AI NMR Extraction for Spin-1 Signals

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Outline

- Polarization Extraction Methods (for ND_3)
- Neural Networks
- Preliminary results (for vector polarization)
- Tensor Polarization
- Observations & Outlook

Extracting Deuteron Polarization

- Can fit a signal by average the dependance on the azimuthal angle
  - $F_\epsilon(R, A, \eta) = \frac{2}{\pi}\int_0^{\pi/2} \frac{\sqrt{3} f_\epsilon(R,A,\eta,\phi)}{\sqrt{3-\eta\cos(2\phi)}} d\phi \approx \frac{1}{J+1}\sum_{j=0}^{J} \frac{\sqrt{3} f_\epsilon(R,A,\eta,\phi)}{\sqrt{3-\eta\cos(2\phi)}}, J = 64, 0 < \phi < 2\pi$
- Polarization Approximated as
  - $P = \frac{r^2-1}{r^2+1+r}, \quad r = \frac{I_+}{I_-}$

Extracting Deuteron Polarization

- Thermal Equilibrium (TE)
  - When lattice (L-Helium) and the target material are at the same temperature, we have Boltzmann equilibrium → $P_{TE} = \frac{4}{3}\tanh(\frac{\hbar\omega_d}{2kT})$
  - Assuming **linearity** of Q-Meter system, relationship between **area** and **polarization** is linear, i.e.,:
    - $P = C\int \frac{\omega_d S(\omega)}{\omega} = CP_{TE}$, where C is a calibration constant
    - NMR Signal: $S(\omega) = \Re\{V(\omega,\chi) - V(\omega,0)\}\chi''(\omega)$, $\chi''(\omega)$ is the **absorption function** and $\chi(\omega)$ is the **magnetic susceptibility**

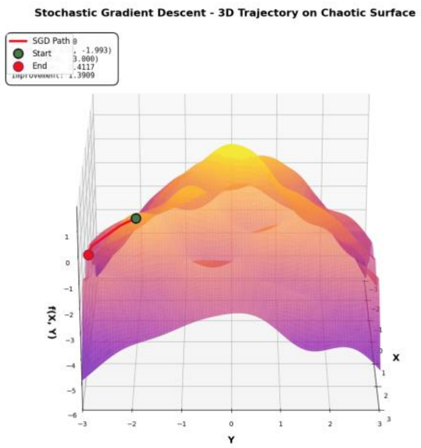
Extracting Deuteron Polarization

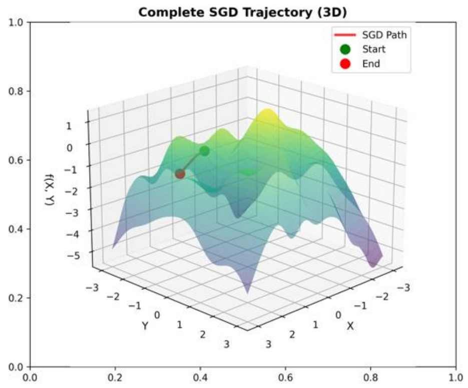
- TE method comes with considerable error (~4% relative error but sometimes as much as 7% for standard spin-1 fitting)
  - Error propagated from change in **area** of TE signal and fitted signal.
  - TE state takes **very** *long* to reach (can take several hours, ie ND3).
  - Dulya type fitting is prone to systematic errors and susceptible to signal-to-noise.
  - Dulya type fitting **not possible for RF manipulated signal**.

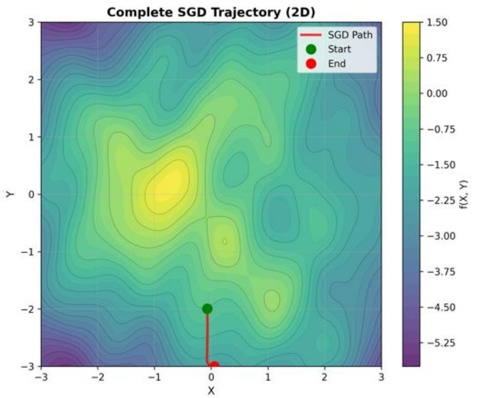
Q-Meter Limitations

- Sources of error:
  - $^{n\lambda}/_{2}$ cable length (Tuning errors)
  - Calibration Constant
  - Changes in **RF** environment
  - **Temperature** Change
  - **Statistical errors** dependent on DAQ

Artificial Neural Networks







$$\hat{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{w} + b, \qquad \boldsymbol{X}, \boldsymbol{w} \in \mathbb{R}^{d}$$

Loss Function: $\mathrm{L}(\mathbf{w}, \mathrm{b})$ (e.g., MSE, MAE)

Minimize: $(\mathrm{w}^{*}, \mathrm{b}^{*}) = \operatorname{argmin}(\mathrm{L}(\mathbf{w}, \mathrm{b}))$

$$\mathrm{w} \leftarrow \mathrm{w} - \eta \sum_{\mathrm{i} \in \mathrm{B}} \partial_{\mathrm{w}} \mathrm{L}^{(\mathrm{i})}(\mathrm{w}, \mathrm{b})$$

$$\mathrm{b} \leftarrow \mathrm{b} - \eta \sum_{\mathrm{i} \in \mathrm{B}} \partial_{\mathrm{b}} \mathrm{L}^{(\mathrm{i})}(\mathrm{w}, \mathrm{b})$$

