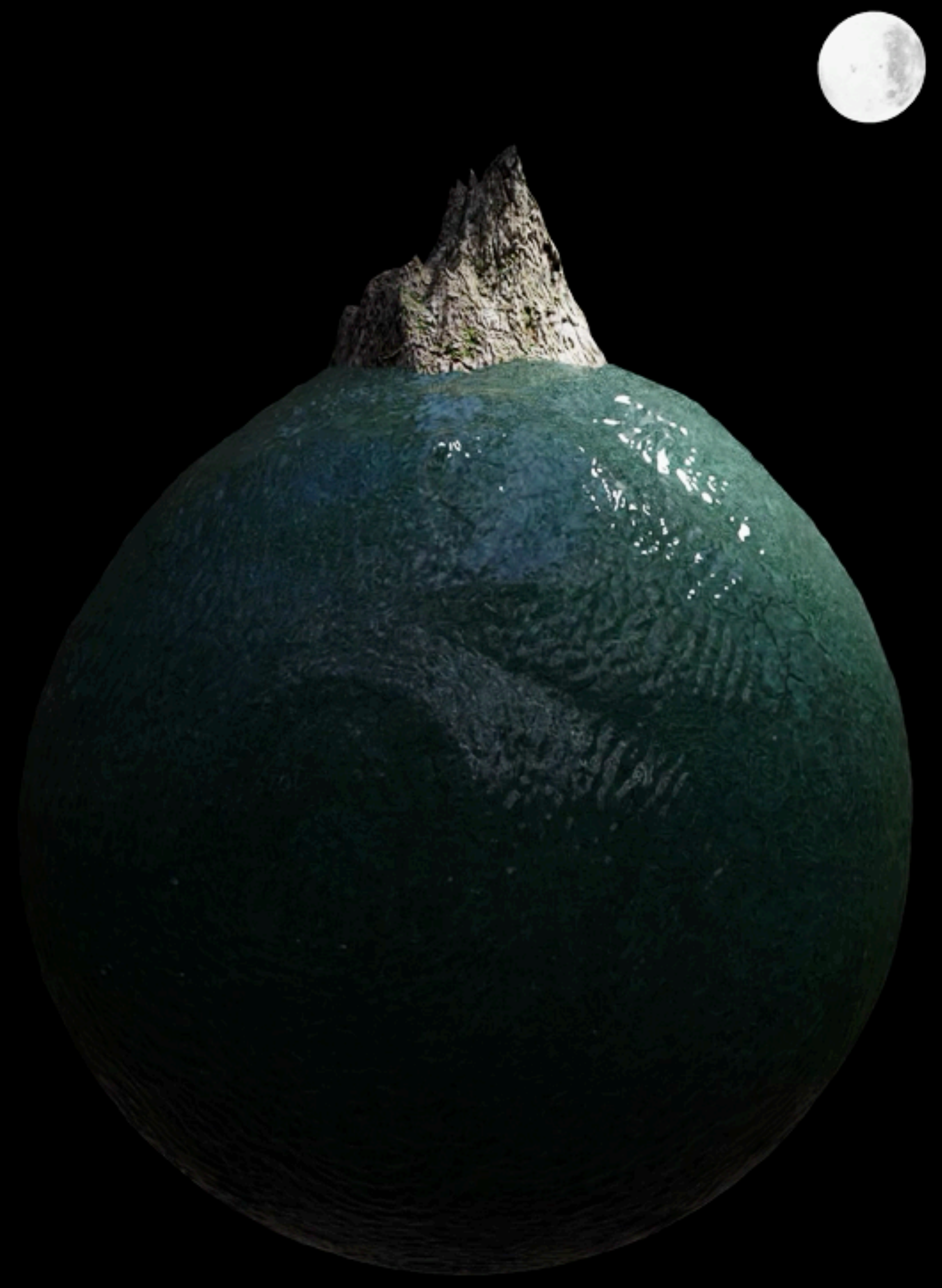
Artificial Neural Networks for Nuclear Structure Corrections



