

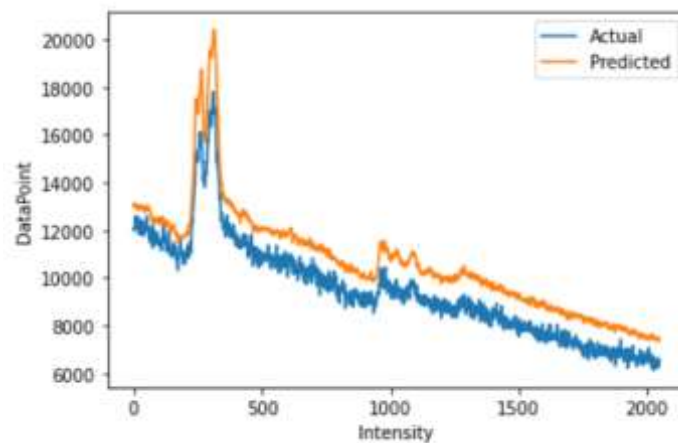
LSTM Higher-Level Approaches

Two approaches have been discussed and implemented so far w.r.t to sequencing the LSTM input and trying to predict a new sequence (i.e., future spectra). We have conceptualized a “randomized spectra scrambling” testing which will be implemented in the upcoming week that would further validate if we would want to go ahead with **Approach 1** or **Approach 2**. We will also be looking if there are any alternative approaches that could be explored.

Approach 1:

Sequencing the data such that the prediction value at a particular Energy level is only influenced by the previous sequences at the same energy level. Here, we try to predict the intensity value at a single Energy level value. We make predictions individually for each Energy level.

	0	1	2	3
0	16890.533203	16871.441406	16935.539062	16695.902344
1	15170.534180	15365.441406	15048.539062	15032.902344
2	15444.534180	15560.441406	15617.539062	15516.902344
3	15270.534180	14962.441406	15048.539062	14950.902344
4	15591.534180	15681.441406	15588.539062	15808.902344
5	15939.534180	15786.441406	16375.539062	16139.902344
6	15933.534180	16274.441406	16383.539062	15959.902344



Approach 2:

Sequencing the data such that the prediction values at a time step depends on the entire spectra at the previous time step. Here, we consider the fact that discrete Energy levels have intensities not completely independent of one another. Hence, we try to predict the entire the spectra a particular time-step based on the entire spectra from previous sequences.

	0	1	2	3
0	16890.533203	16871.441406	16935.539062	16695.902344
1	15170.534180	15365.441406	15048.539062	15032.902344
2	15444.534180	15560.441406	15617.539062	15516.902344
3	15270.534180	14962.441406	15048.539062	14950.902344
4	15591.534180	15681.441406	15588.539062	15808.902344
5	15939.534180	15786.441406	16375.539062	16139.902344
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