Uncertainty quantification of spin-parity assignments in ^{19}Ne unbound states

Ben Wood

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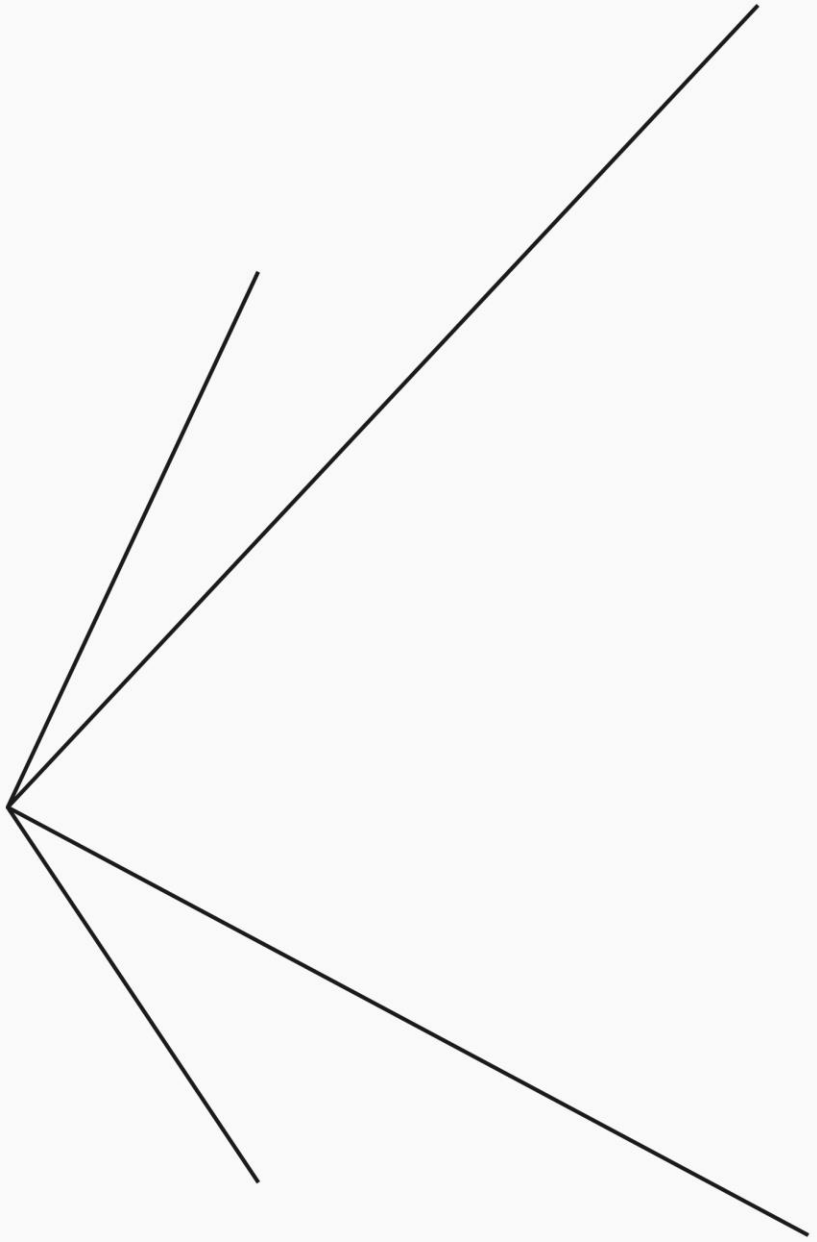
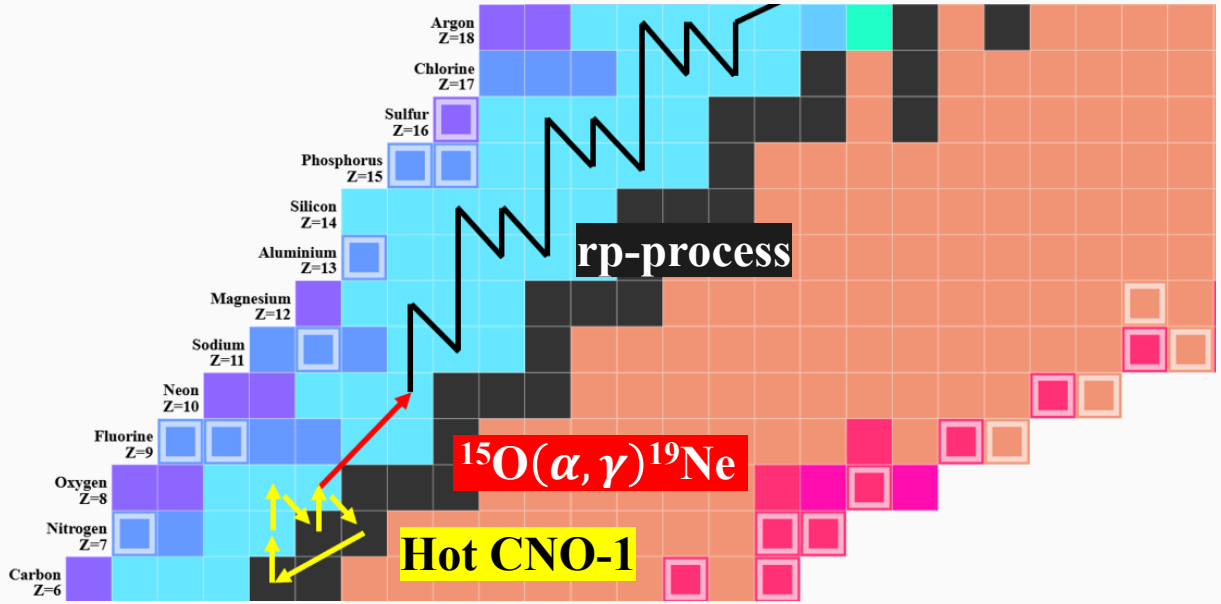
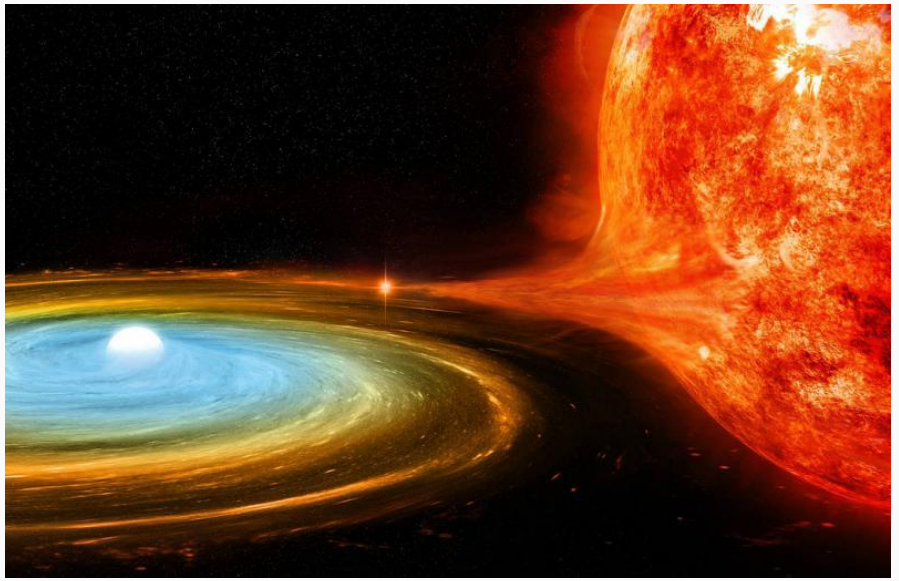


Background: ^{19}Ne unbound structure

- X-ray bursts: rapid thermonuclear burning on accreting neutron stars
- $^{15}O(\alpha,\gamma)^{19}Ne$ controls breakout from hot CNO to rp-process
- Reaction rate dominated by near α-threshold ^{19}Ne resonances



Reaction pathways for hot CNO-1 cycle and rp-process, with breakout reaction.



Artistic impression of neutron star accreting matter from nearby companion [1]

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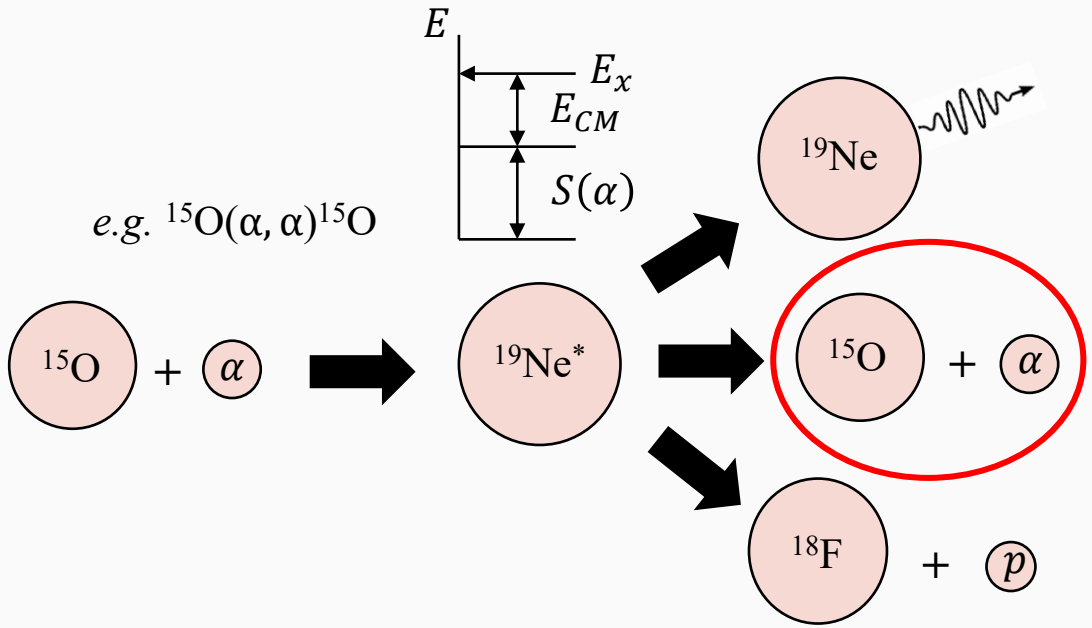
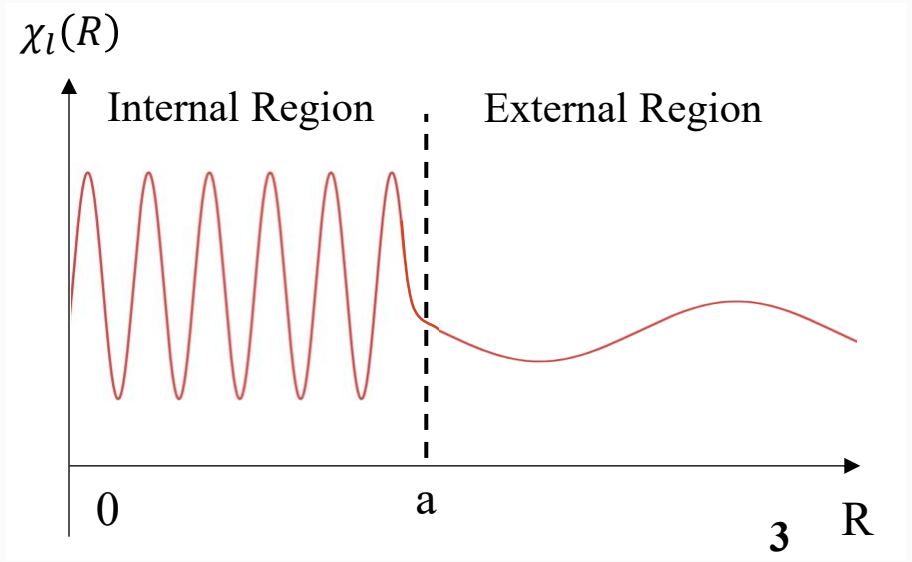
Background: *R*-matrix theory

- Compound reactions described by discrete resonances coupled to reaction channels
- Internal region (R < a):
  - Nuclear potential
  - Complicated many-body interaction
  - Parameterised as: $$\mathbf{R}(E) = \sum_{n=1}^{N} \frac{\gamma_n^2}{\epsilon_n - E}$$
- External region (R > a):
  - Coulomb potential only
  - Match *R*-matrix at channel radius
  - Calculate scattering amplitude and cross-sections





