Decoding Quantum States through Nuclear Magnetic Resonance

Google Summer of Code 2021 Student Talk

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Mentors:
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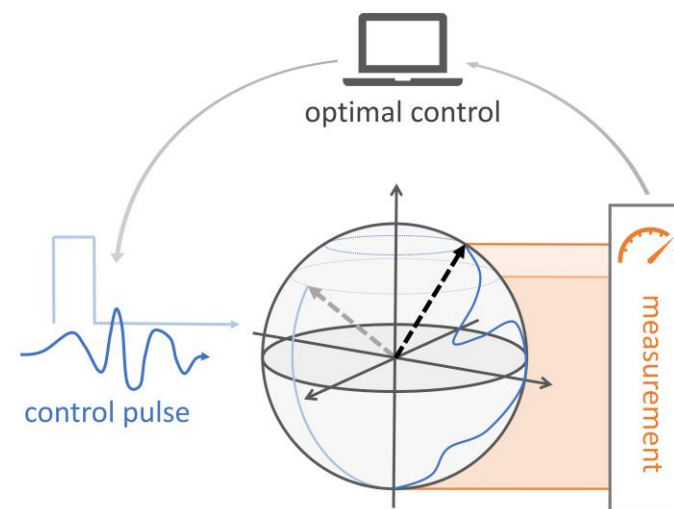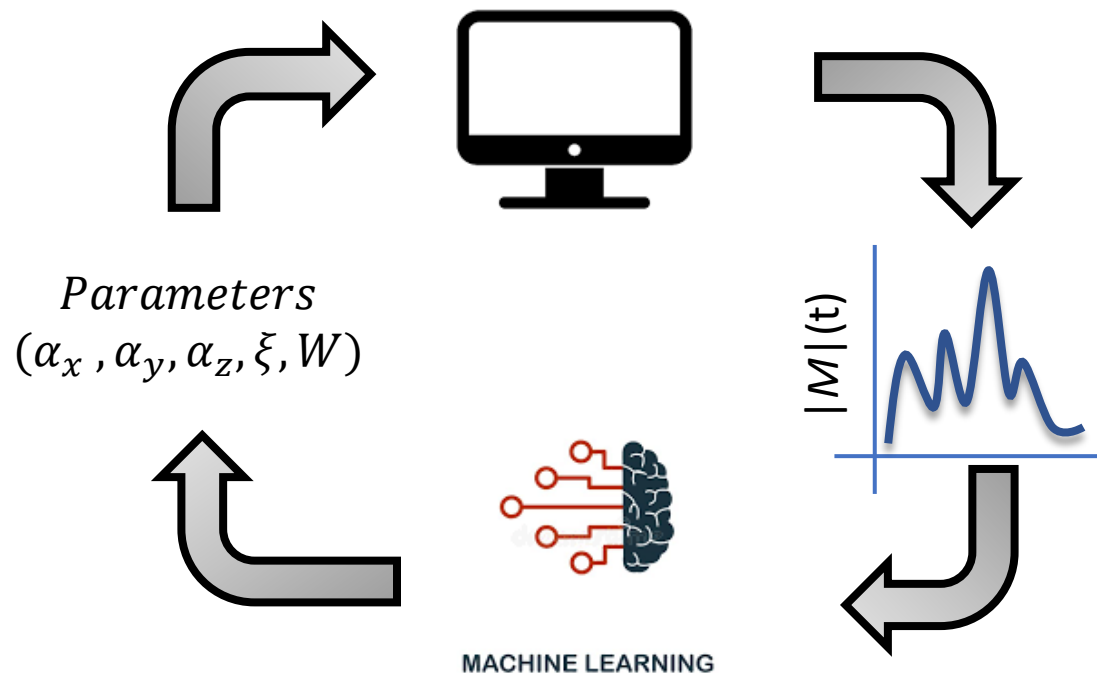*Department of Physics, Indian Institute of Science Education and Research Pune, India
