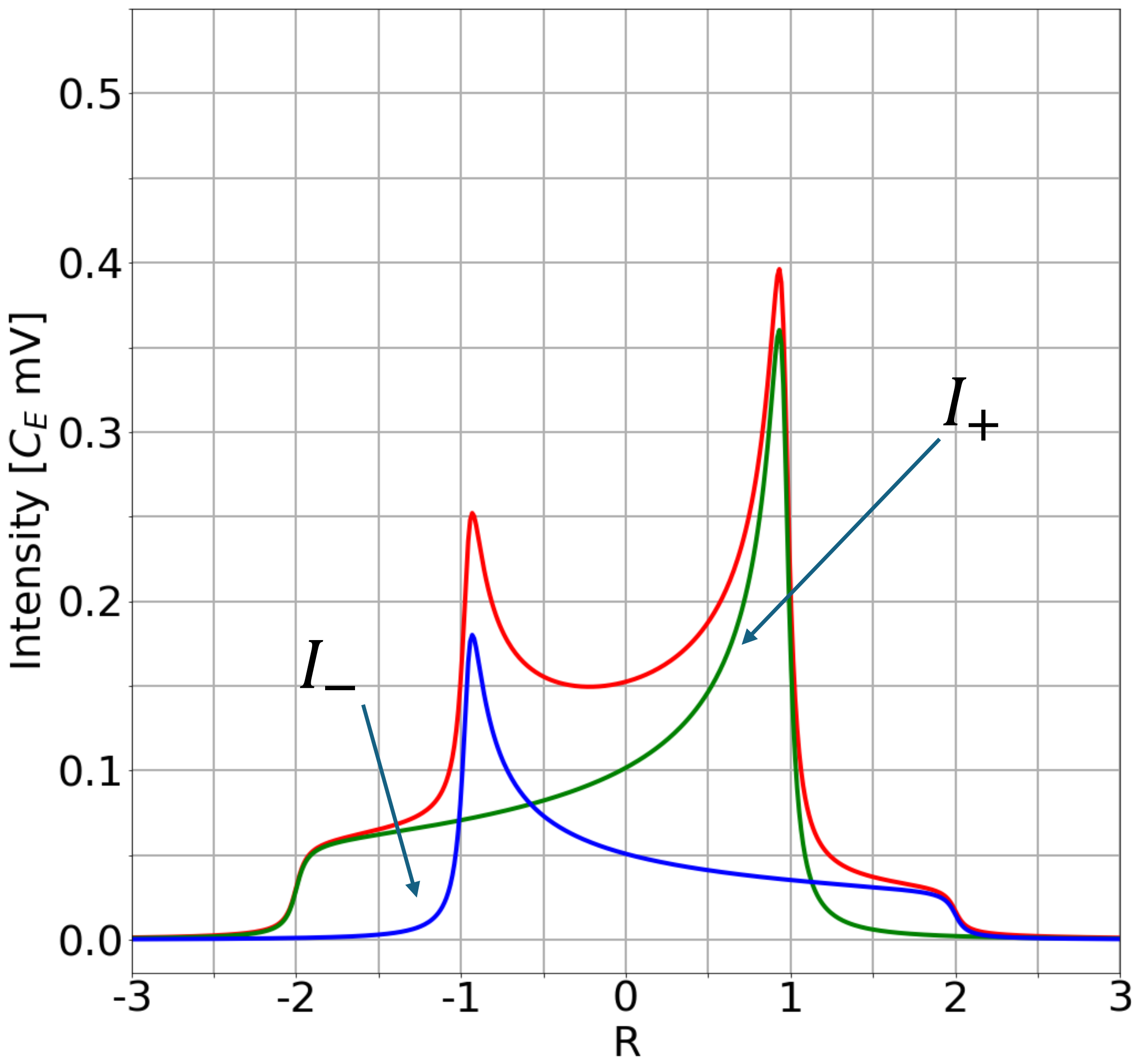
Q-Meter Based NMR

- Q-meter couples to the **magnetic susceptibility** of target material (e.g. Solid Ammonia)
  - Signal passes through λ/2 length cable (358.0 cm for 5T for NH3), so the Q-meter has a **tuning range** of λ/2 to 7λ/2
  - With a **frequency range** of 3-300 MHz
- Within these limits, we expect a **linear relationship** between Polarization and scale (ideal settings gives **2% relative error**)



Deuteron Lineshape

- The Deuteron lineshape has two corresponding **absorption lines**, I_+ and I_-, which are associated with the analytical function for ε = ±1
  - **Absorption lines** arise due to the interaction of the Deuteron's **quadrupole moment** with the **electric field gradient** (EFG), which creates non-degenerate eigen states in the energy levels.
  - **Quadrupole** splitting → two overlapping absorption lines in the NMR spectra (**Pake Doublet**).
  - This Pake doublet is particular to spin-1 material without **cubic symmetry** (Deuteron, Butanol).