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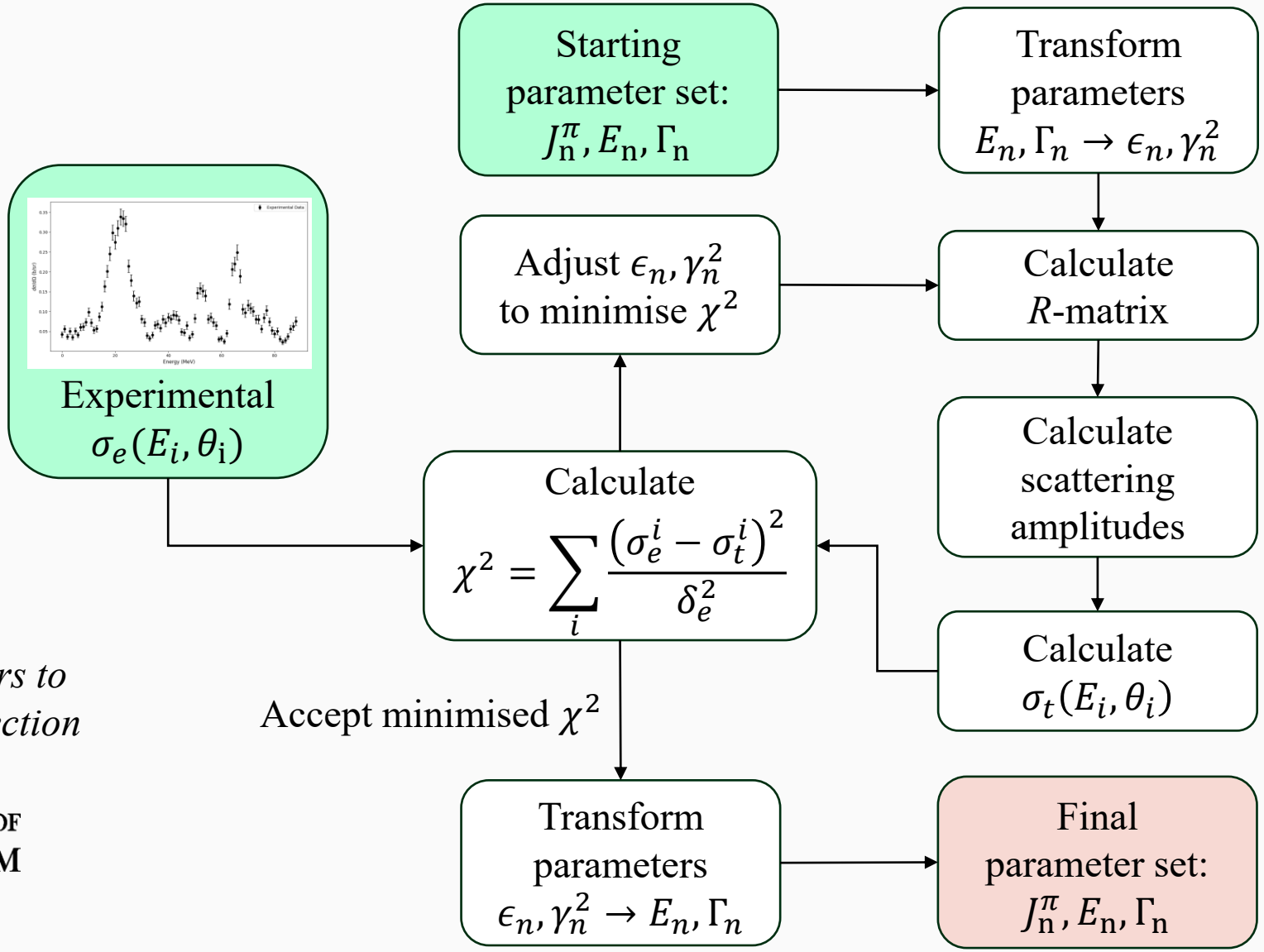
Background: *R*-matrix phenomenology



Note: $\sigma(E, \theta)$ refers to differential cross section

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Motivation

- Discrete spin-parity assignments:
  - Require confident prior information
  - Tedious trial-and-error
  - Degenerate solutions
  - Difficult uncertainty quantification

- Continuous energy and width parameters:
  - Dependent on starting parameters
  - Stuck in local minima
  - Underestimated uncertainties

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- Continuous energy and width parameters:
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- This work:
  - Predict J^{π} assignments sequentially with ML
  - Quantify assignment uncertainties
  - Refine E, Γ parameters with AZURE2 fit
  - **Improve confidence of ^{19}Ne unbound structure**

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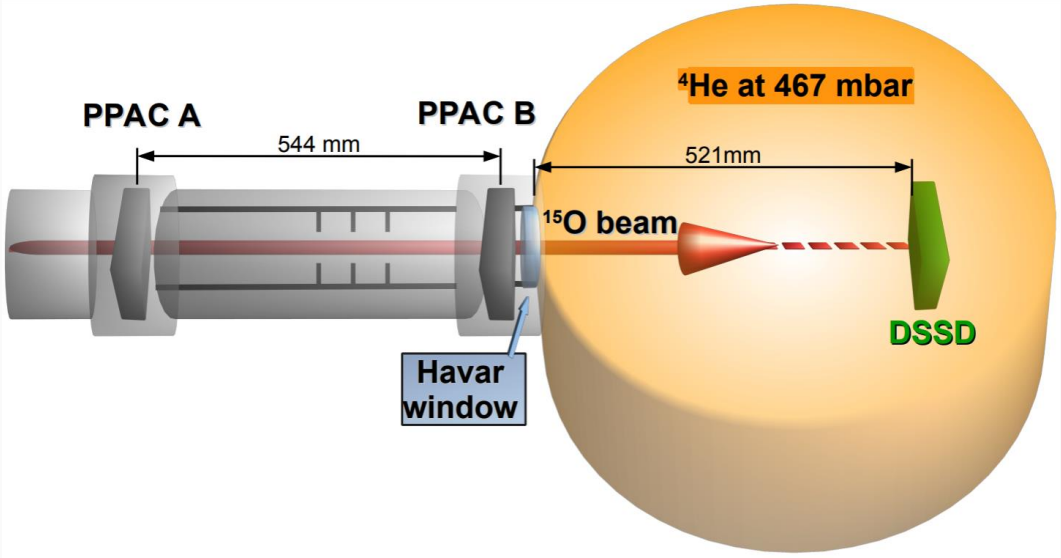
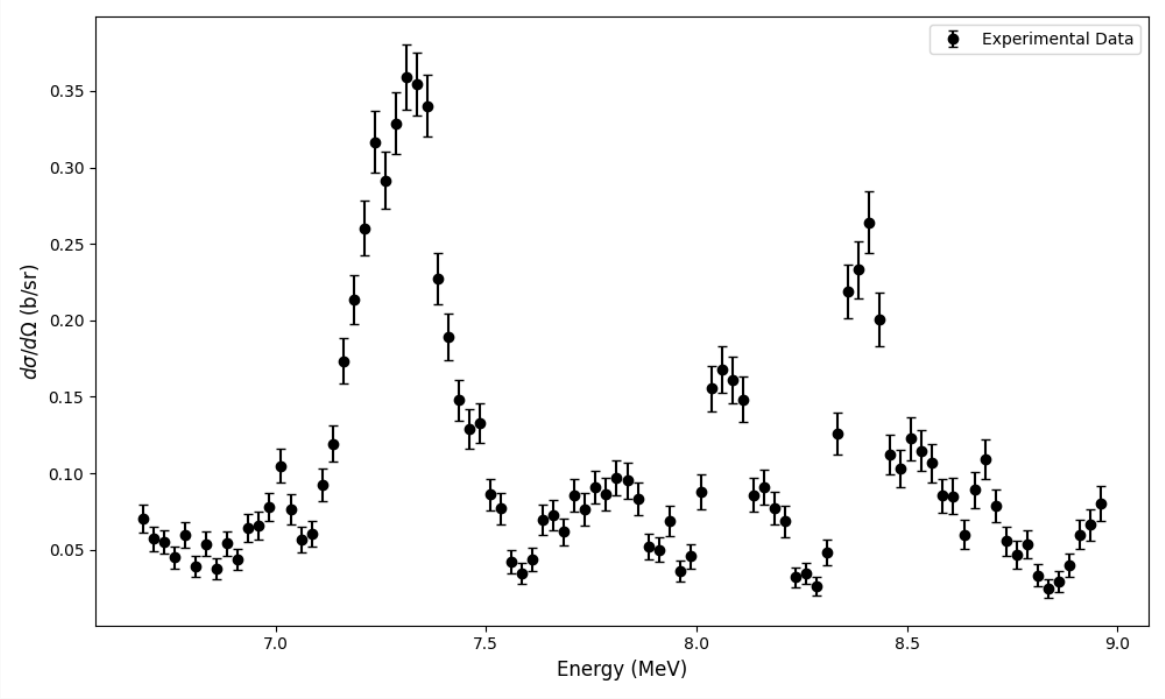
Experimental data

- TTIK ^{15}O beam on ^{4}He gas
- DSSD detects scattered α's at $\sim 0°$
- TOF and detected energy for PID
- 50 keV FWHM energy resolution



Experimental setup for resonant scattering [2]



Experimental differential cross-section spectrum [2]

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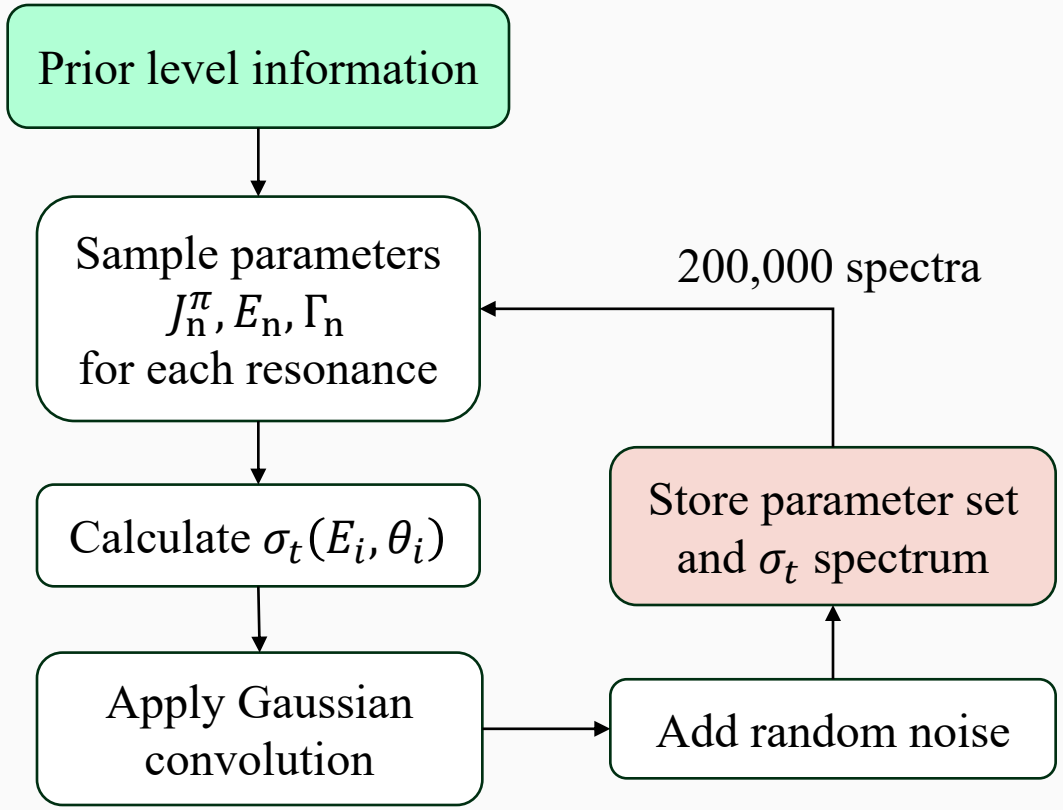
Synthetic data generation