A comprehensive story of ANNs in nuclear physics

Tim Egert, Johannes Gutenberg University Mainz, 31.7.2025

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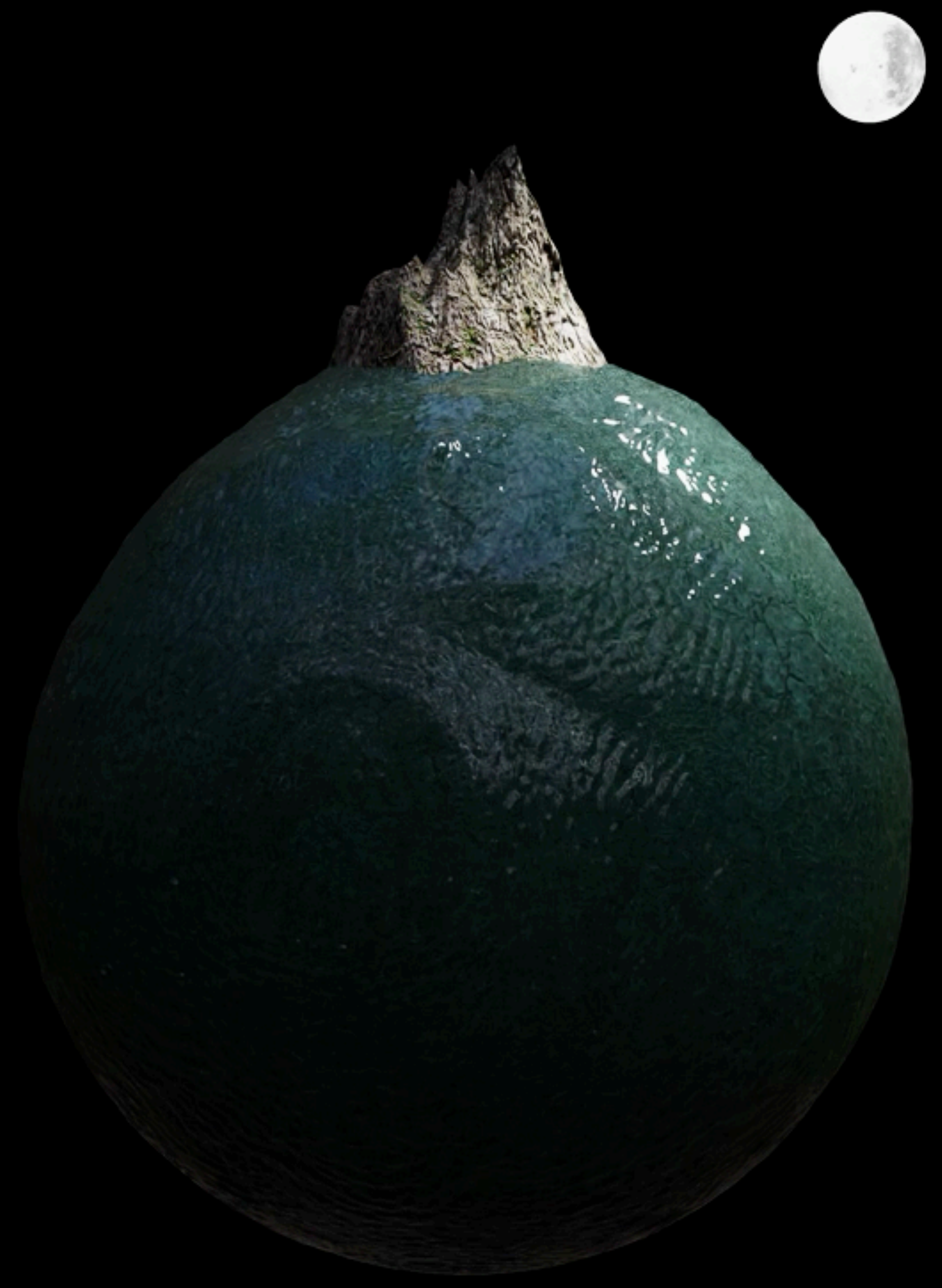