https://doi.org/10.1016/S0168-9002(97)00317-3

Deuteron Lineshape

- The Pake Doublet is mathematically described by the **energy levels**:

$$E_m = -\hbar\omega_D m + \hbar\omega_Q(3\cos^2\theta - 1 + \eta\sin^2\theta\cos 2\phi)(3m^2 - 2)$$

- The peaks correspond to the **principle axis** of the coupling interaction being **perpendicular** (θ = π/2) to the magnetic field.
- The opposing end (**the pedestal**) corresponds to the configuration when the principle axis of the coupling interaction is **parallel** (θ = 0) to the magnetic field

$$\mathscr{F} = \frac{1}{2\pi\mathscr{X}}\left[2\cos(\alpha/2)\left(\arctan\left(\frac{\mathscr{Y}^2-\mathscr{X}^2}{2\mathscr{Y}\mathscr{X}\sin(\alpha/2)}\right)+\frac{\pi}{2}\right) + \sin(\alpha/2)\ln\left(\frac{\mathscr{Y}^2+\mathscr{X}^2+2\mathscr{Y}\mathscr{X}\cos(\alpha/2)}{\mathscr{Y}^2+\mathscr{X}^2-2\mathscr{Y}\mathscr{X}\cos(\alpha/2)}\right)\right],$$