- $^{15}\mathrm{O}(1/2^-) + \alpha(0^+)$
- Channel spin: $s = 1/2 \oplus 0 = 1/2$
- Orbital angular momentum: $l = 0,1,2, \ldots$
- $J = l \oplus s = |l \pm 1/2|, \quad \pi = (-1)^{l+1}$

- For each resonance:
  - Choose J^{π} up to $l = 6$
  - Add random noise to E_{prior}
  - Calculate $\Gamma_W(l, E)$
  - Select Γ up to $\Gamma_W(l, E)$
  - Include random background poles

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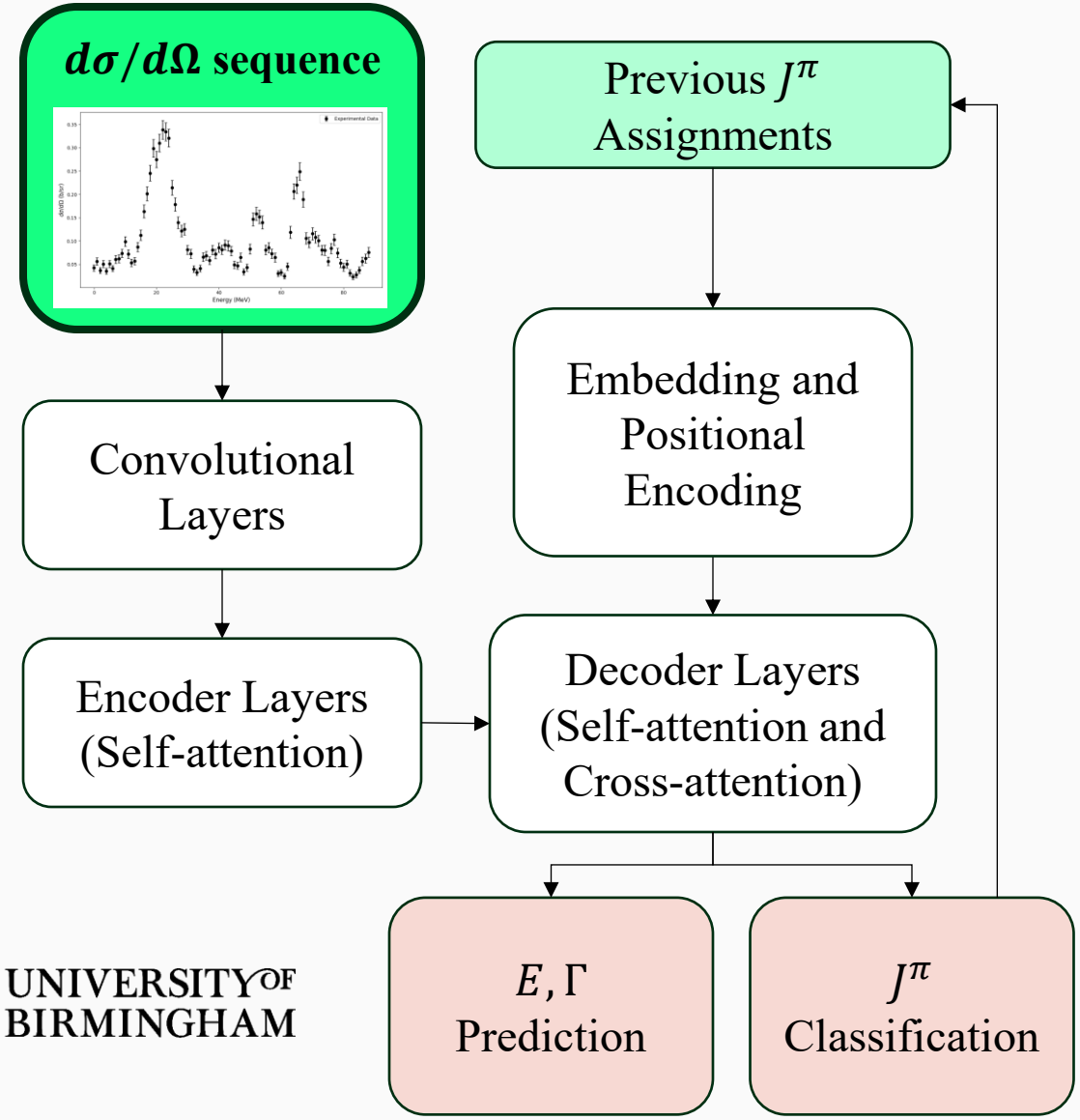
ML Architecture



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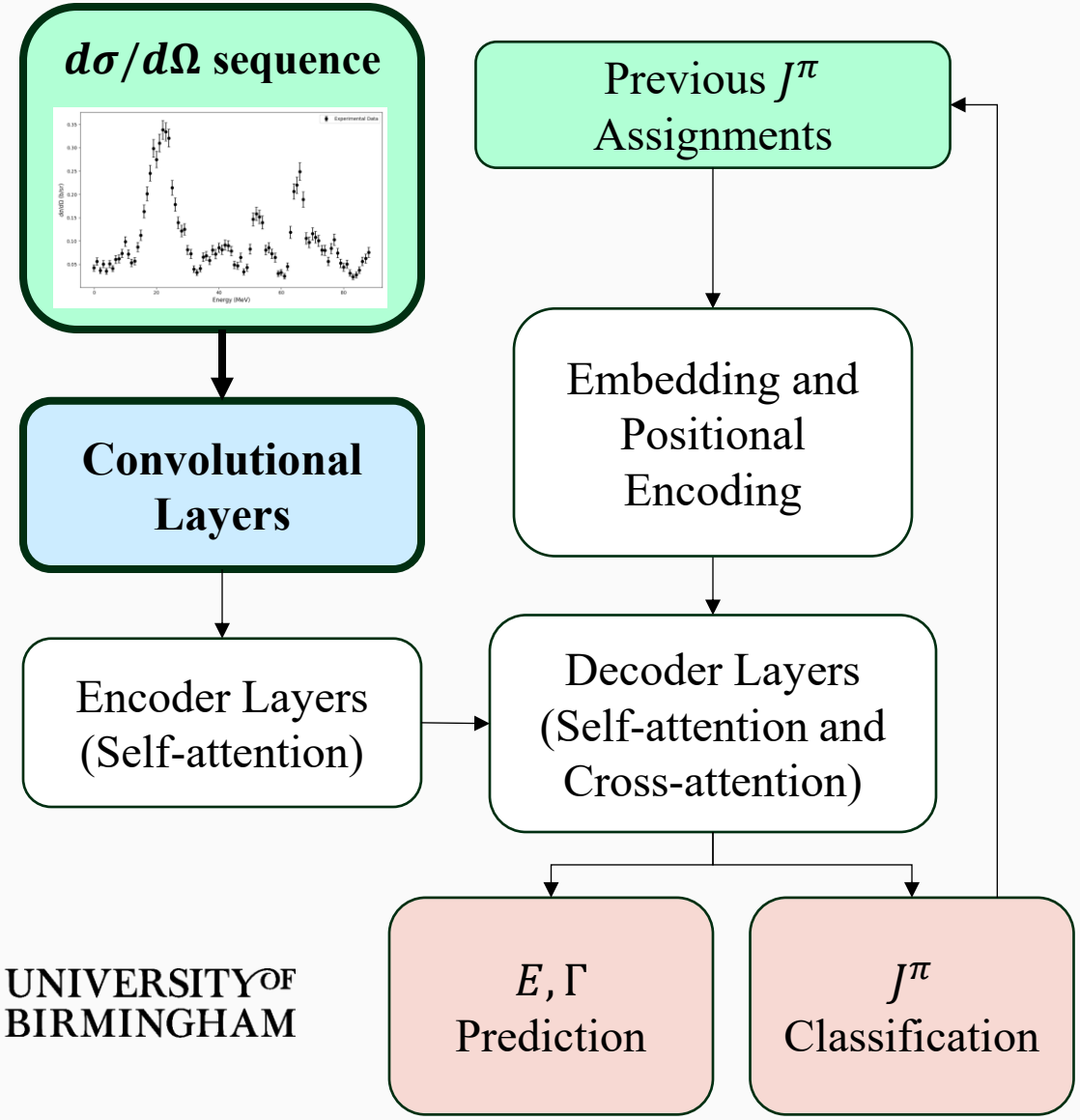
Encoder-decoder transformer: Vaswani *et. al.* [3]

ML Architecture



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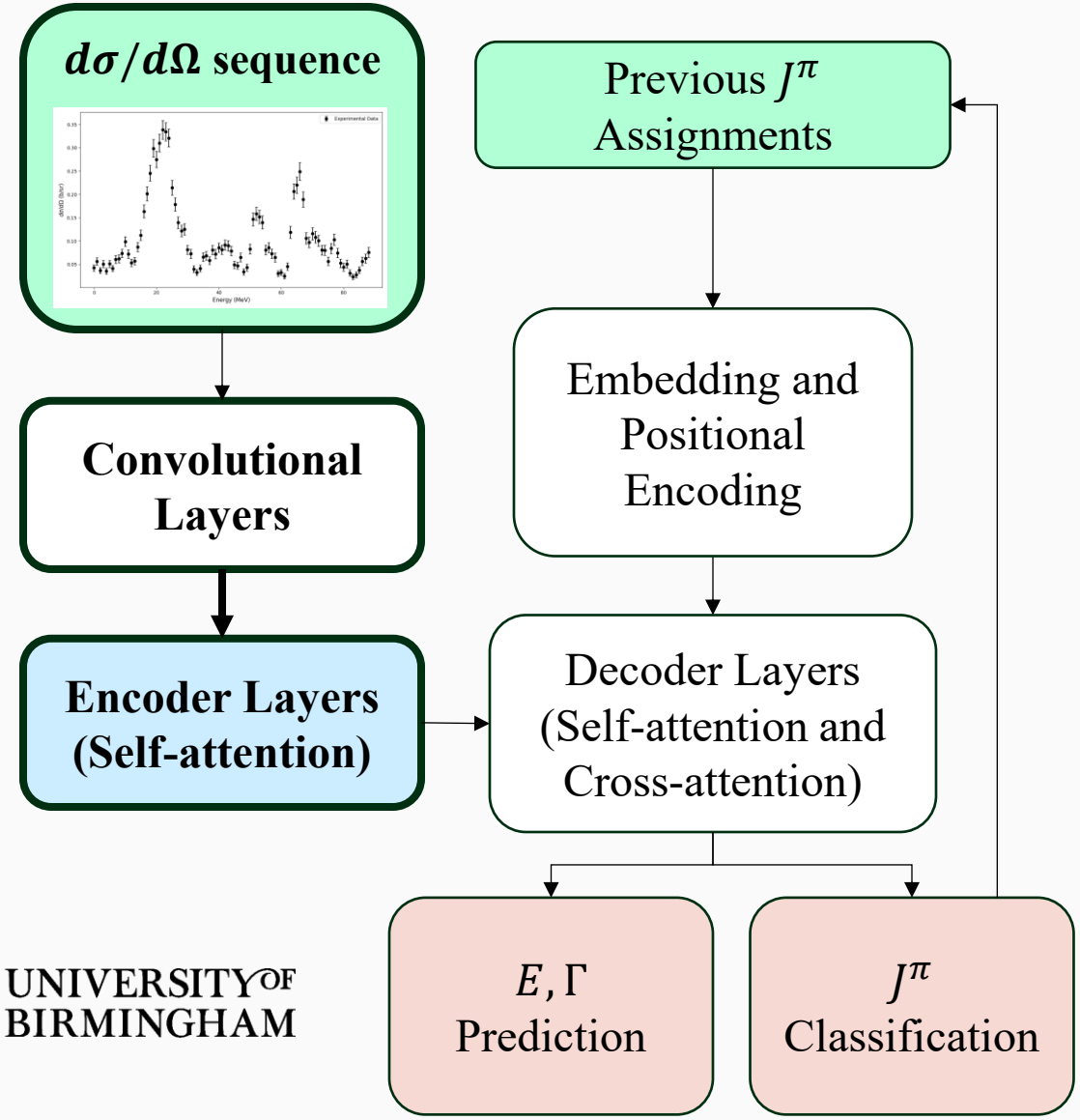
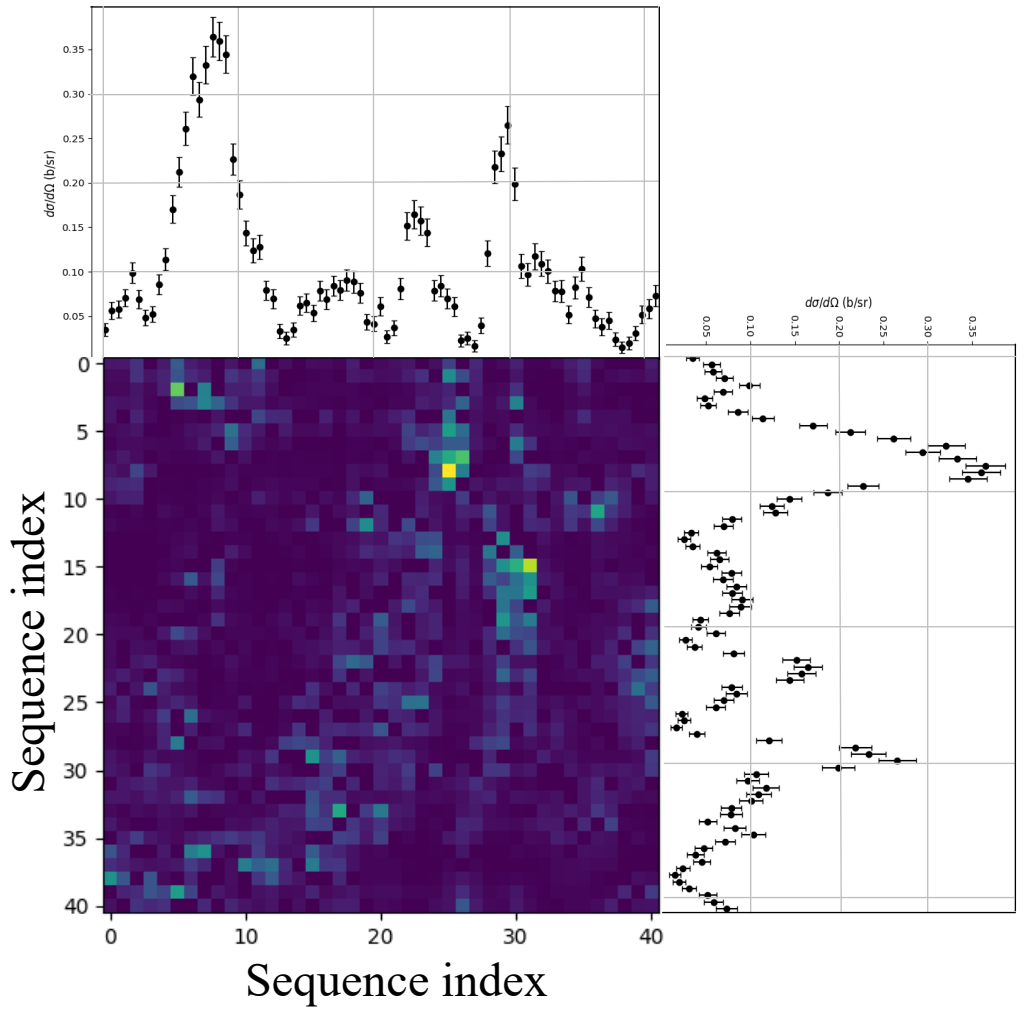