Goals

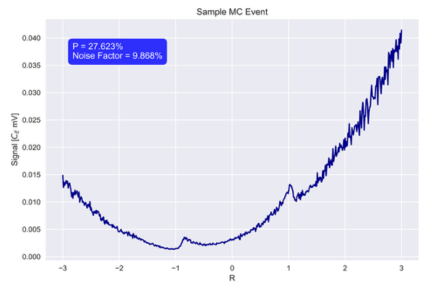
- (Reduce fit errors) **increase accuracy and precision** (for spin ½ and 1)
- **Achieve reliable results** even with large range of noise and shifts
- Develop flexible software that improves reliability even when **working Q-meter outside its design specifications**
- Enable ***real-time*** polarization readings
- Apply to **ss-RF/AFP type manipulations**

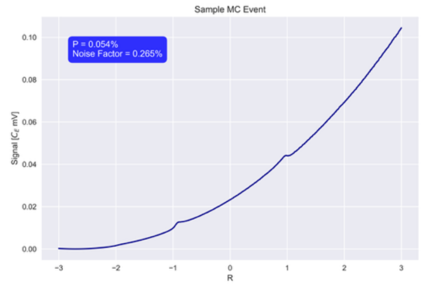
Why Neural Networks?

- Most Flexible ML approach to regression problems (UAT)
- Very fast inference is possible (~ms scale updates with standard GPU)
  - More accurate real-time polarization monitoring
- Can do more with multidimensional information
- Common libraries help to leverage basic hardware

Data Generation

- Generated 1M data points varying over polarization and noise level (0% - 10% relative error per bin)
  - $SNR = \frac{|Max(Lineshape)|}{|Max(Noise)|}$
- Deuteron lineshape generated by analytical function
- Baseline simulated from Q-Meter circuitry parameters
  - U: Voltage
  - Z_{Stray}: Stray capacitance
  - $C(\omega)$: Capacitance
  - I: Current
  - $\phi(\omega)$: Phase
  - η: Filling Factor (of coil)
  - $\lambda/2$: Cable length
- Data generated under various conditions of parameters to generalize