$$\mathscr{X}^2 = \sqrt{\Gamma^2 + (1 - \varepsilon R - \eta\cos 2\phi)^2}$$

$$\mathscr{Y} = \sqrt{3 - \eta\cos 2\phi}$$

$\eta\cos 2\phi \sim 0.04$ $\Gamma \sim 0.05$

$$\cos\alpha = (1 - \varepsilon R - \eta\cos 2\phi)/\mathscr{X}^2$$

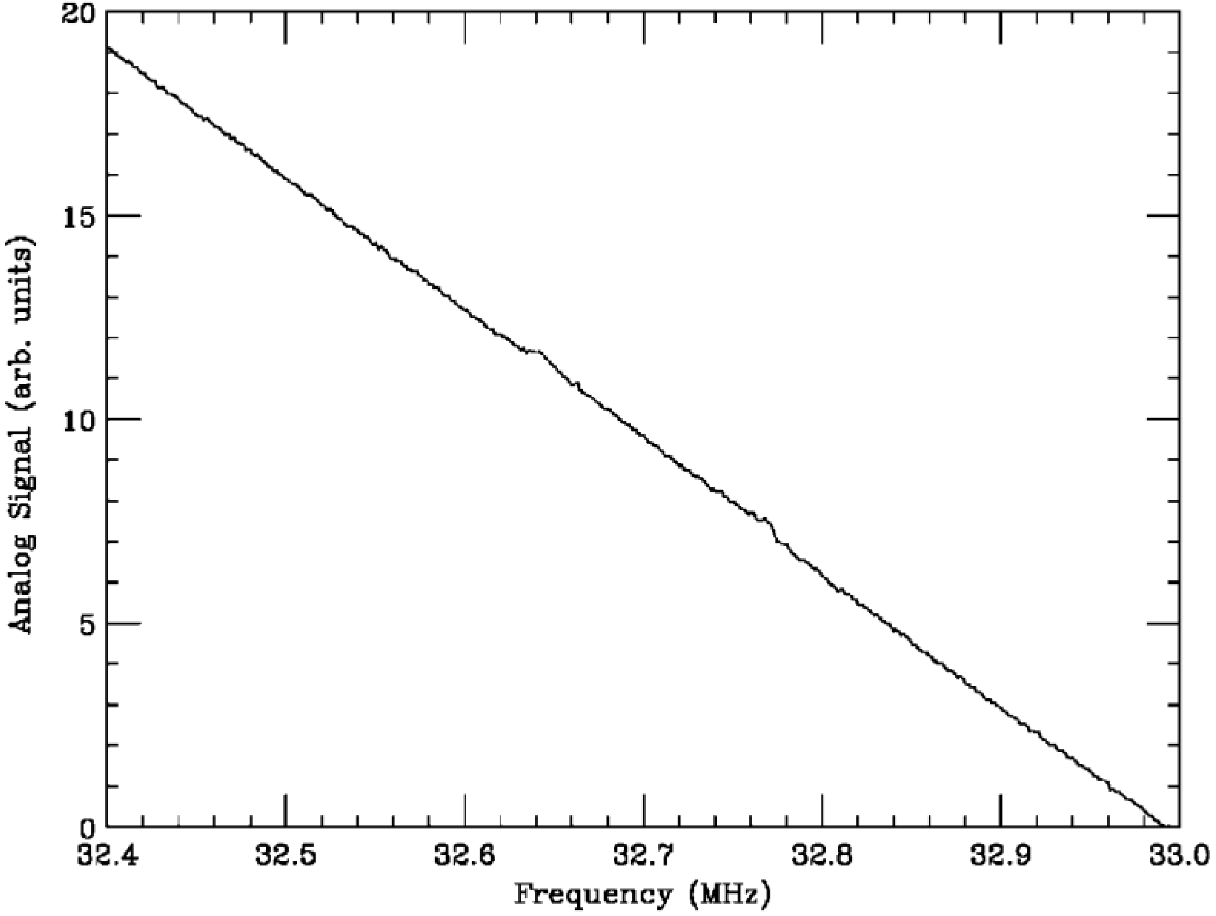
$$P = (r^2 - 1)/(r^2 + r + 1)$$

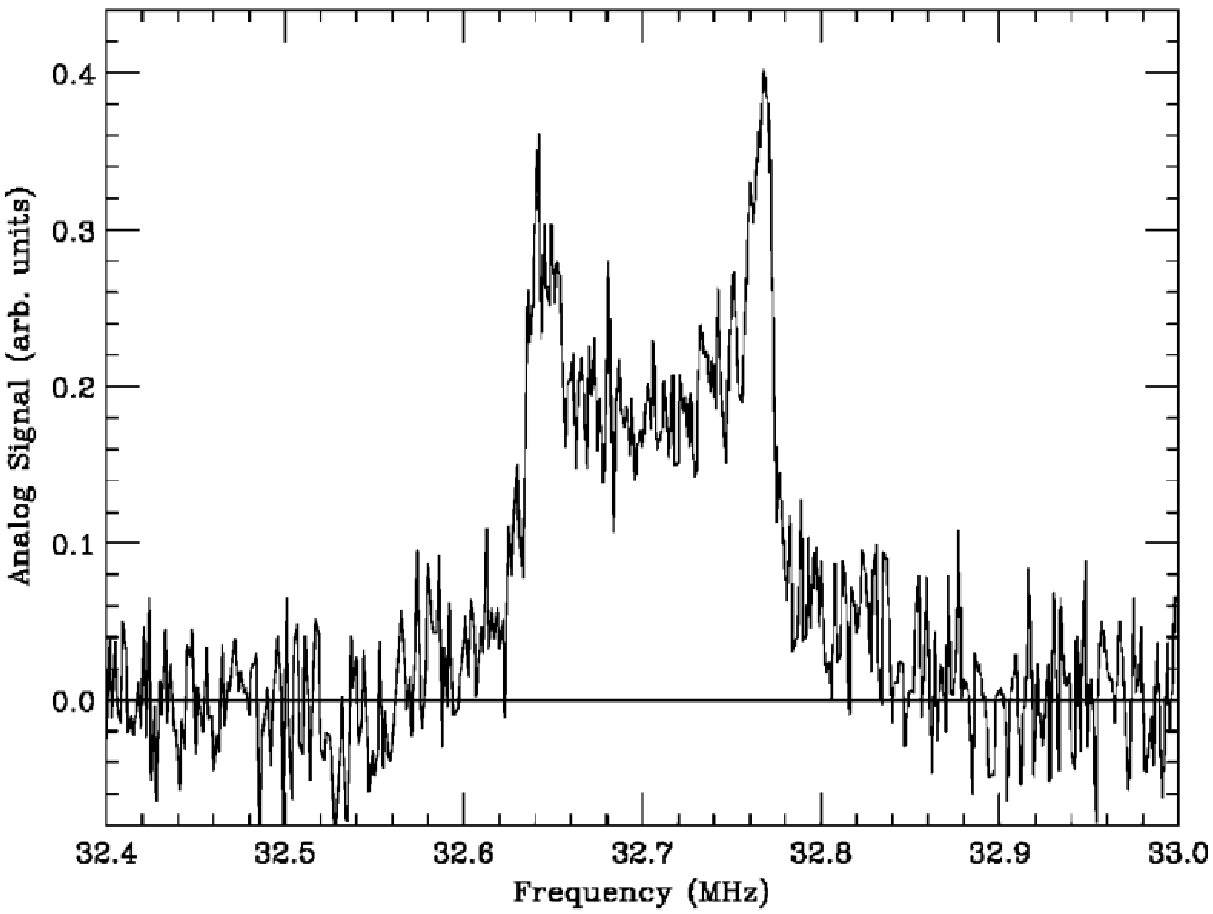
$$r = {}^{I_+}/_{I_-}$$

$$P = \mathscr{K}\int \frac{\omega_d S(\omega)}{\omega}\, d\omega,$$

Real Example of Deuteron Signal

$$P_{TE} = \frac{4}{3}\tanh(\hbar\omega_d/2kT)$$





Court, G.R. & Houlden, Michael & Bültmann, S. & Crabb, D.G. & Day, Day & Prok, Y.A. & Penttila, S.I. & Keith, Christopher. (2004). High precision measurement of the polarization in solid state polarized targets using NMR. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment. 527. 253-263. 10.1016/j.nima.2004.02.041.