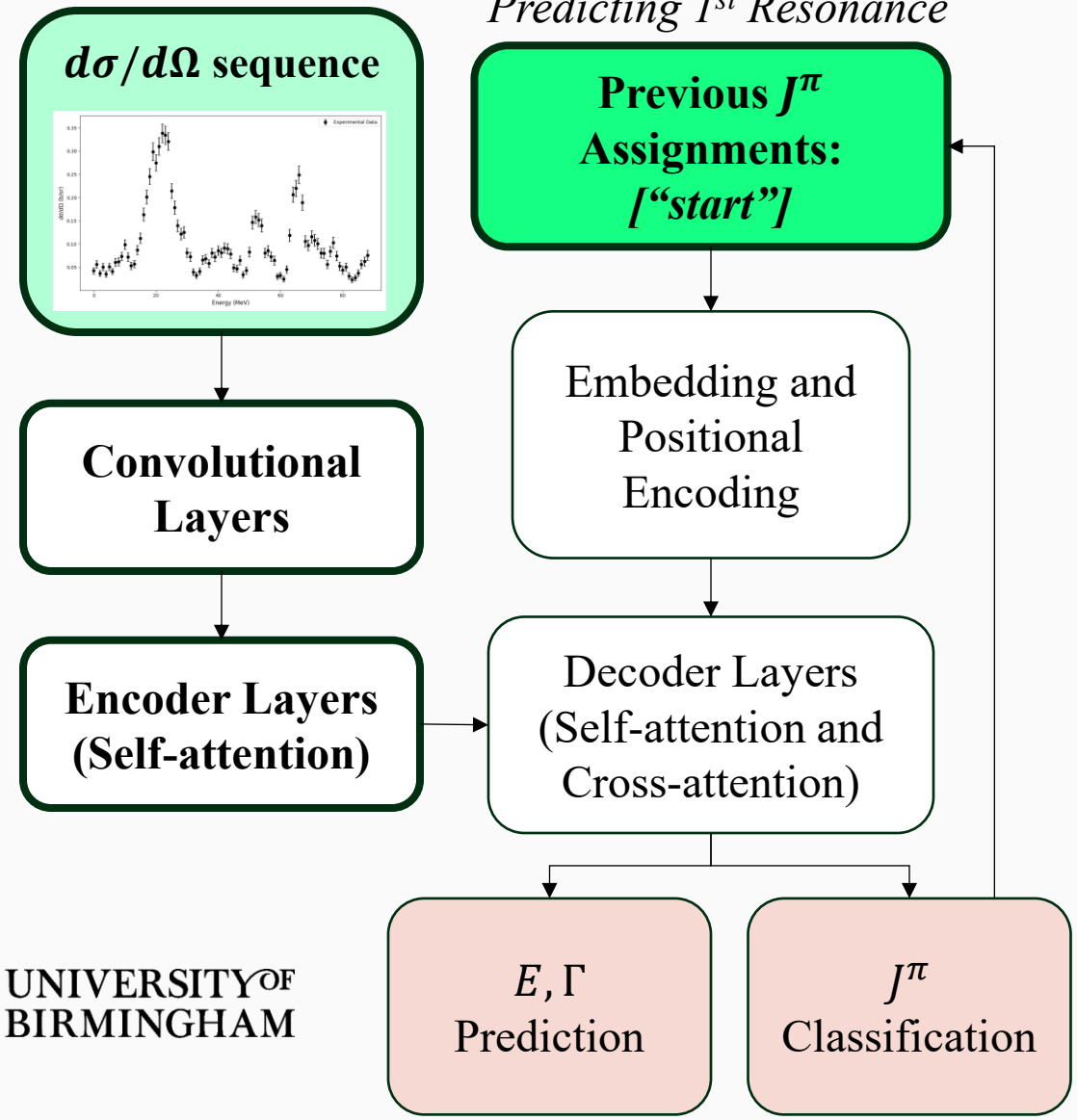
Encoder self-attention:
Captures correlations across input spectrum



Encoder-decoder transformer: Vaswani *et. al.* [3]

ML Architecture

Predicting 1st Resonance



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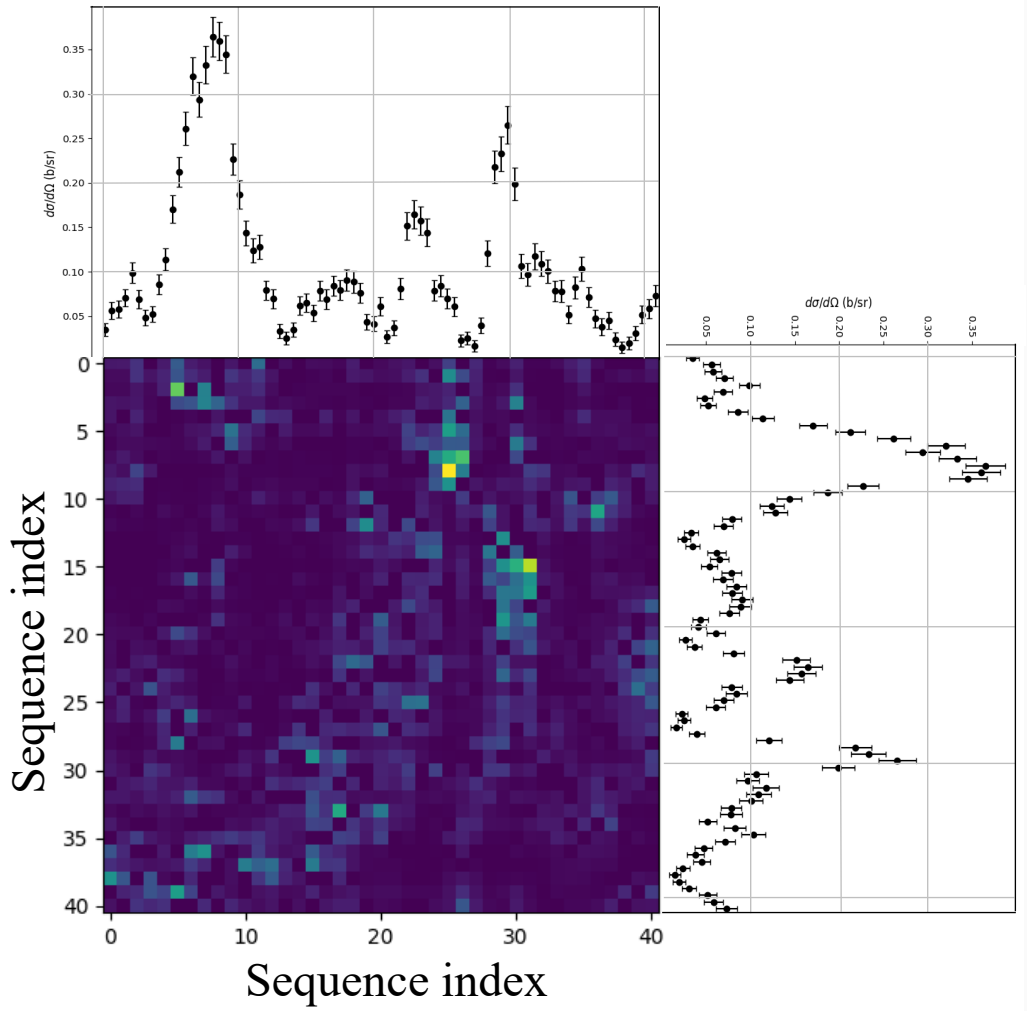