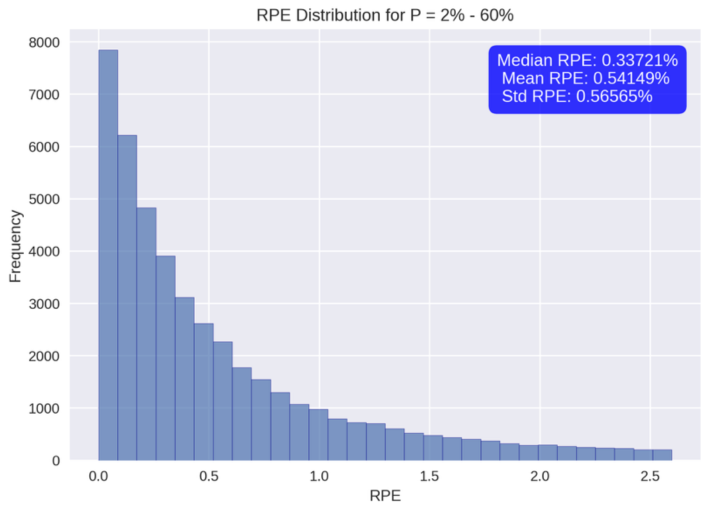


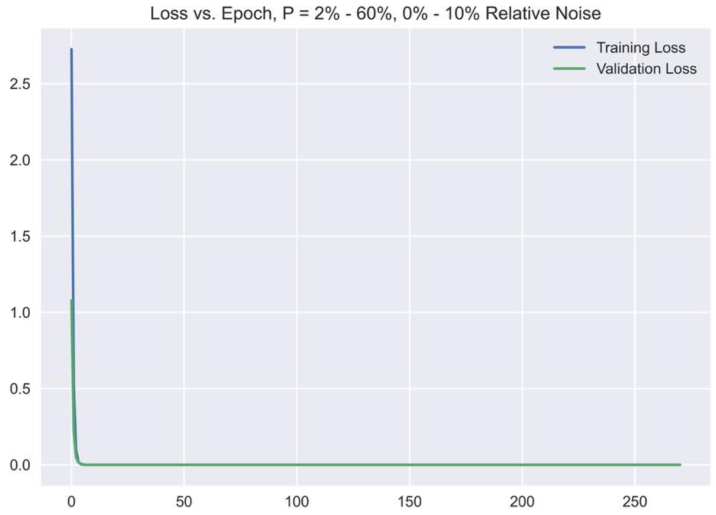


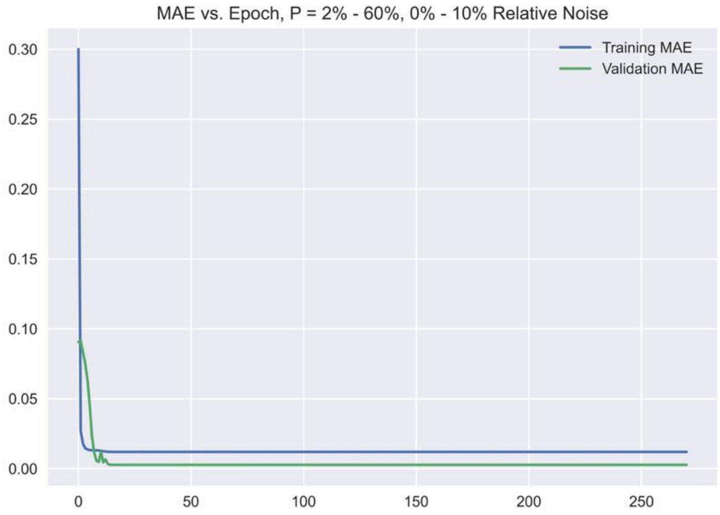
Preliminary Results

Results for P = 2% - 60%

Relative Error ~ 0 – 10% per bin
SNR ~ 1-2

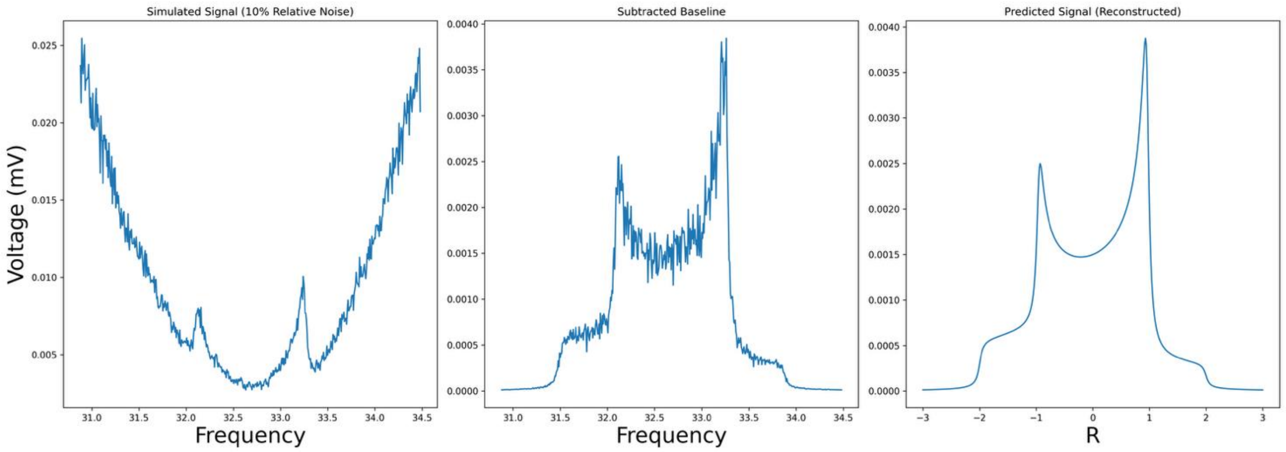




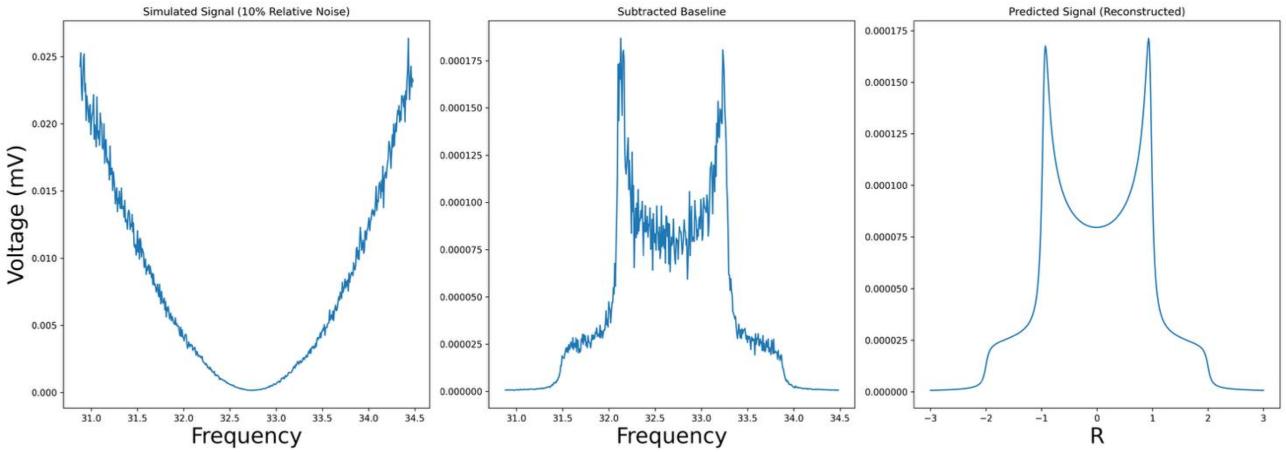