[++]Department of Physics, Brown University, Providence, Rhode Island 02912-1843, USA
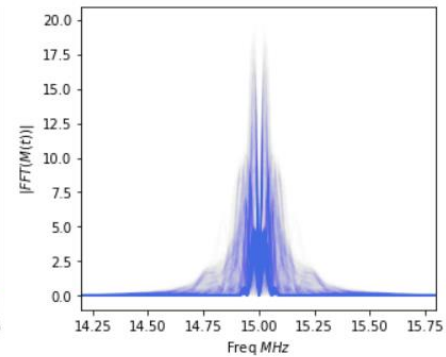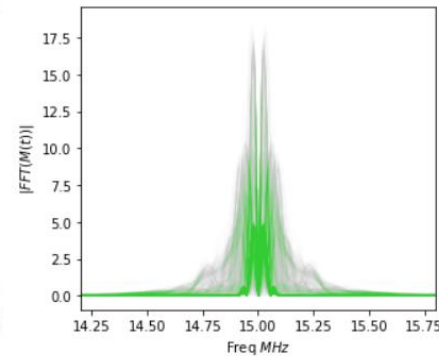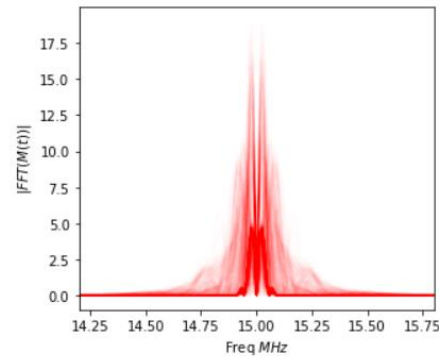[+++]Department of Physics and Astronomy, Dartmouth College, Hanover, NH 03755, USA
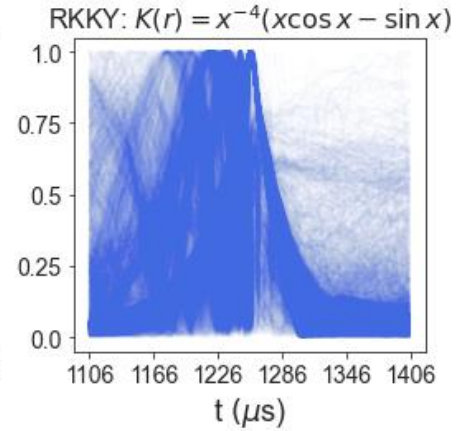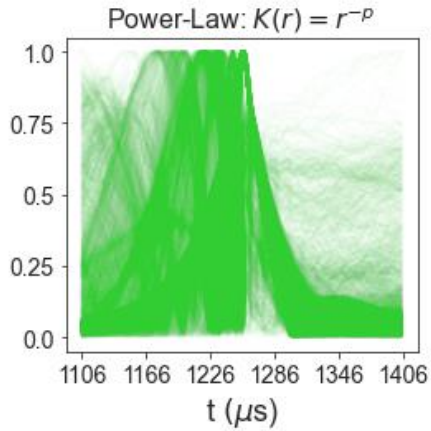
The Problem:

Artificial Intelligence → Develop Novel Quantum Materials and Quantum Control using NMR

$Parameters$
$(\alpha_x, \alpha_y, \alpha_z, \xi, W)$

$|M|(t)$

MACHINE LEARNING

optimal control

control pulse

measurement

https://qusco-itn.eu/2020/06/19/intro_nvc/

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DATASET

Spin Echo insilico experiment data

Radial Kernel Types

$\xi_{rkky} = 13$
$\xi_g = 8$
$p = 1.447$

Gaussian : $K(r) = e^{r/\xi^2}$

Power-Law: $K(r) = r^{-p}$

RKKY: $K(r) = x^{-4}(x\cos x - \sin x)$

METHODS :

DATA
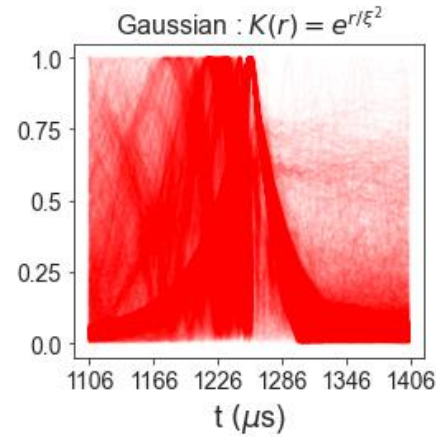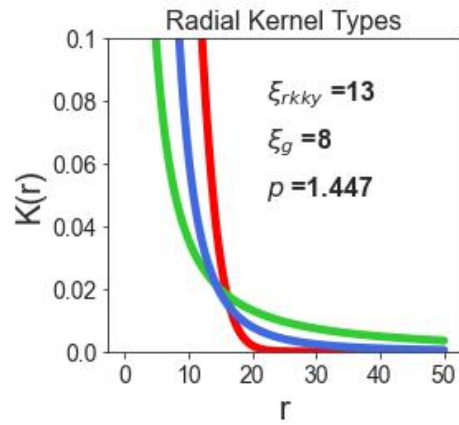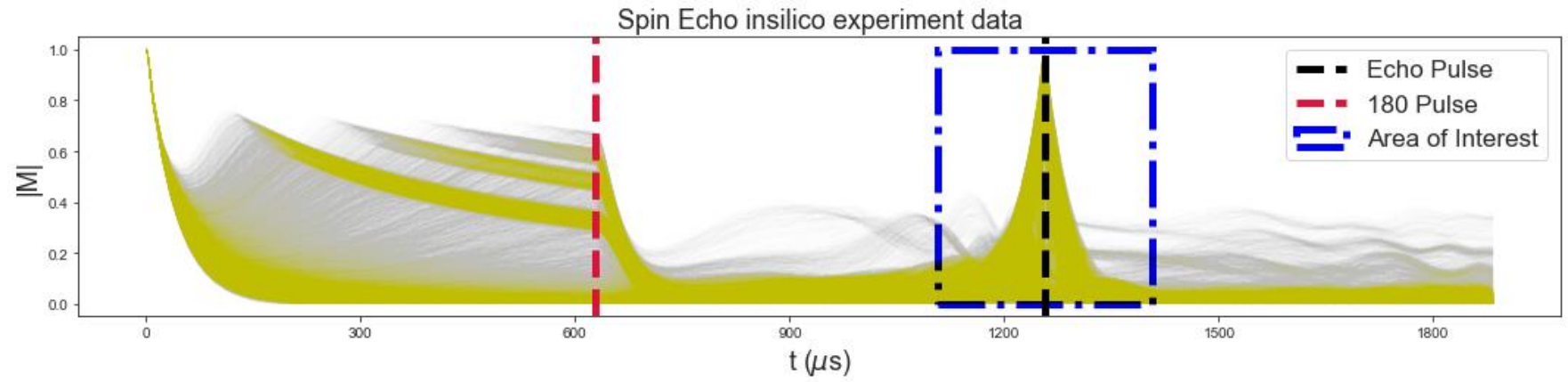
Pointwise features   Polynomial features
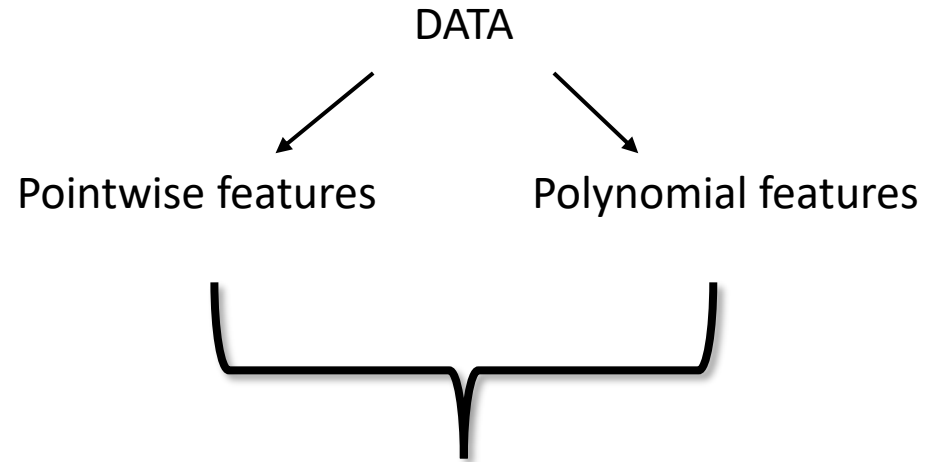
(I) Regression
(II) Classification
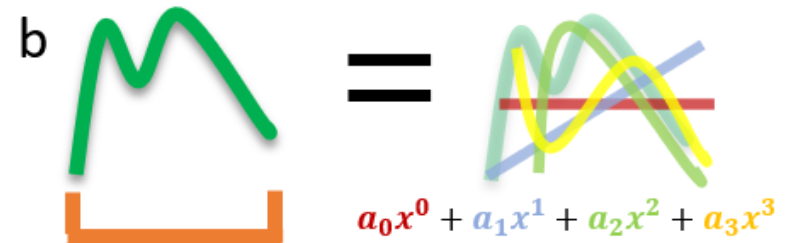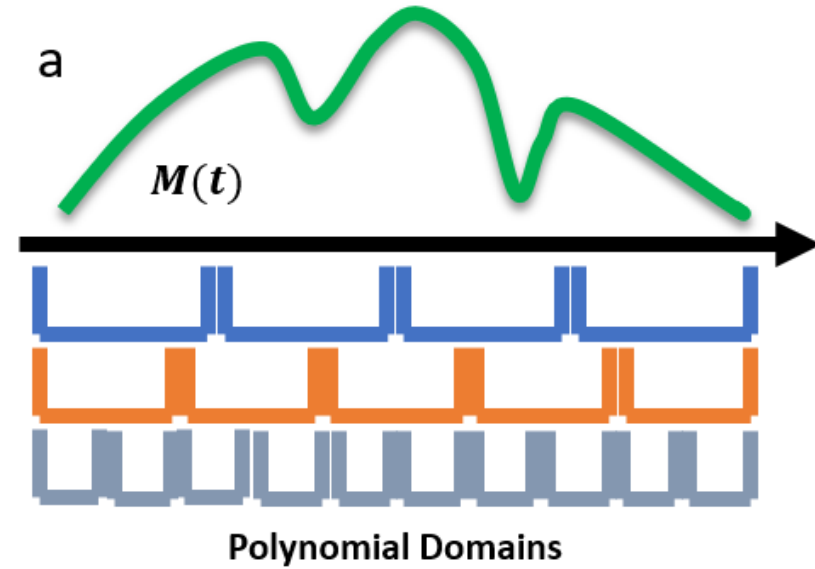
Polynomial Feature Extraction