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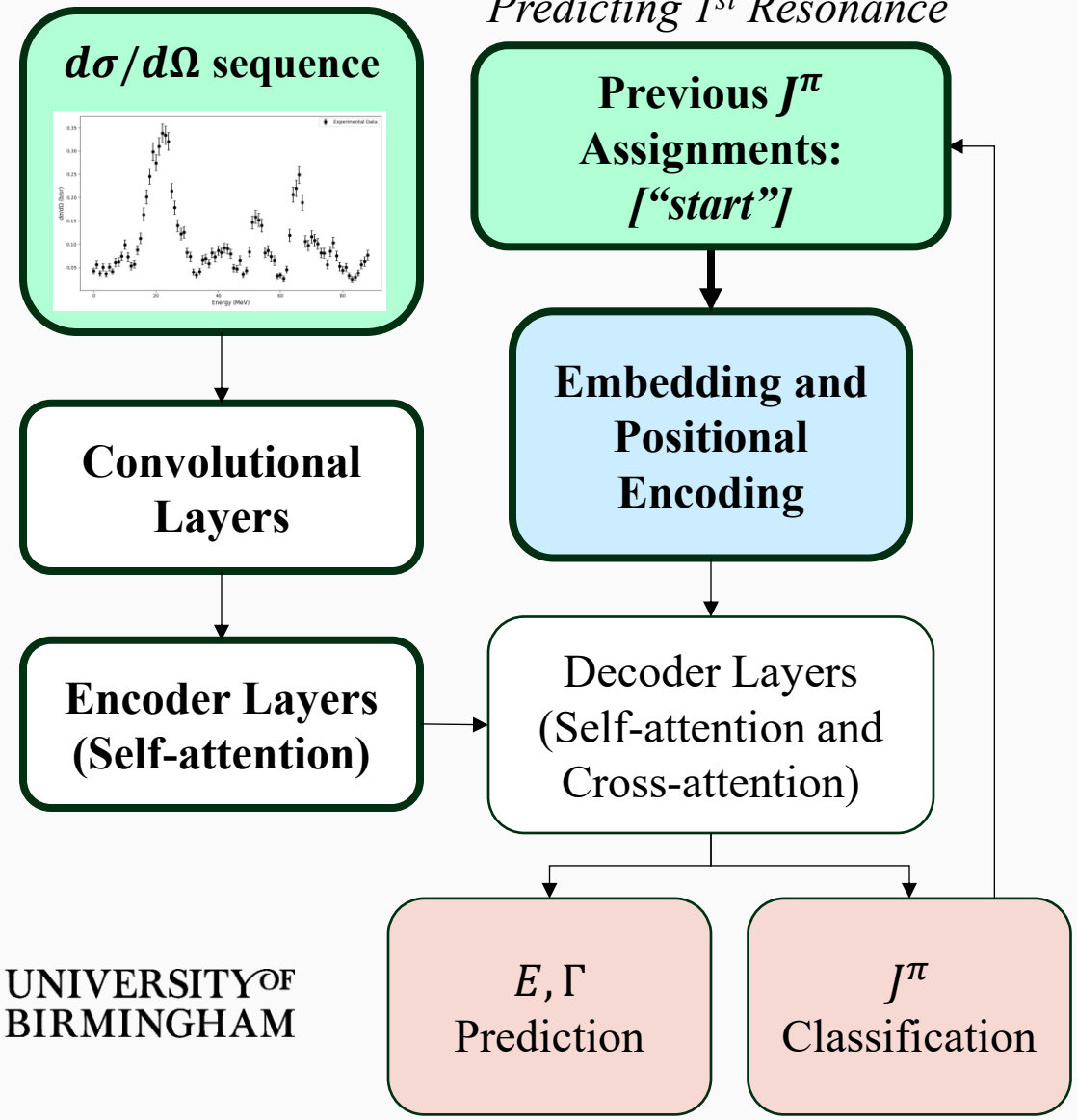

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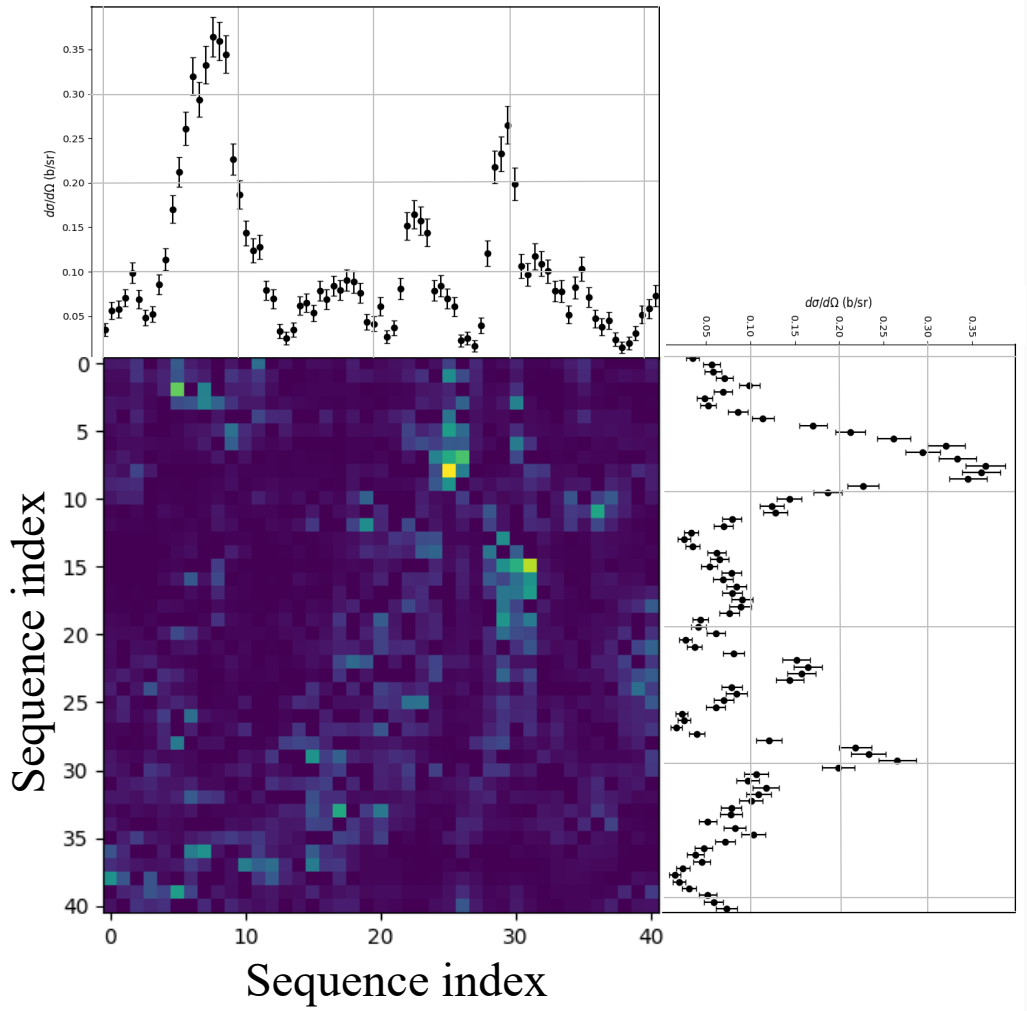

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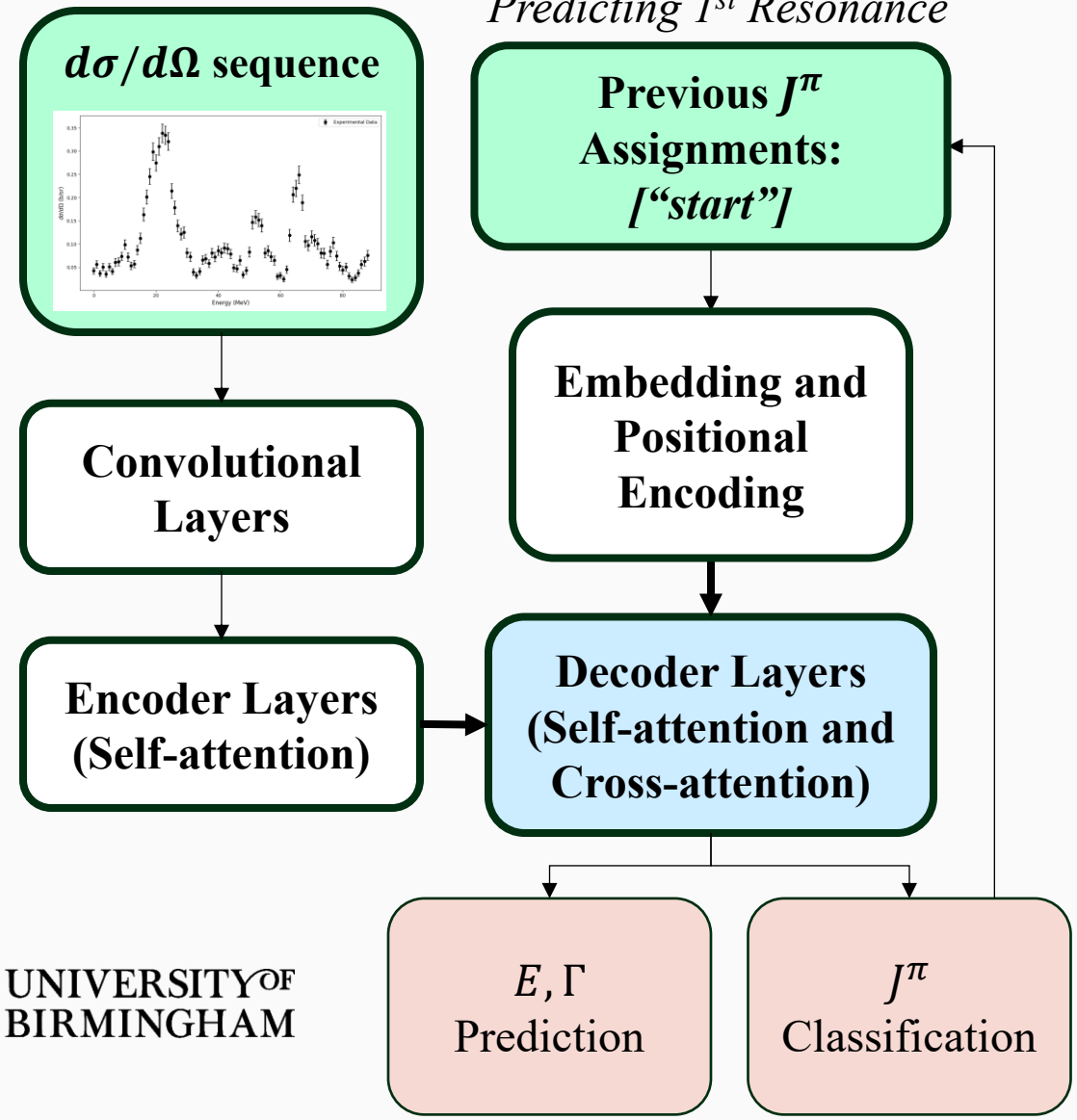
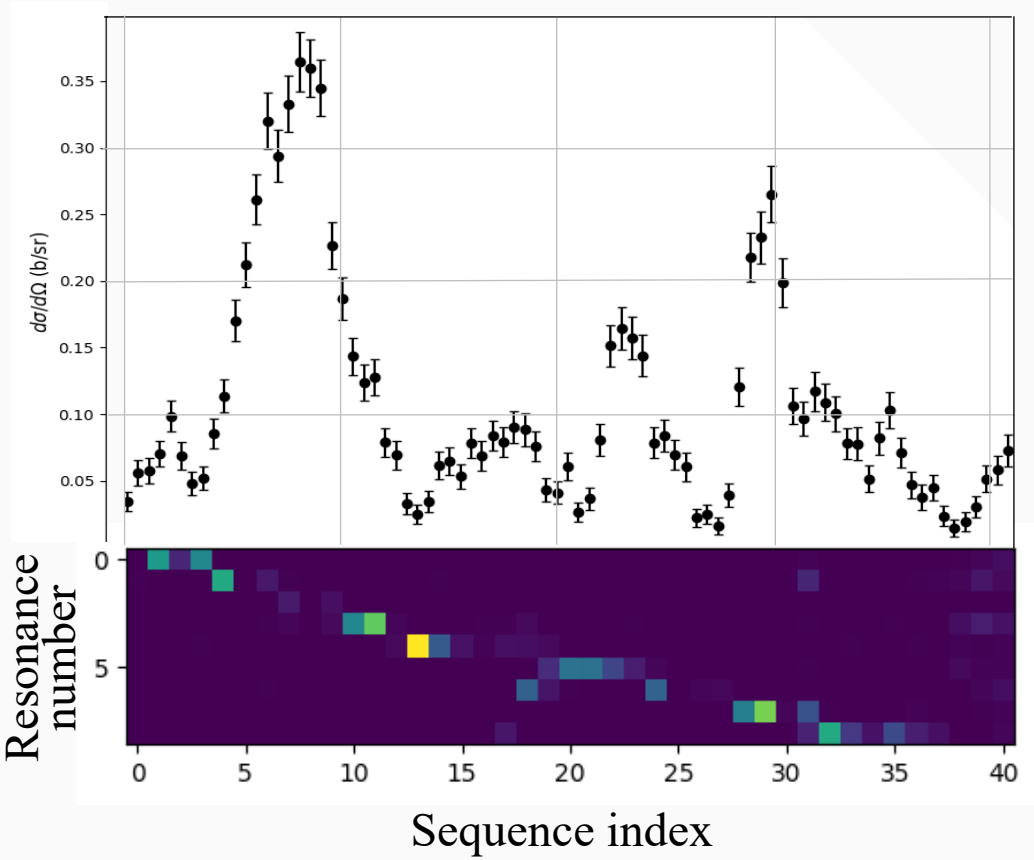