Median RPE: **0.34%**
Mean RPE: **0.54%**
STD: **0.57%**

Simulated (P = 41.47%) and Predicted (P = 41.72%) Signal
RPE = 0.59%

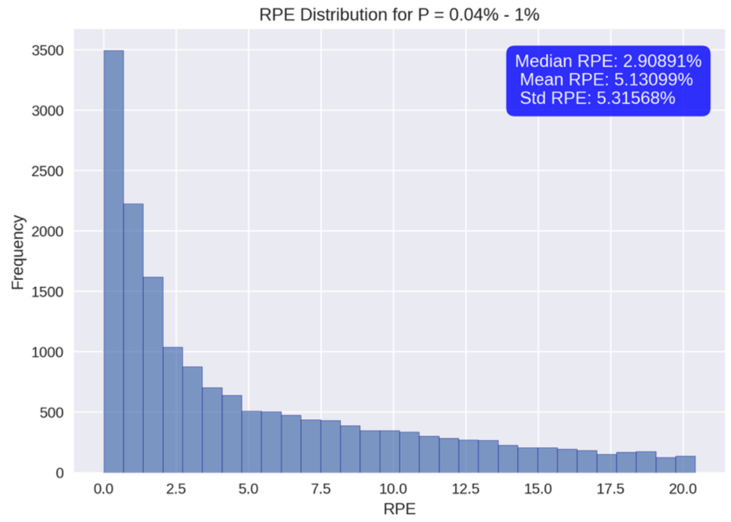


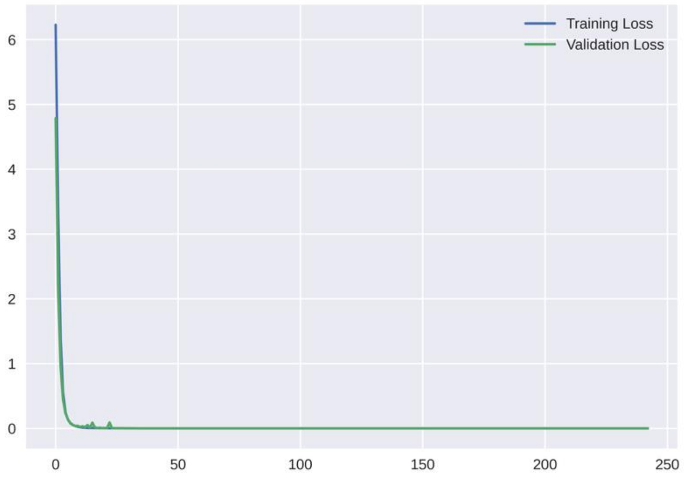
Simulated (P = 2.219%) and Predicted (P = 2.217%) Signal
RPE = 0.09%