$$a_0x^0 + a_1x^1 + a_2x^2 + a_3x^3$$
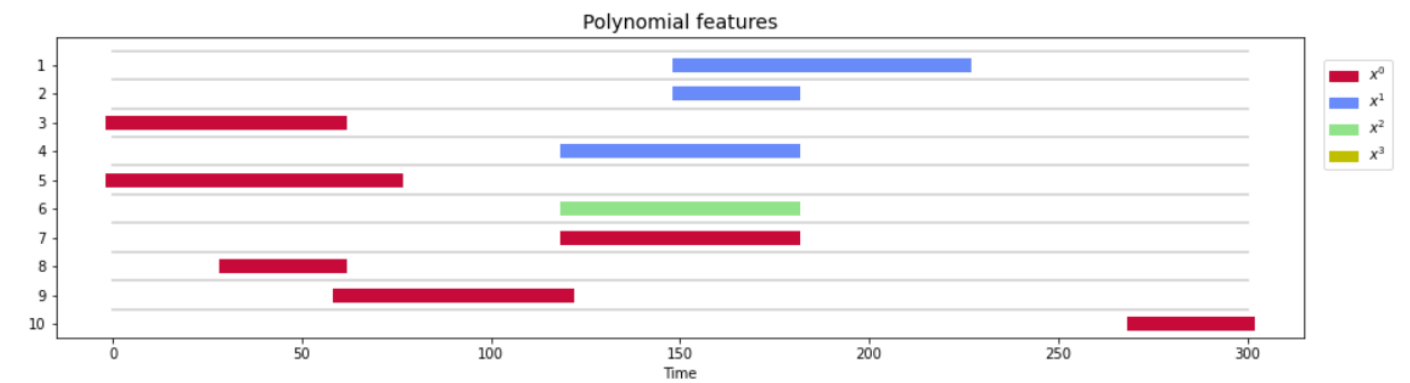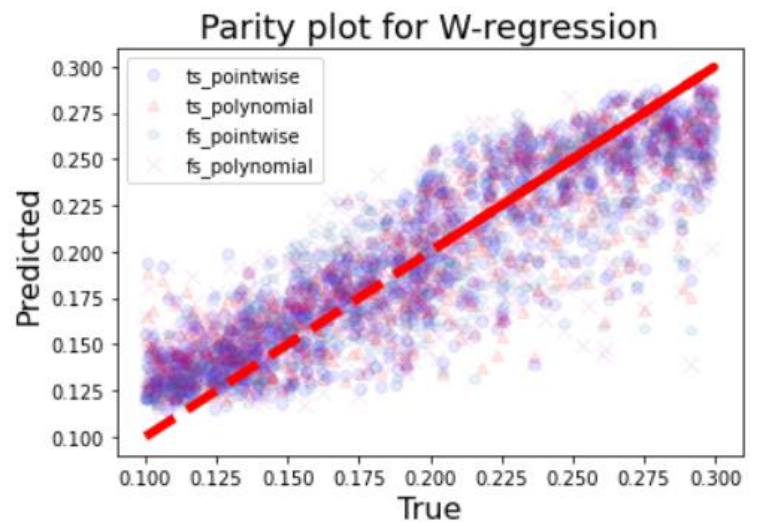
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Results – Regression on W
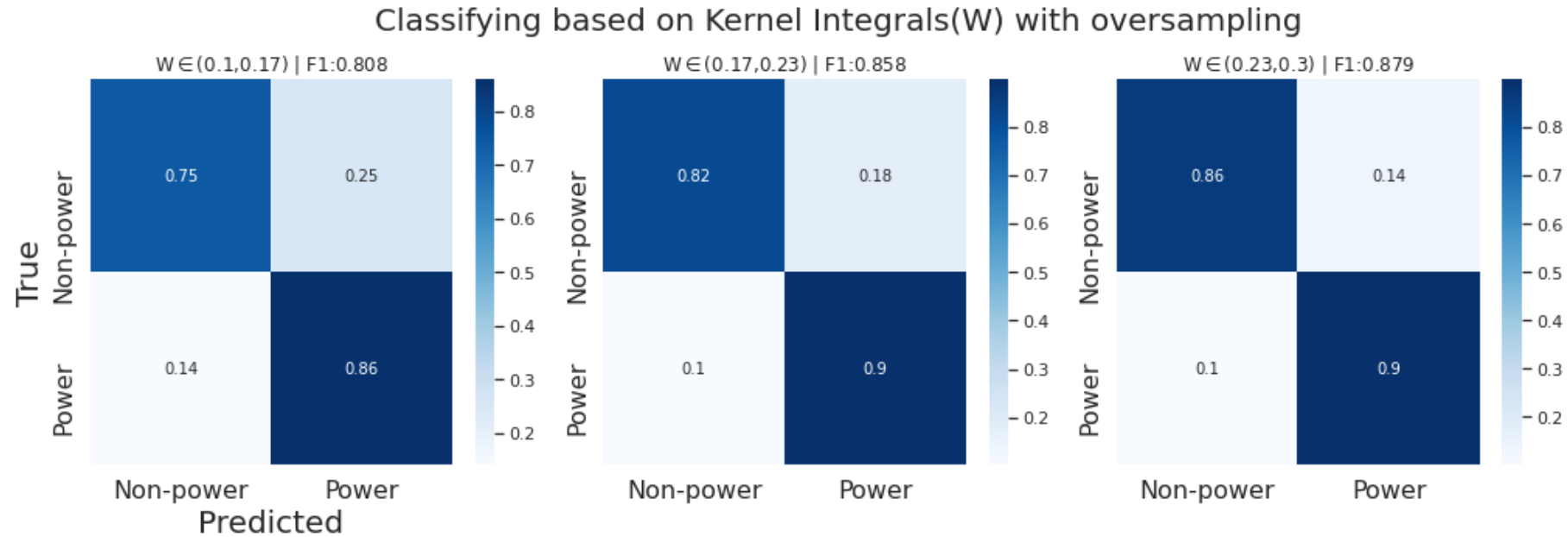