Measuring Polarization

- **Thermal Equilibrium** (Previous technique)
  - When we have the lattice (**L-Helium**) and the target material at the same temperature, we can obtain the TE polarization by the equation:
    - $P_{TE} = \frac{4}{3}\tanh(\hbar\omega_d/2kT)$
  - Then for any polarization not in TE
    - $P = C \times P_{TE}$, where C is the **calibration constant** calculated
- Using TE method comes with **considerable** error (~ 7% relative error) from the change in area of the TE signal and the fitted signal.

https://doi.org/10.1016/j.nima.2013.06.103

Limitations for Deuteron polarization determination

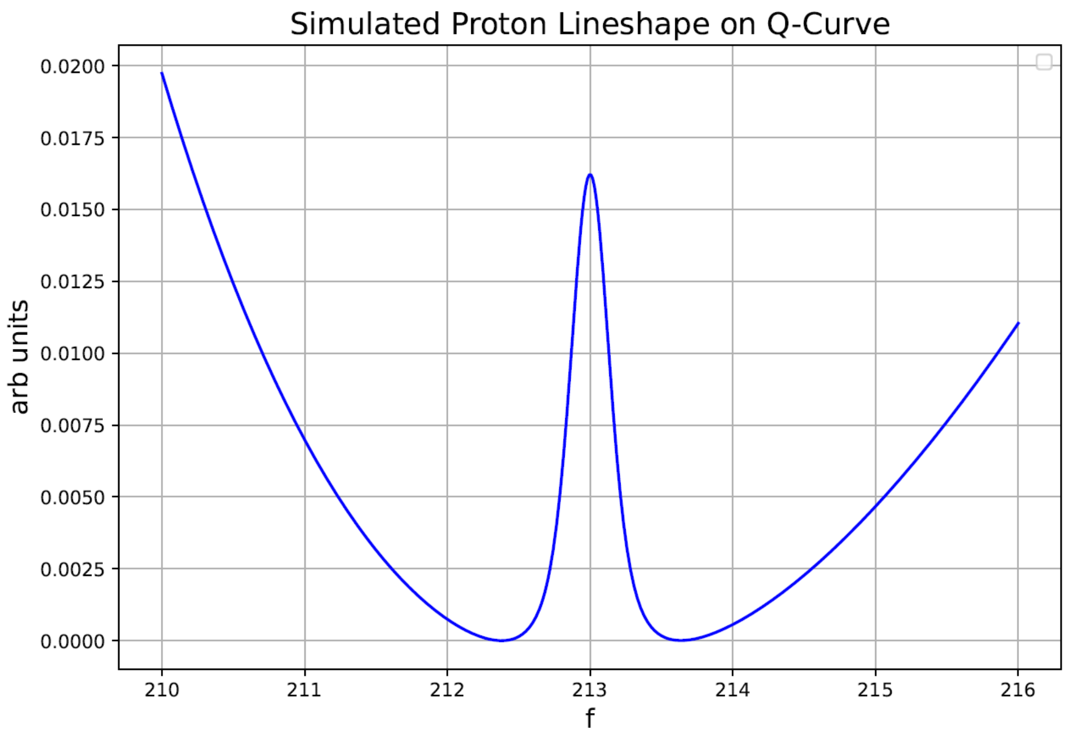
- The Liverpool Q-meter system allows for relative accuracy a deuteron signal's polarization (error of about 1%). However, in the experimental setting, this is far worse, especially at low polarizations. Normally in the experimental setting, we'd expect a relative uncertainty of about 7%
- Sources of error:
  - $n\lambda/_2$ cable length
  - Q-meter configurations (calibration constant)
  - Changes in **RF** environment
  - **Temperature** Change
  - **Statistical errors** dependent on DAQ
- Here, we're concerned with trying to overcome complications caused by the first and third sources
  - Also concerned with statistical error (variation in predictions by NN)

https://doi.org/10.1016/j.nima.2013.06.103.