Decoder cross-attention:
Selects relevant parts of spectrum for sequence prediction



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Encoder-decoder transformer: Vaswani *et. al.* [3]

ML Architecture

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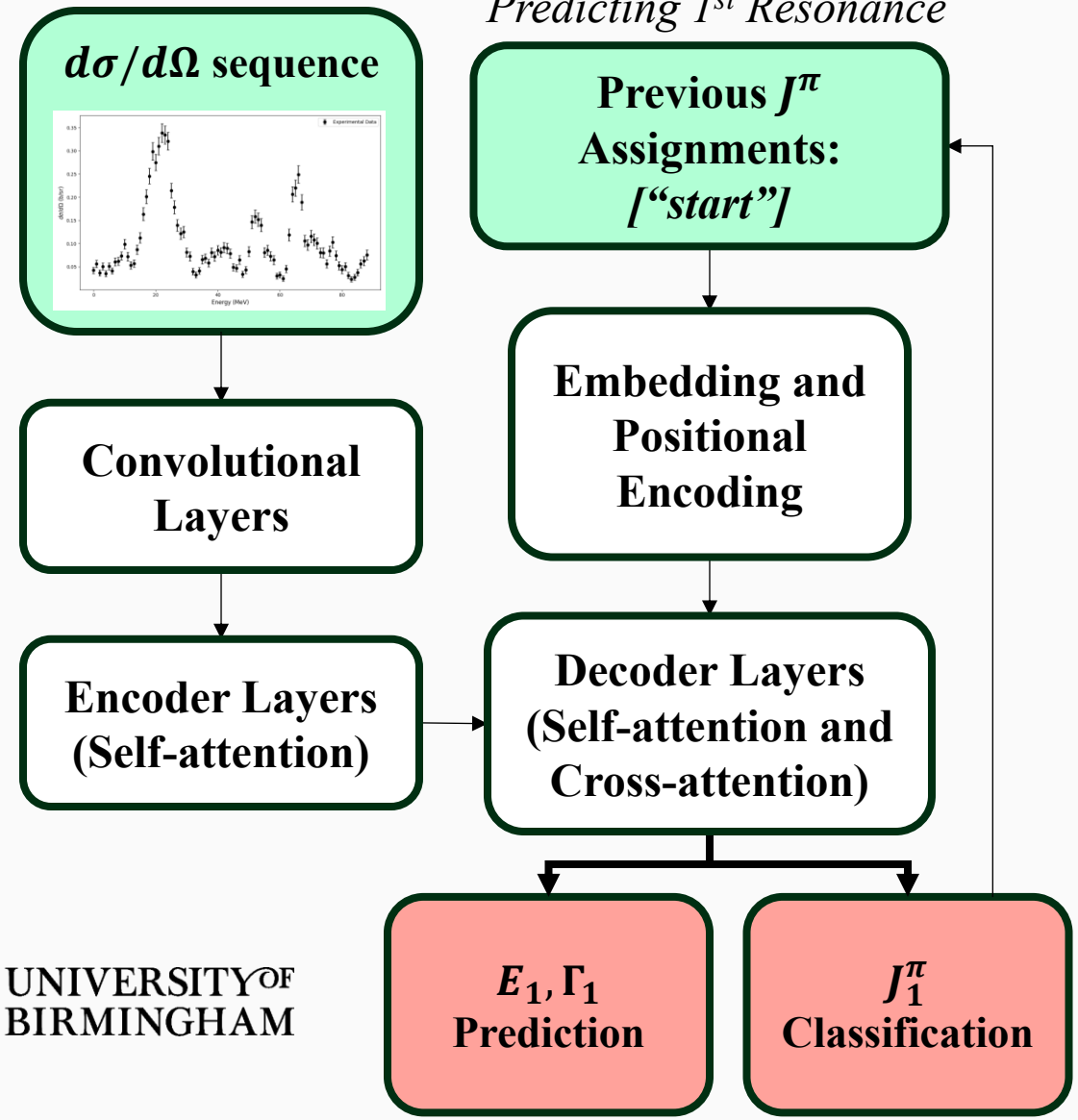

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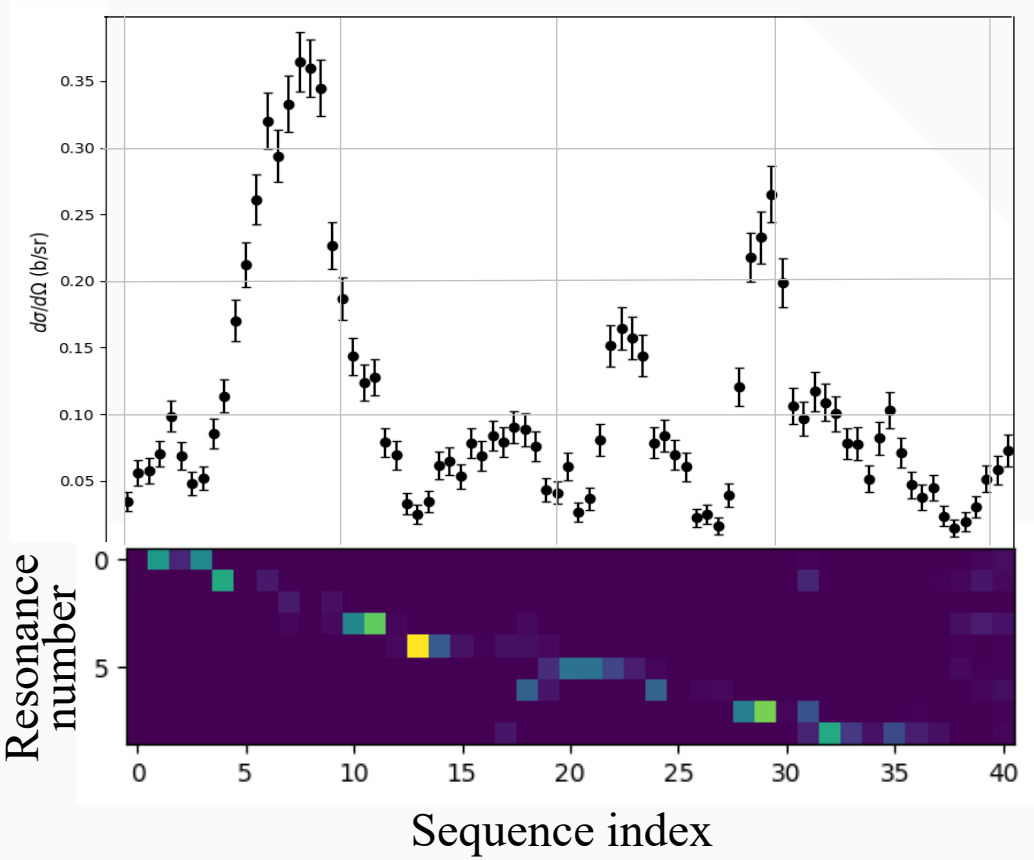

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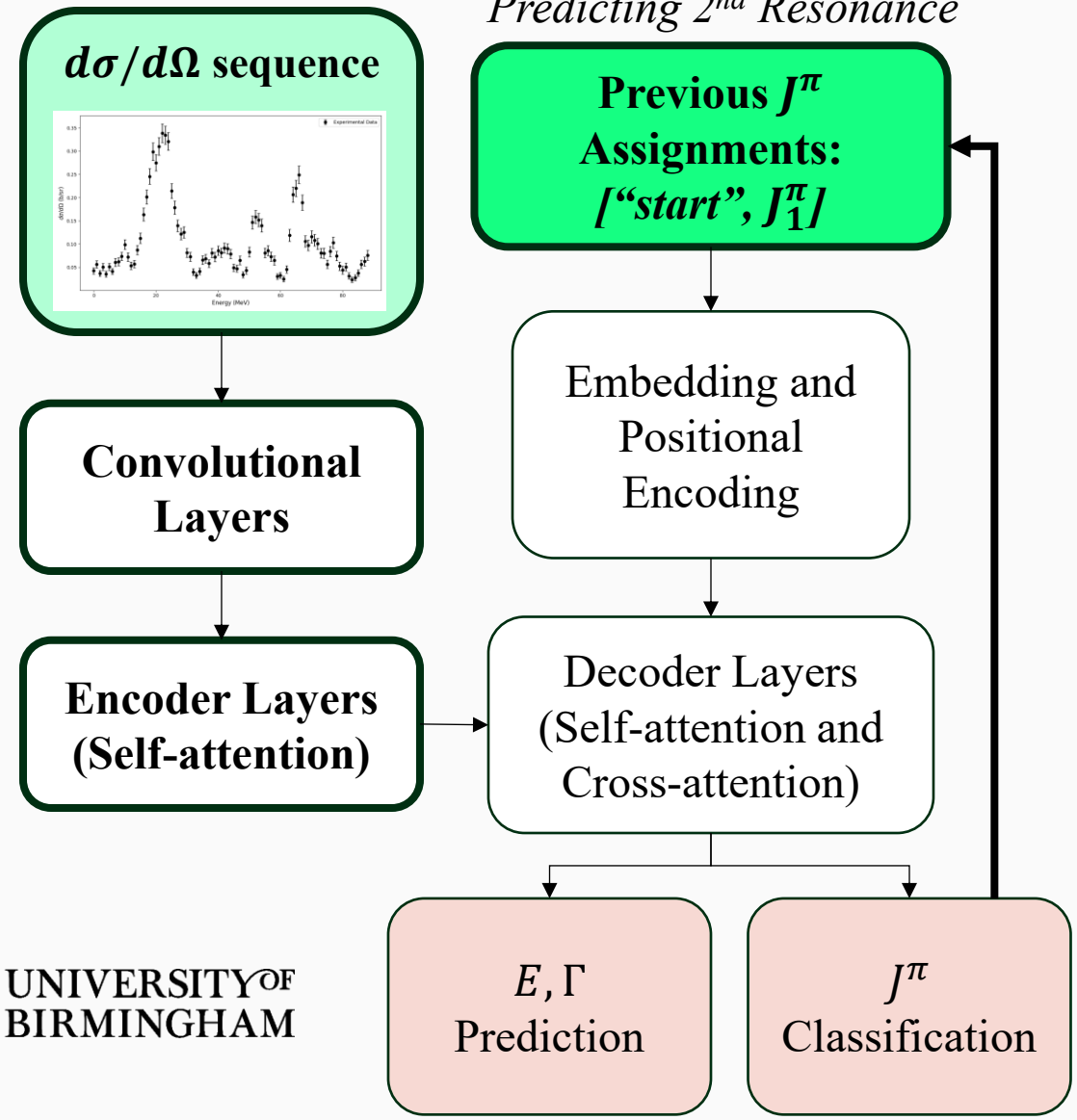
Encoder-decoder transformer: Vaswani *et. al.* [3]