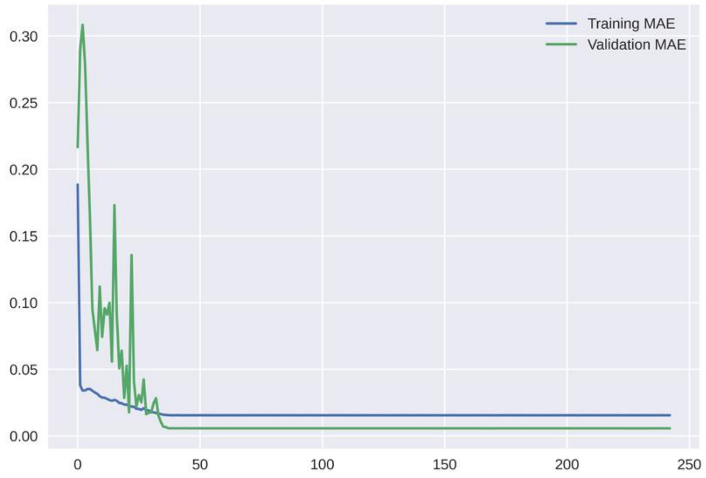


Results for P = 0.04% - 2%

Relative Error ~ 0 – 1% per bin
SNR ~ 1-2

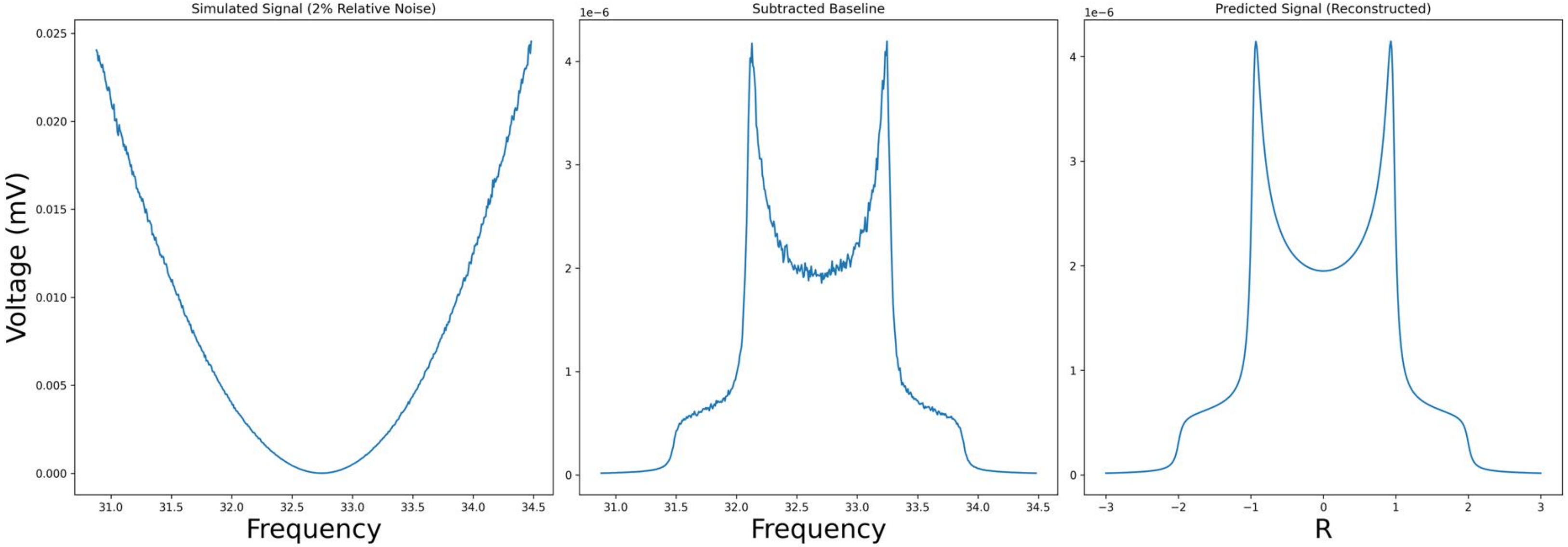






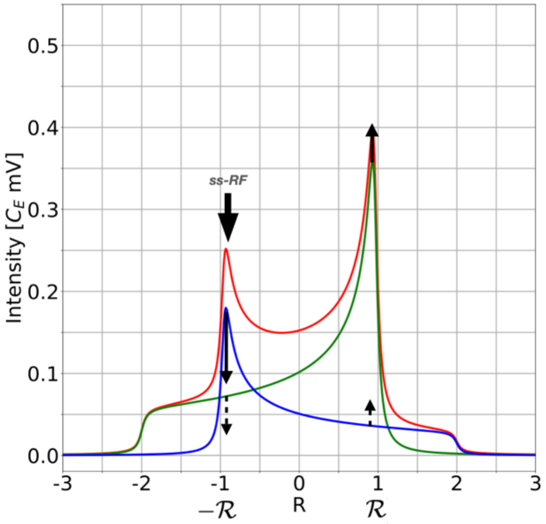
Median RPE: **2.9%**
Mean RPE: **5.13%**
STD: **5.32%**

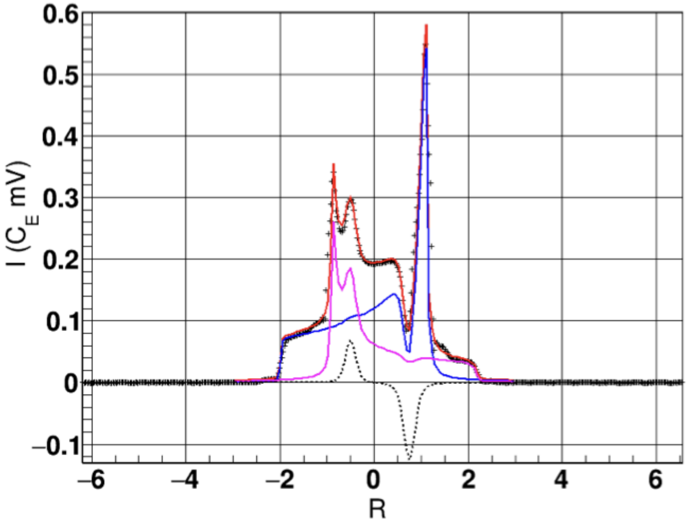
Simulated (P = 0.05402%) and Predicted (P = 0.05425%) Signal
RPE = 0.43%



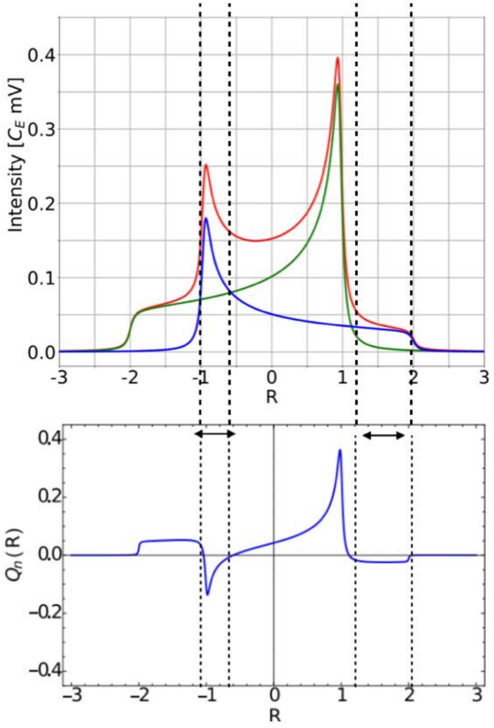
Tensor Polarization

Semi-Saturated Radiofrequency (ss-RF)