Proton (NH3)

- Single crystal has cubic symmetry with a space group of $P2_13$
- Larmor Frequency of ~213MHz for 5T
- Predict **Area** instead of polarization
- Described by **Voigt** function

$$V(x;\sigma,\gamma) \equiv \int_{-\infty}^{\infty} G(x';\sigma)L(x-x';\gamma)\,dx'.$$



Differences between lineshape and area method

Lineshape

- Predict **Polarization** given a lineshape
  - **Specific** to lineshape
  - **Less** accurate/precise
  - **Direct** measurement of polarization

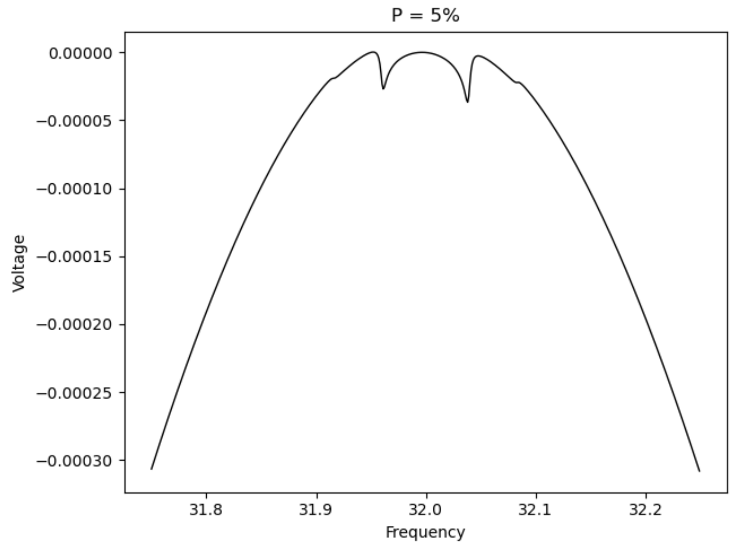
Area

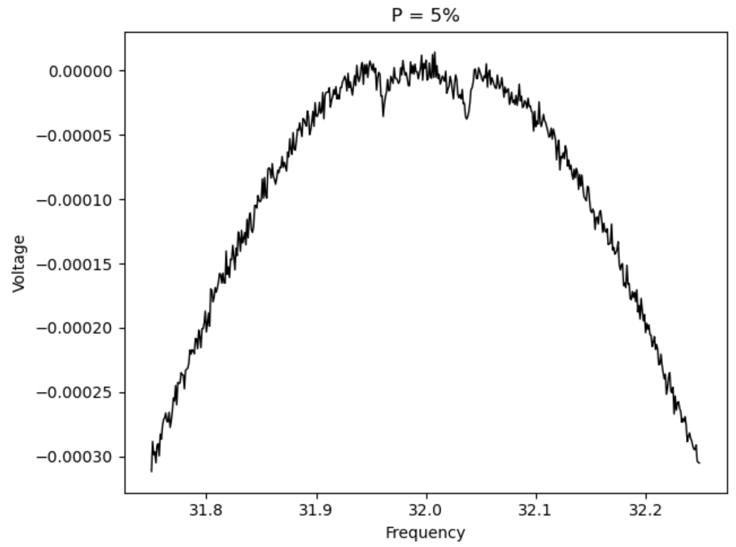
- Predict **Area** underneath curve
  - Can generalize to **any** spin-1 target specimen
  - **More** accurate/precise
  - **Indirect** measurement of polarization

Why Artificial Neural Networks (ANN)?