ML Architecture

Predicting 2nd Resonance



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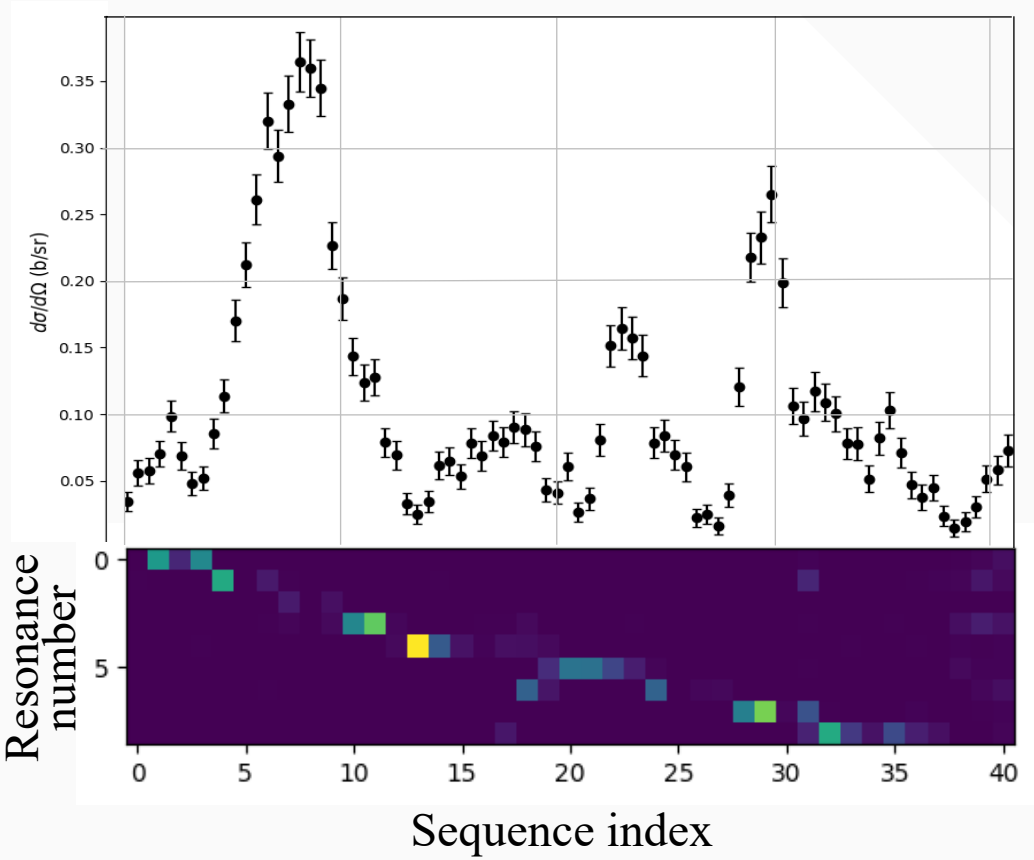

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Encoder-decoder transformer: Vaswani *et. al.* [3]

Uncertainty analysis

- Aleatoric uncertainty:
  - Measurement uncertainties
  - Ambiguous assignments
  - Irreducible

e.g. Classifier trained on animal pictures

Prediction: Cat

True label: Dog

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- Epistemic uncertainty:
  - Out of distribution training data
  - Insufficient training
  - Reducible

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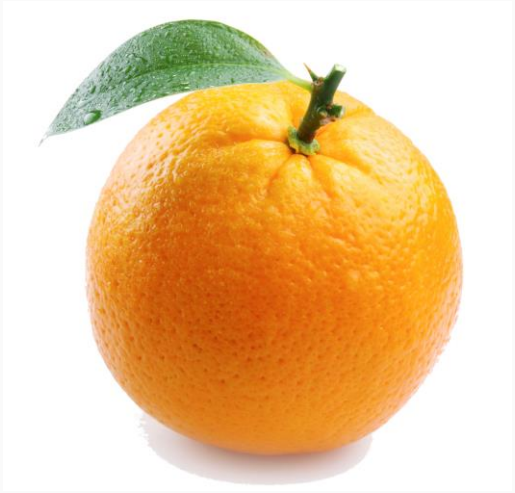

Prediction: Tiger

True label: Orange

Uncertainty analysis

- Aleatoric uncertainty:
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  - Ambiguous assignments
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  - Out of distribution training data
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- **Entropy decomposition [4]**
- Shannon Entropy:

$$H(Y) = -\sum_{y \in Y} p(y) \log\big(p(y)\big)$$

e.g. Classifier trained on animal pictures

Prediction: Cat

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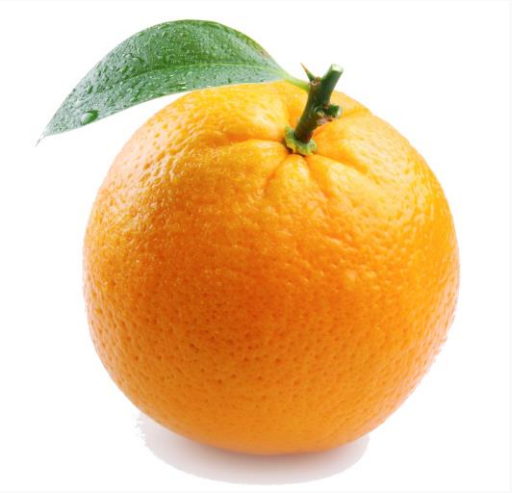

Prediction: Tiger

True label: Orange

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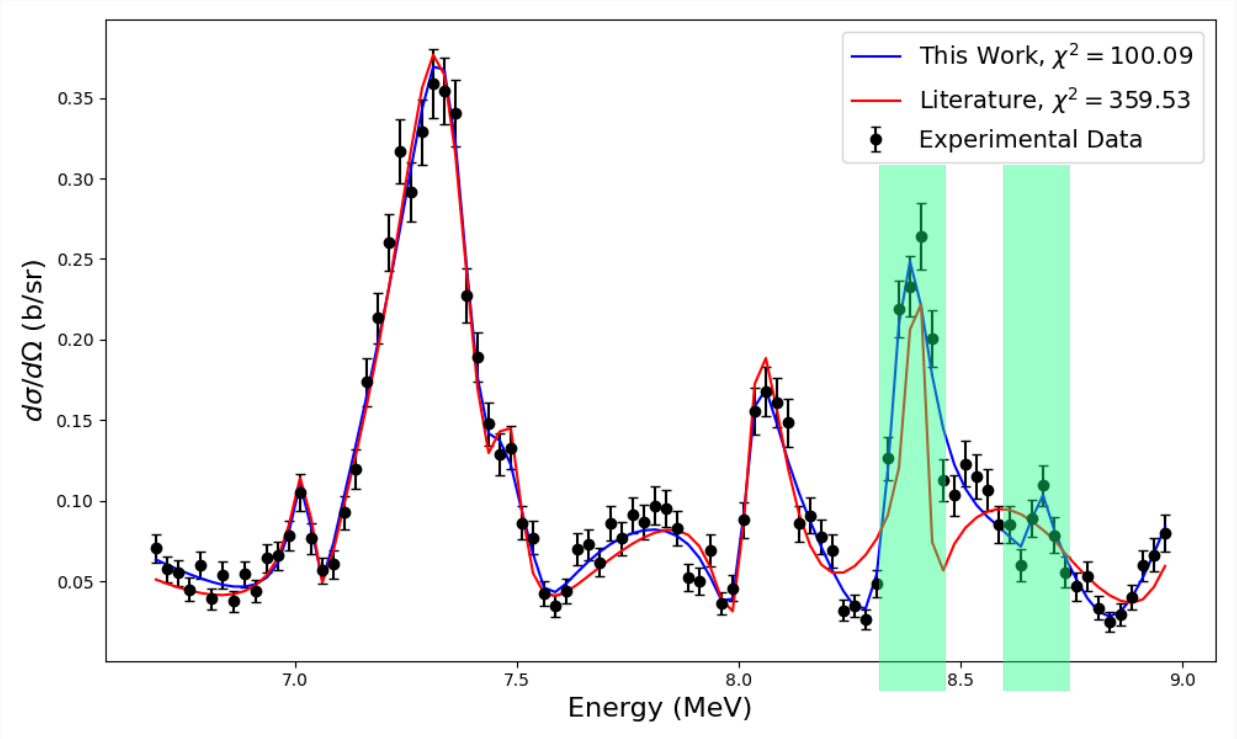
Experimental predictions

- Refine predicted parameters with conventional *R*-matrix fit
- Compare fit to previously reported parameters [2]

Literature		This work			
E / MeV	J^π	J^π	Conf. / %	E / MeV	Γ / keV
7.030(4)	$7/2^+$	$7/2^+$	33.4	7.030	19.6
7.153(9)	$3/2^+$	$3/2^+$	97.6	7.157	491
7.378(7)	$7/2^+$	$7/2^+$	59.2	7.376	162
7.469(7)	$5/2^+$	$5/2^+$	26.8	7.512	54.1
7.568(27)	$3/2^+(1/2^+)$	$3/2^+$	32.0	7.517	116
8.022(4)	$9/2^+$	$9/2^+$	38.9	8.018	64.2
8.223(7)	$5/2^+$	$5/2^+$	66.0	8.208	502
8.428(2)	$13/2^-(11/2^+)$	$5/2^+$	36.8	8.514	606
8.680(1)	$(9/2^-)(7/2^-)$	$11/2^+$	19.6	8.668	10.8

Preliminary results – no finalised errors on energies or widths



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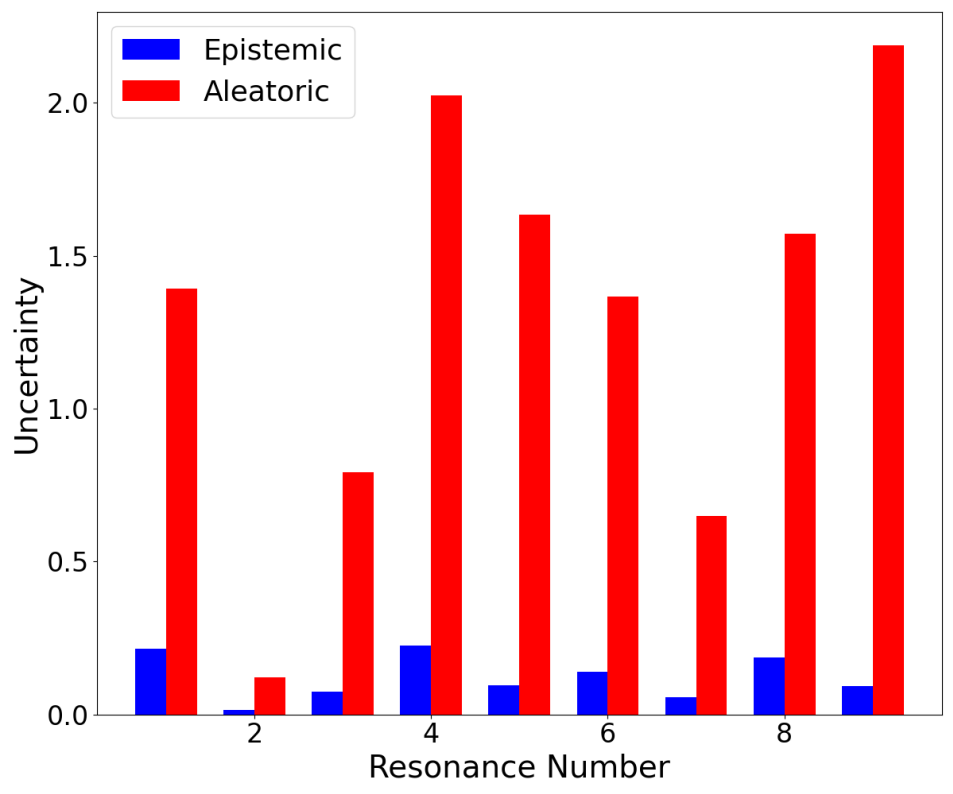
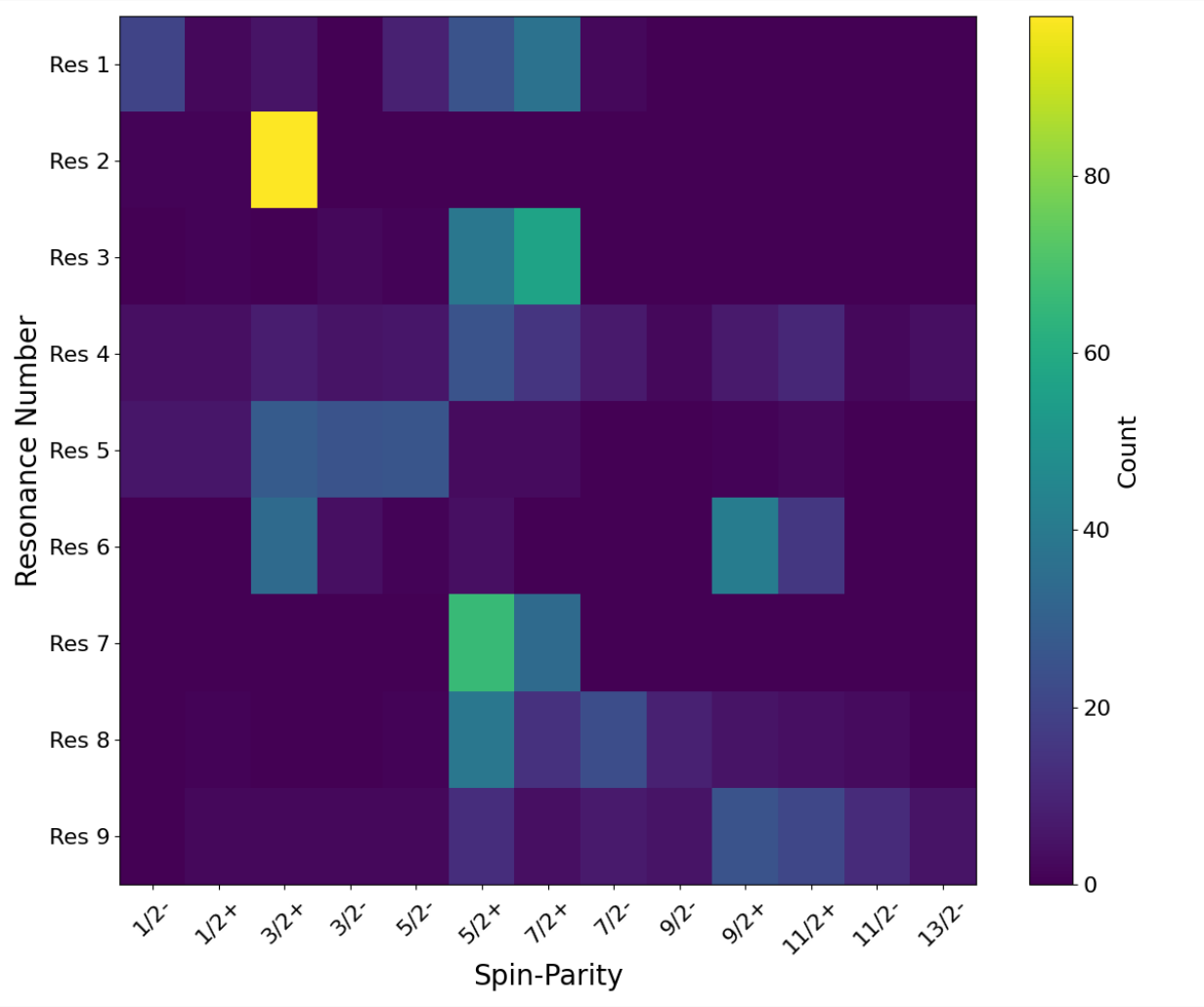
Uncertainty analysis