Relaxation Pathways

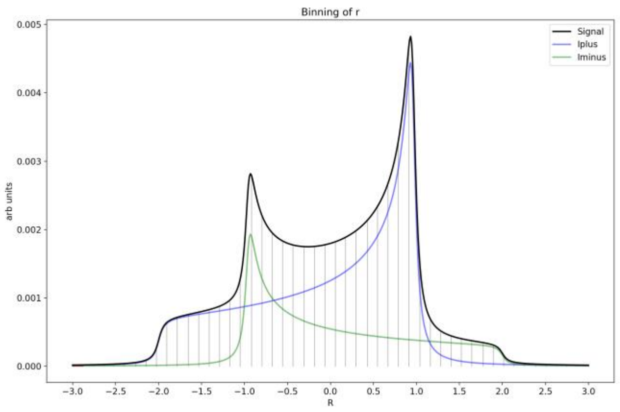


https://arxiv.org/abs/1707.07065

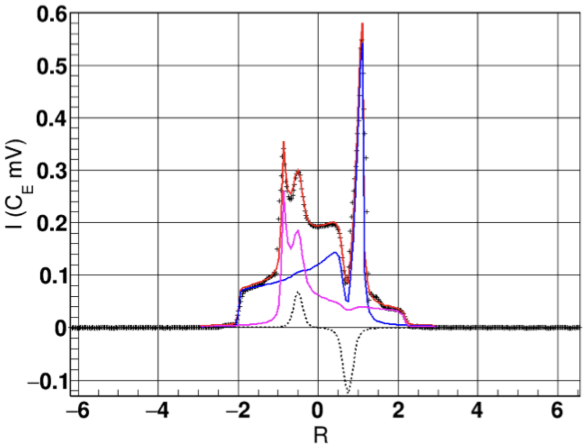
Principles of ss-RF

$$r = \frac{I_+}{I_-} \rightarrow r_i = \frac{I_{+,i}}{I_{-,i}}$$

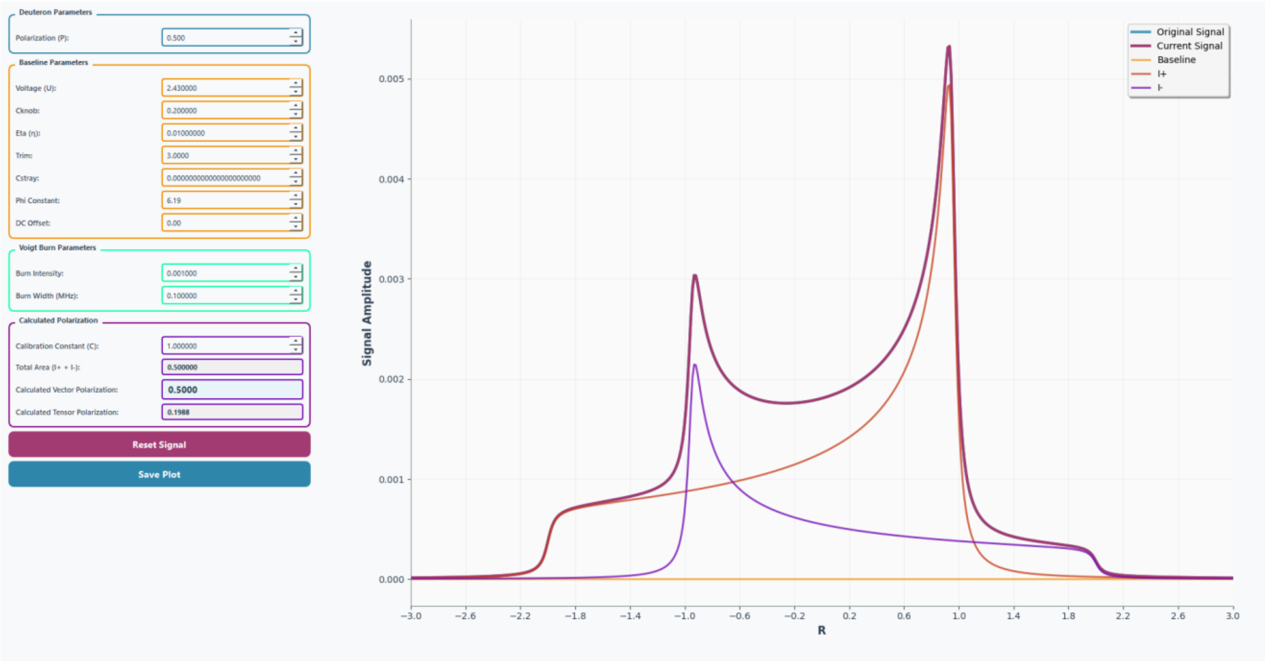
$$P_i = C_i\left(I_{+,i} + I_{-,i}\right)$$
$$P_{zz,i} = C_i(I_{+,i} - I_{-,i})$$

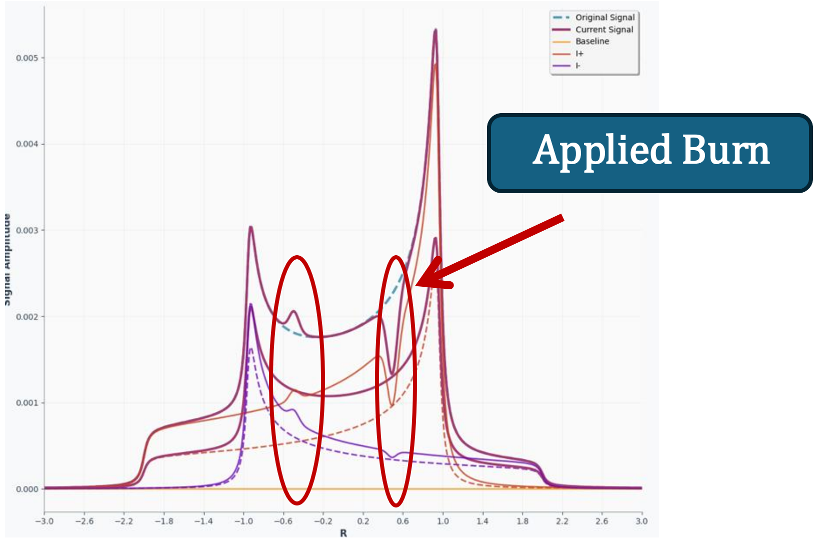


- Spin-Temperature Consistency
  - Hole burning locally erases non-equilibrium state biases by restoring partial equilibrium
  - Burning acts as *mirror image* of DNP, driving spin transition in **opposite** direction
- Differential Binning
  - Partitioning signal into frequency beams and manipulating/measuring each subset
- Rates Response
  - Peak achieved from hole burning is ½ area of burned area (in high RF power limit)