Neural Networks: A Possible Solution

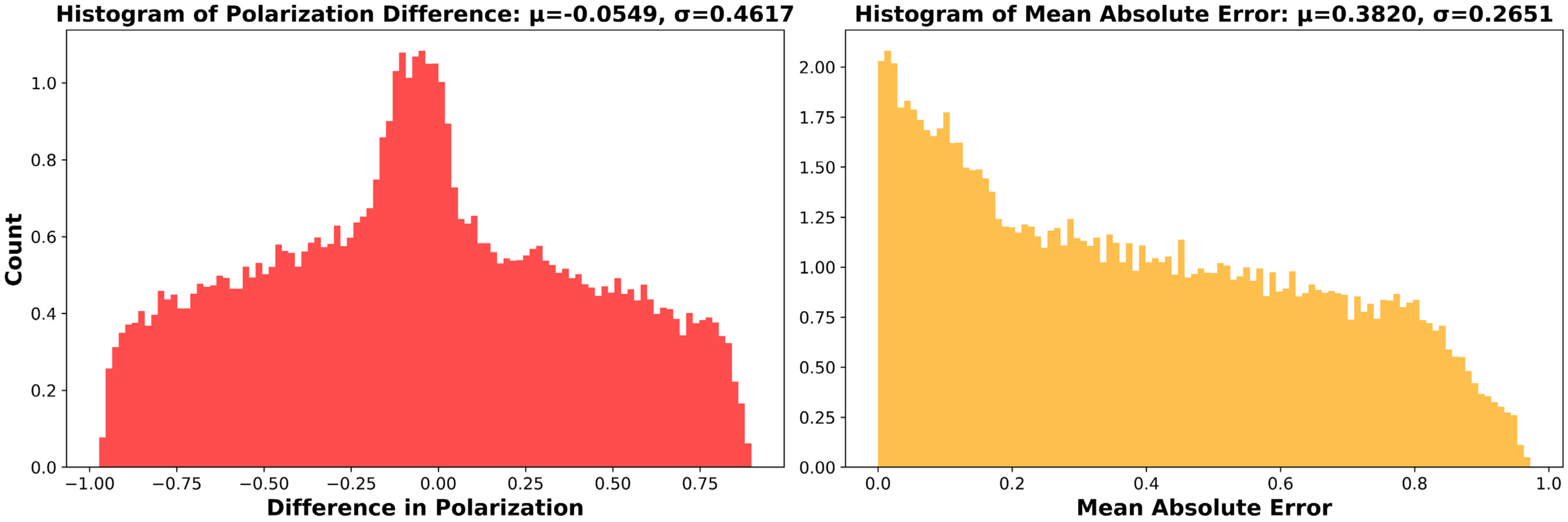
- By training a neural network (NN) on sample data that replicates experimentally accurate noise levels that evolve through time, we can go beyond the capability of the Q-meter and make up for where it lacks.
- Using to optimize precision and accuracy, regardless of Signal-to-Noise Ratio (SNR)
- SNR: ratio of maximum of amplitude of signal to maximum of amplitude of noise, represents how overwhelming the noise is
- By training an NN to associated a specific polarization with its associated signal over 500 data bins, we can accurately predict polarization for a given noisy signal





Preliminary Results

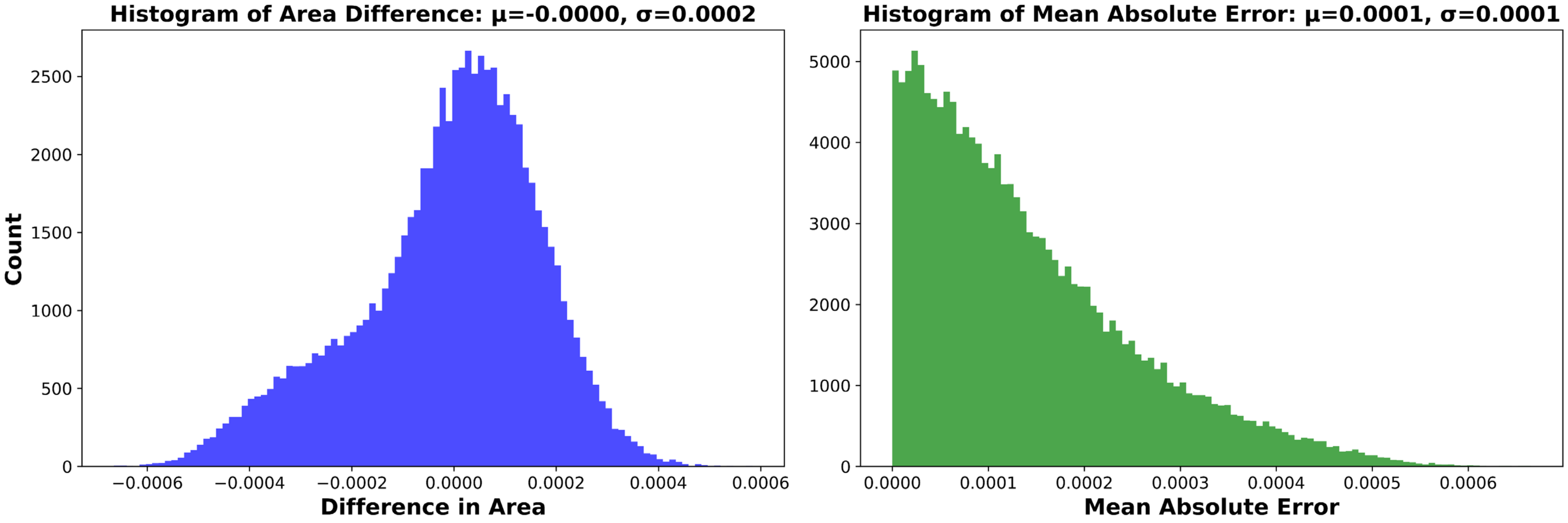
ND3



(a) (b)