Dominated by aleatoric uncertainties: irreducible ambiguity from experimental uncertainties



Some uncertainty from choice between two, some completely uncertain

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Conclusions and Future Work

- Developed ML model to predict ^{19}Ne resonance parameters
- Predicted parameters improve fit compared to reported values
- Identified inherently ambiguous assignments due to large measurement uncertainties

- Decompose uncertainties of energy and width parameters
- Predict variable number of resonances
- Test with multi-angle datasets (e.g. ^{16}O + α)

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Questions?

References:

[1]: NASA/CXC/M.Weiss

[2]: Torresi, D., Wheldon, C., Kokalova, T., Bailey, S., Boiano, A., Boiano, C., Fisichella, M., Mazzocco, M., Parascandolo, C., Pierroutsakou, D. and Strano, E., 2017. Evidence for O 15+ α resonance structures in Ne 19 via direct measurement. Physical Review C, 96(4), p.044317.

[3]: Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, Ł. and Polosukhin, I., 2017. Attention is all you need. Advances in neural information processing systems, 30.

[4]: Wimmer, L., Sale, Y., Hofman, P., Bischl, B. and Hüllermeier, E., 2023, July. Quantifying aleatoric and epistemic uncertainty in machine learning: Are conditional entropy and mutual information appropriate measures?. In Uncertainty in artificial intelligence (pp. 2282-2292). PMLR.

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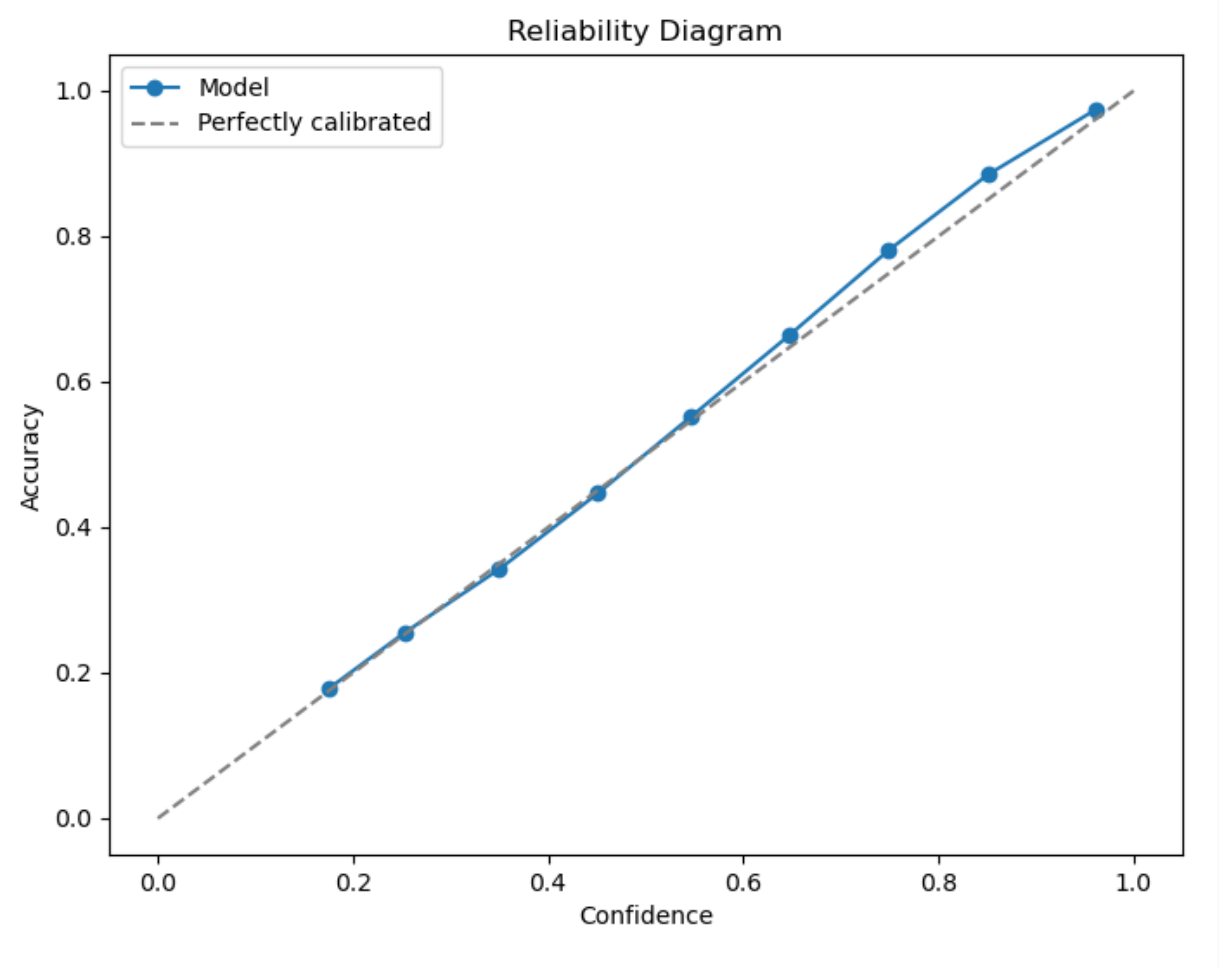
Backup Slides: Calibration



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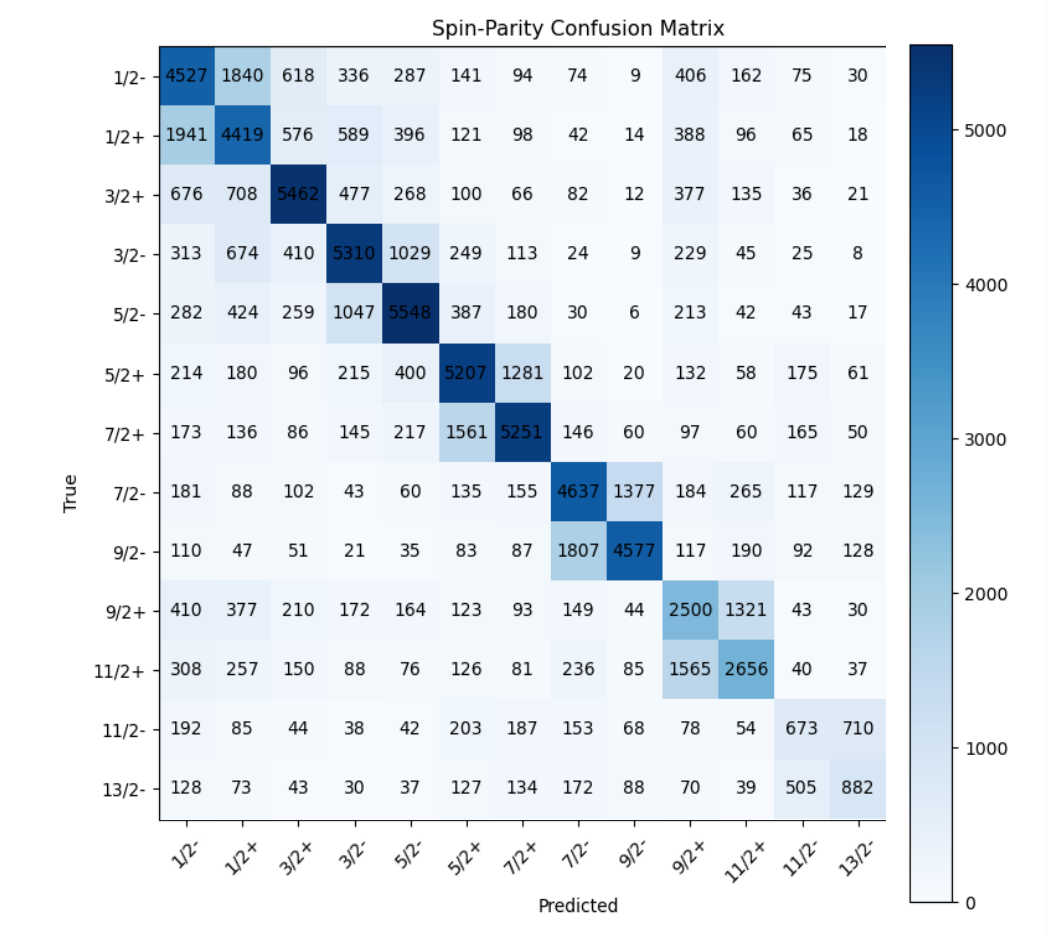
Backup Slides: Confusion Matrix



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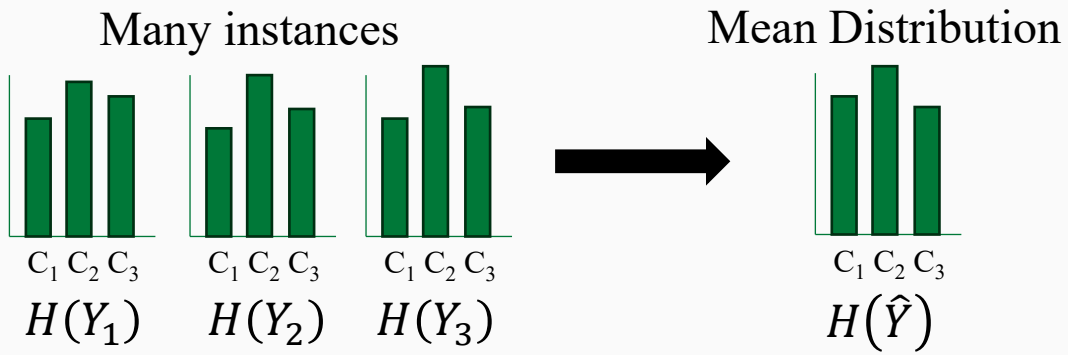
Backup Slides: Entropy Decomposition

Shannon Entropy: $H(Y) = -\sum_{y \in Y} p(y) \log\big(p(y)\big)$



Epistemic = Total - Aleatoric