Burning Simulation





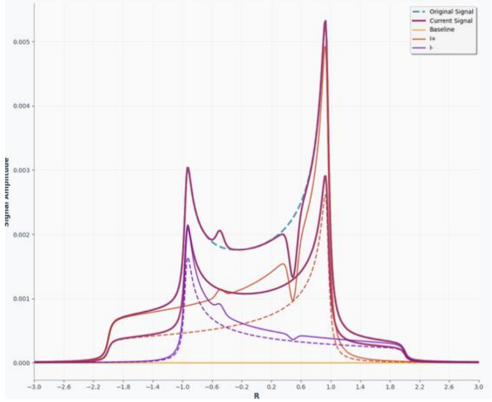
Calculated Vector Polarization: **0.4975**

Calculated Tensor Polarization: 0.1990

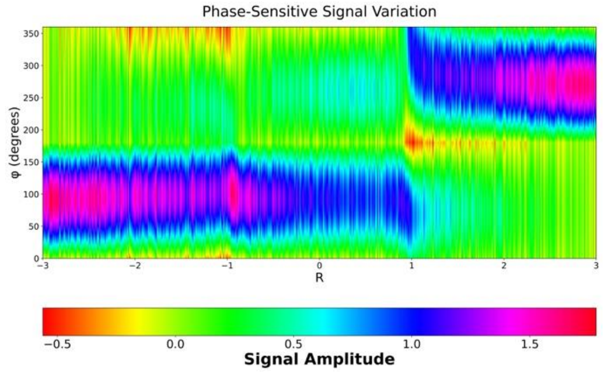
Calculated Vector Polarization: **0.5000**

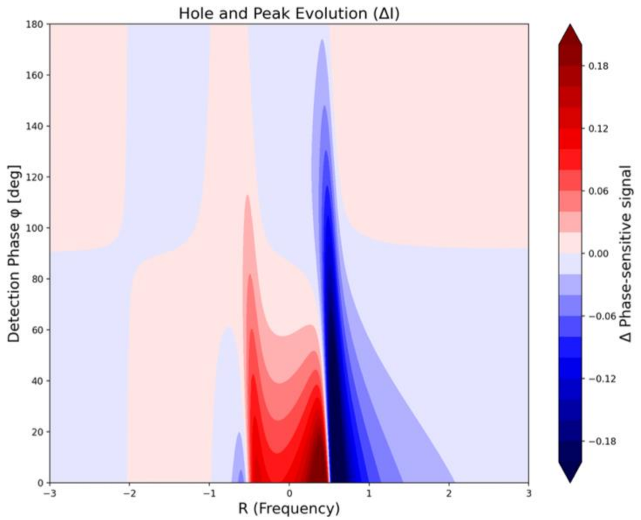
Calculated Tensor Polarization: 0.1988

Future Machine Learning Endeavors



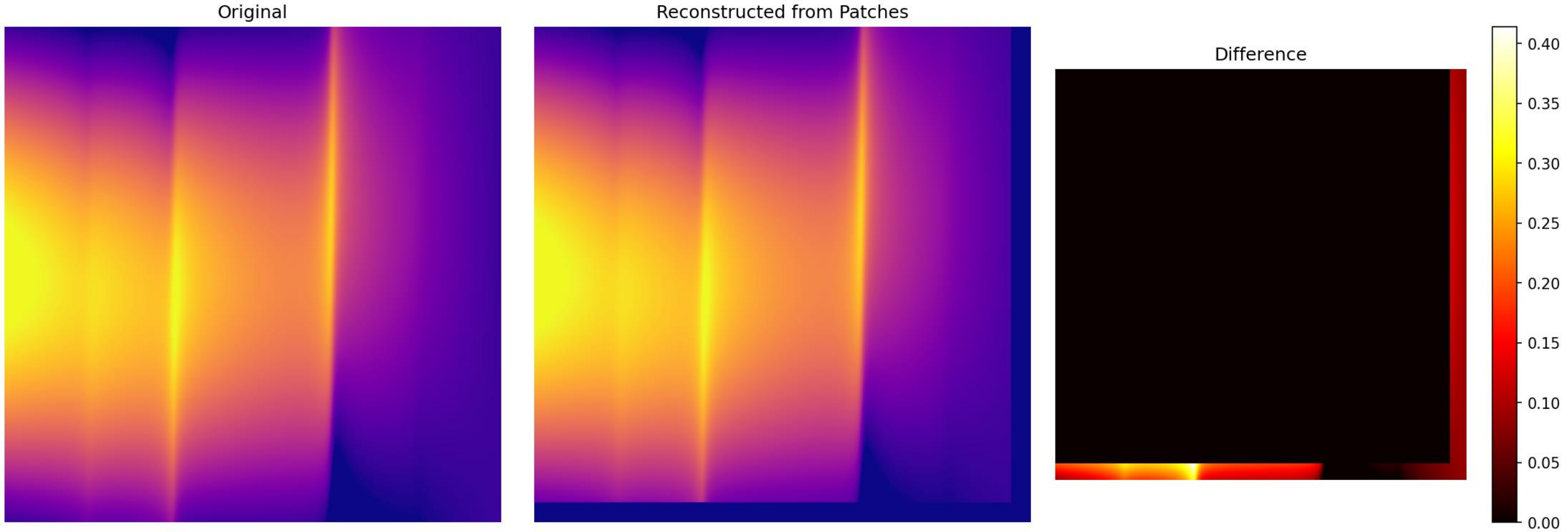
- **1D Case:**
  - (bin P and P_{zz} in R domain only) to extract P and P_{zz} *invariantly* of RF manipulation
- **2D Case:**
  - Calculate P and P_{zz} along R ***and*** ϕ
  - → Train model with smaller, synchronized, phase-shifted tiemsteps
  - → *More information* to train on!