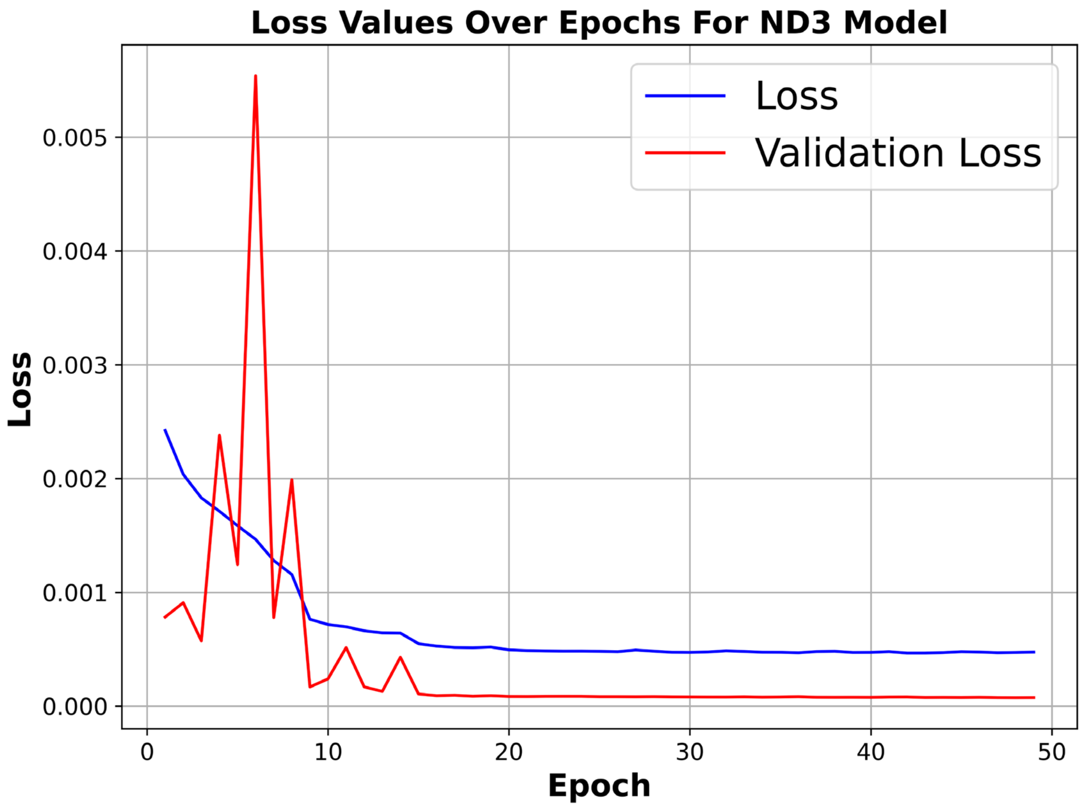
Polarization range: ~ 0 – 100 %

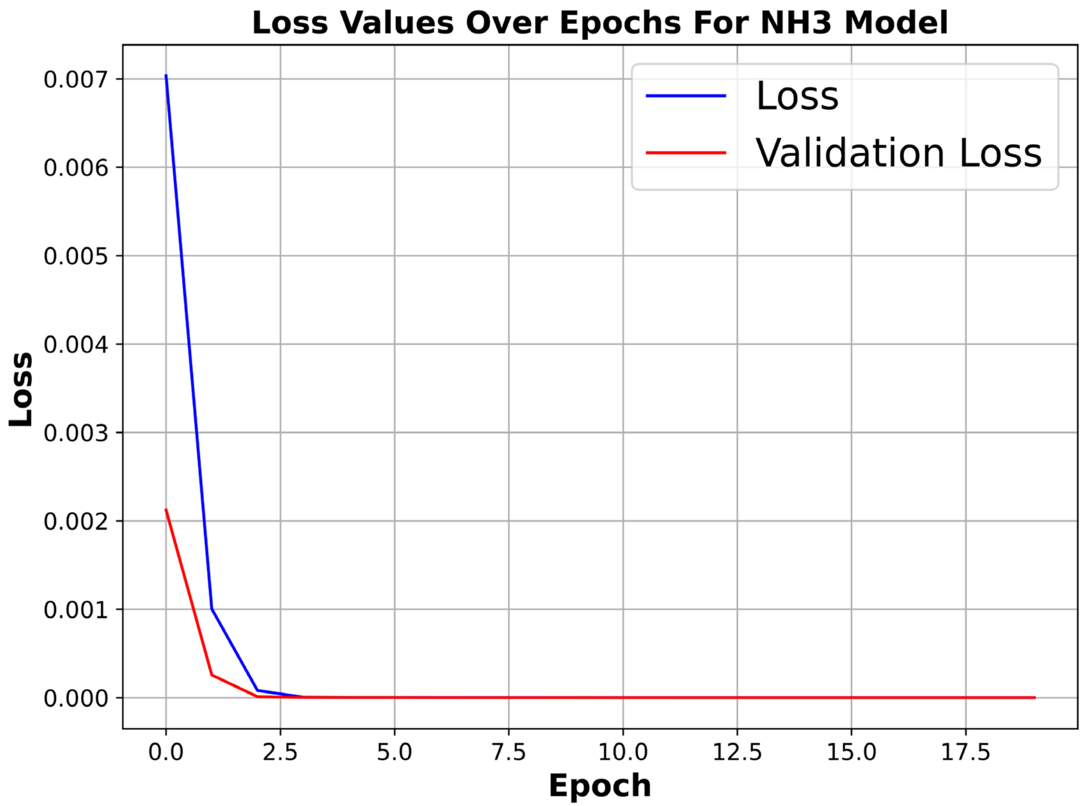
NH3



(a) (b)

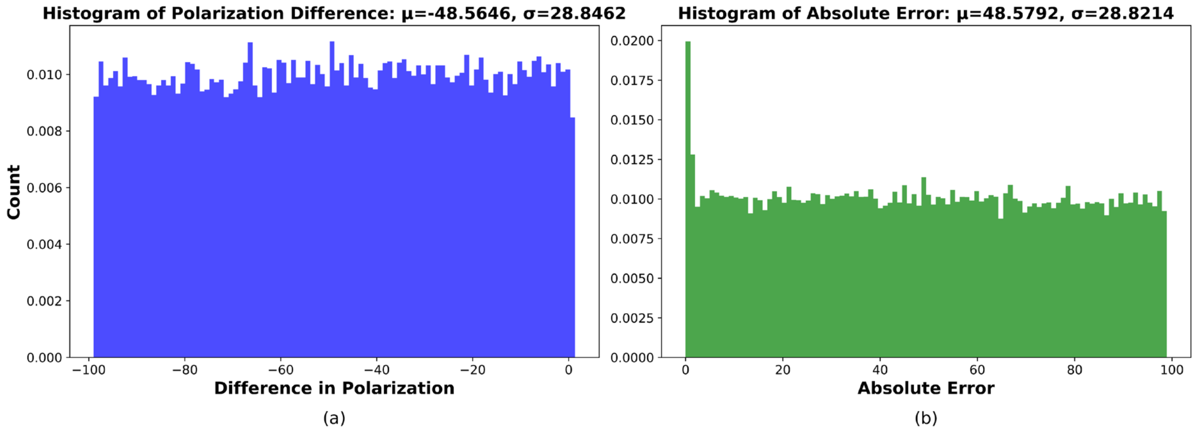
Area range: ~ 0 - .1


Loss Values Over Epochs For ND3 Model
Loss
Validation Loss
0.005
0.004
0.003
0.002
0.001
0.000
0
10
20
30
40
50
Epoch
Loss

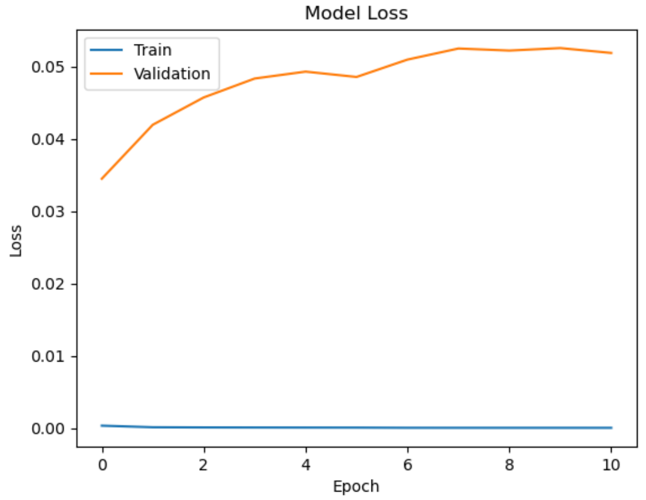

Loss Values Over Epochs For NH3 Model
Loss
Validation Loss
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Epoch
Loss

Future

Need to improve this!



- Need to increase amount of training data
  - Need to tune for this larger amount, especially for ND3



- ANN techniques for NMR (especially extracting area) are universal for all spin-1 specimen.
- The adaptability of the ANN allows for changes in baseline and scanning range of an NMR to quickly and easily be considered

Thank you!

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