The use of Deep Learning for PWRA estimation, performance analysis and comparison with other technique

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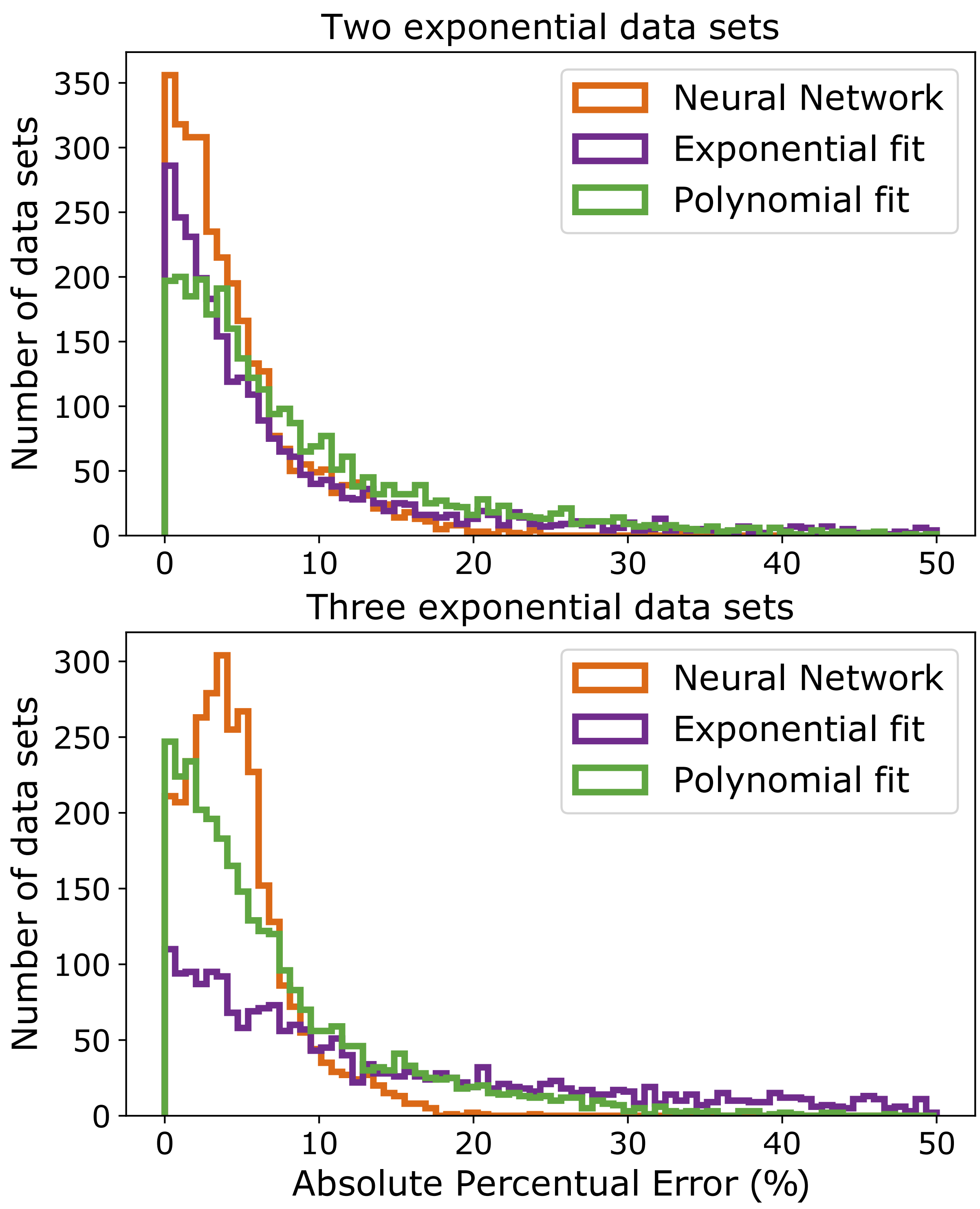
Scope:

The spin-lattice relaxation (T1, or T1ρ) of abundant nuclei in solids, is heavily affected by the spin diffusion process, often generating a non-exponential relaxation decay. The Population Weighted Rate Average (PWRA) is not affected by spin diffusion [1] and therefore its correct measurement could be exploited to obtain reliable dynamic information [2] even in the presence of spin diffusion.
The scope of this work is trying to apply and compare the following different PWRA estimation methods:
1) Exponential fitting
2) Polynomial fitting
3) Neural Network Ensemble

$$PWRA = \frac{\sum_n w_n R_{1(\rho)n}}{\sum_n w_n}$$



Conclusions:

Deep Learning has low mean absolute percentual estimation error compared to multi exponential fitting or polynomial fitting, and it also produces fewer outliers

Data	Method	Mean Absolute Percentual Error	1st Quartile APE	2nd Quartile APE	3rd Quartile APE	Max APE	Inter Quartile Range APE	Mean Squared Error 10^{-3}	Bias 10^{-3}	Standard deviation
2 exp	Exponential fit	174.57	1.95	5.16	15.06	1.28 e+05	13.11	196.32	61.7	0.44
	Neural Network	6.99	1.77	4	8.2	101.85	6.43	0.04	-0.46	0.01
	Polynomial fit	9.12	2.59	5.69	11.83	103	9.23	0.04	-0.55	0.01
3 exp	Exponential fit	2690.68	5.94	22.73	69.22	2.15 e+06	63.28	930858	802.83	30.5
	Neural Network	6.54	1.4	3.11	6.67	58.57	5.27	0.07	-2.38	0.01
	Polynomial fit	7.33	2.16	4.97	9.88	55.97	7.72	0.04	-1.66	0.01

Methods:

- Test data: Synthetic relaxation dacays generated using 2 or 3 exponential function with 3 combination of relaxation times ranging form 15 to 45 au, 5 weight combination and two white noise intensity 15 and 50. Linearly sampled on 41 points rangeing from 0.01 to 40 au. Globally 3000 sets of data were generated and tested with the three different methods.
- Exponential fit: We fit 2 or 3 exponential components to our data using the software Mathematica
- Polynomial fit: We fit 4^{th} order polynomials to estimate the gradient of the decay at t=0 which is equal to minus the PWRA
- Neural Network Ensemble: We train 50 NN (7 Dense layers) to estimate the PWRA from the experimental data, and then we take the average between their estimations

[1] A.M. Kenwright, B.J. Say, Solid State NMR 7, 86 (1996).
[2] M. Geppi, R.K. Harris, A.M. Kenwright, B.J. Say, Solid State NMR 12, 15 (1998).

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