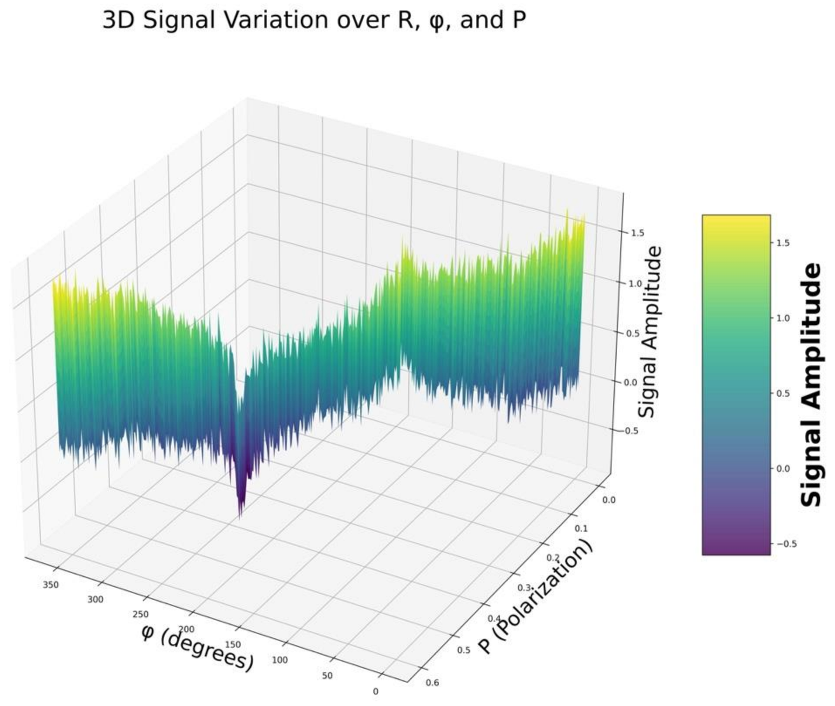


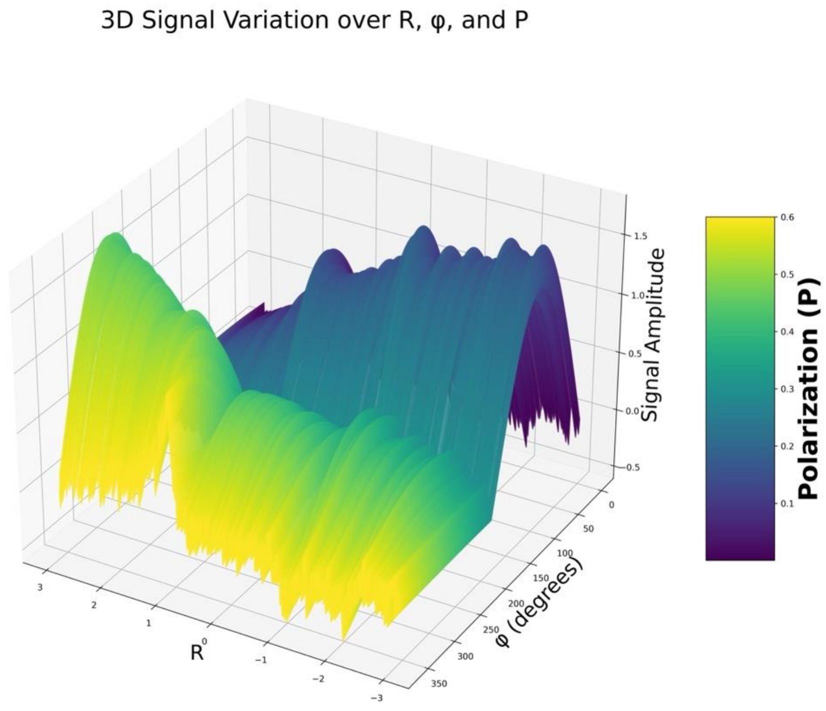


Thank you!

Leftovers


Original
Reconstructed from Patches
Difference
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00


3D Signal Variation over R, φ, and P
φ (degrees)
P (Polarization)
Signal Amplitude


3D Signal Variation over R, φ, and P
R
φ (degrees)
Signal Amplitude
Polarization (P)