Parity plot for W-regression

Feature importance based on mean decrease in impurity for W regression

Pointwise features

Polynomial features
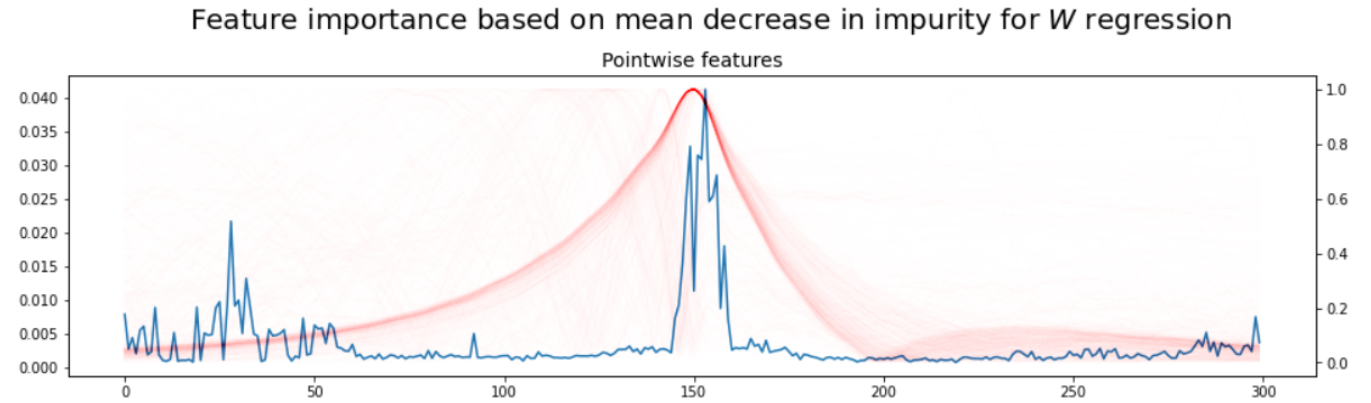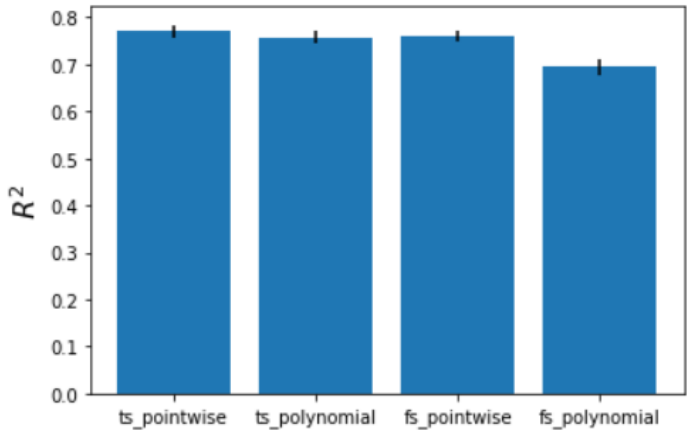
Results – Classification based on interaction type

Classifying based on Kernel Integrals(W) with oversampling

➢ We are able to classify long-range interactions (Power-law) and short-range interactions (Gaussian and RKKY) solely based on the the shape of the Echo Curve with an F1 score of ~0.88
➢ With knowledge of the type of interaction, we were able to predict the value of the kernel integral with an R^2 of ~0.8

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THANK YOU

Github Repository : Anantha-Rao12/Decoding-Quantum-States-with-NMR