[Credit: Vinny Ravuri]

A comprehensive story of ANNs in nuclear physics

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From the Beginning

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Muonic atoms → Lamb shift → charge radii

Motivation

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$$\delta_{LS} = \delta_{QED} + \mathscr{A}_{OPE} \cdot r^2_{nucl} + \delta_{TPE}$$

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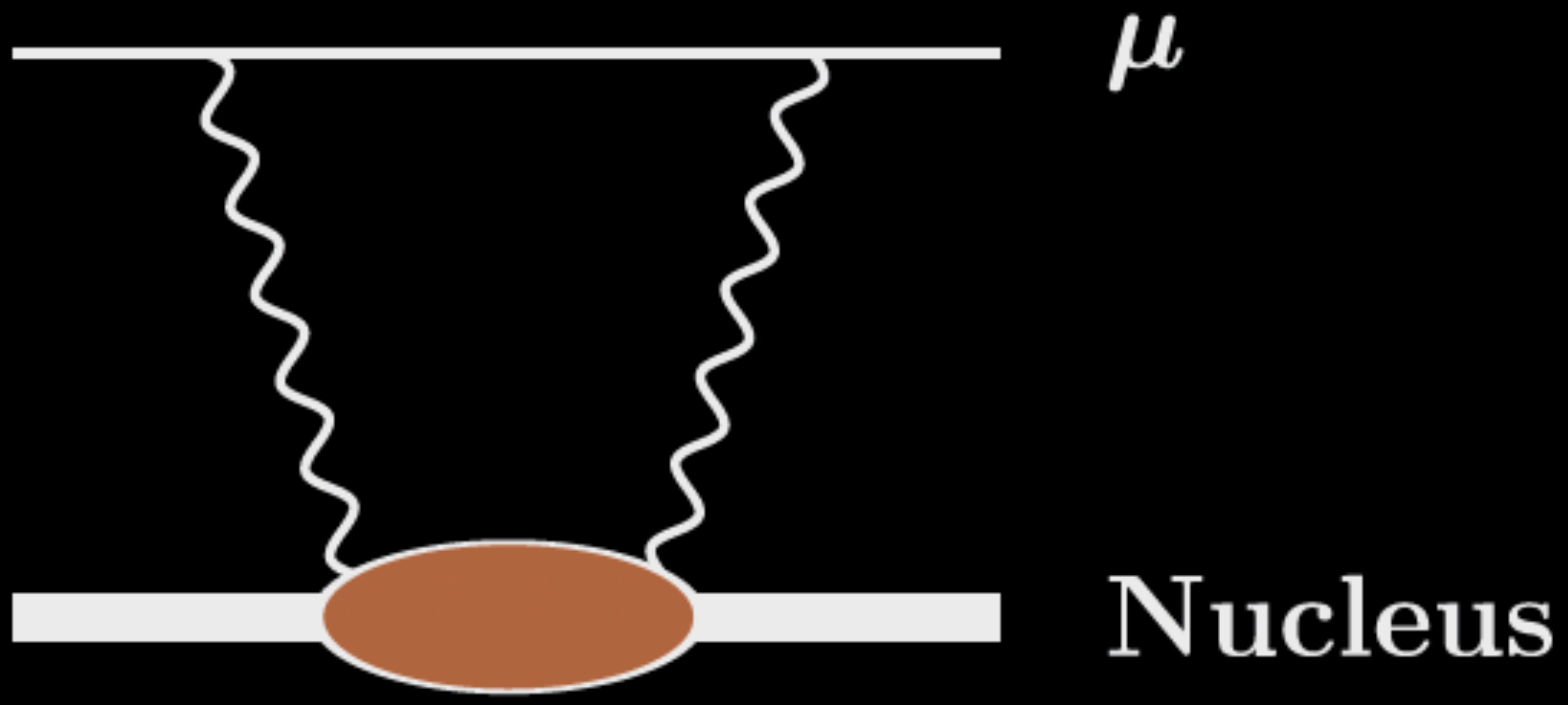
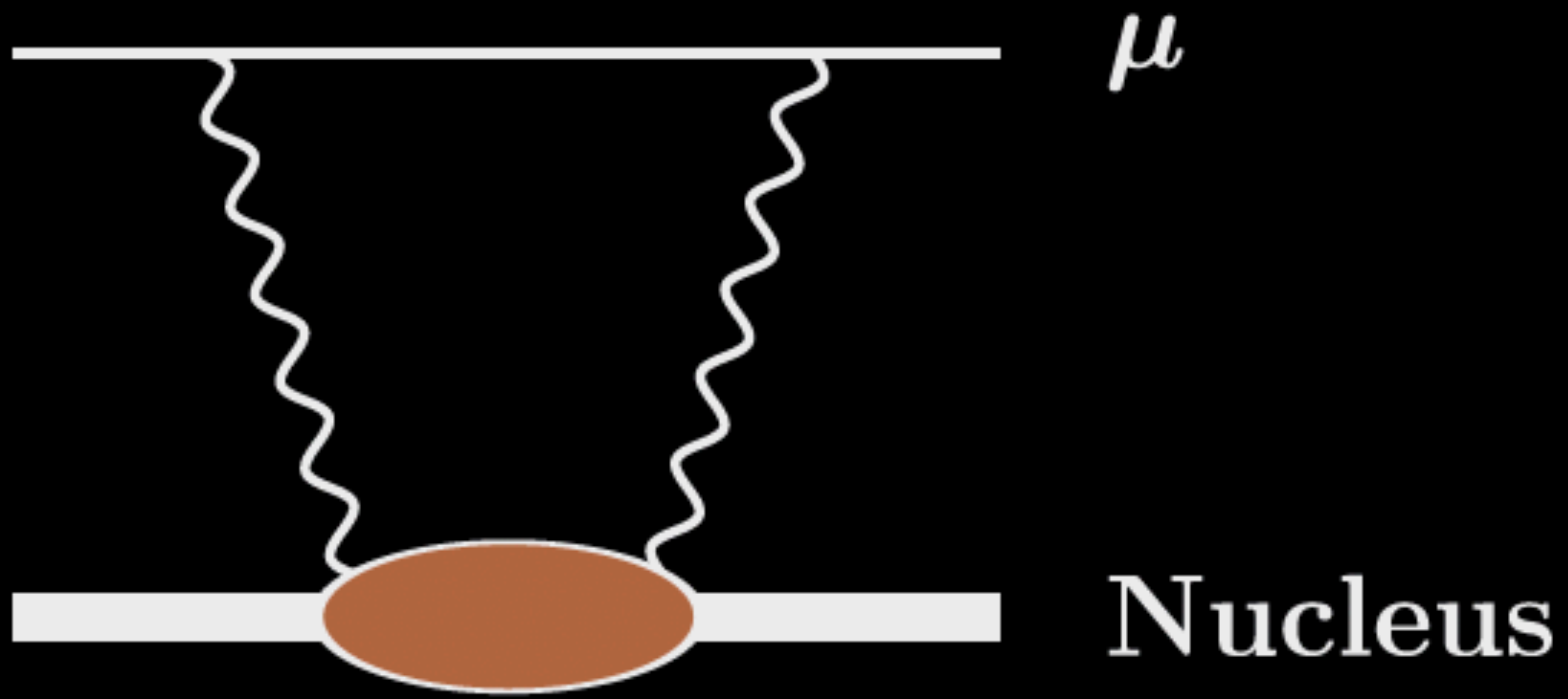


[Ji, Bacca, Barnea, Hernandez and Dinur, J: Phys. G: Nucl. Part. Phys. 45 (2018)]

Motivation

$$\delta_{LS} = \delta_{QED} + \mathscr{A}_{OPE} \cdot r^2_{nucl} + (\delta_{Zem} + \delta_{pol})$$



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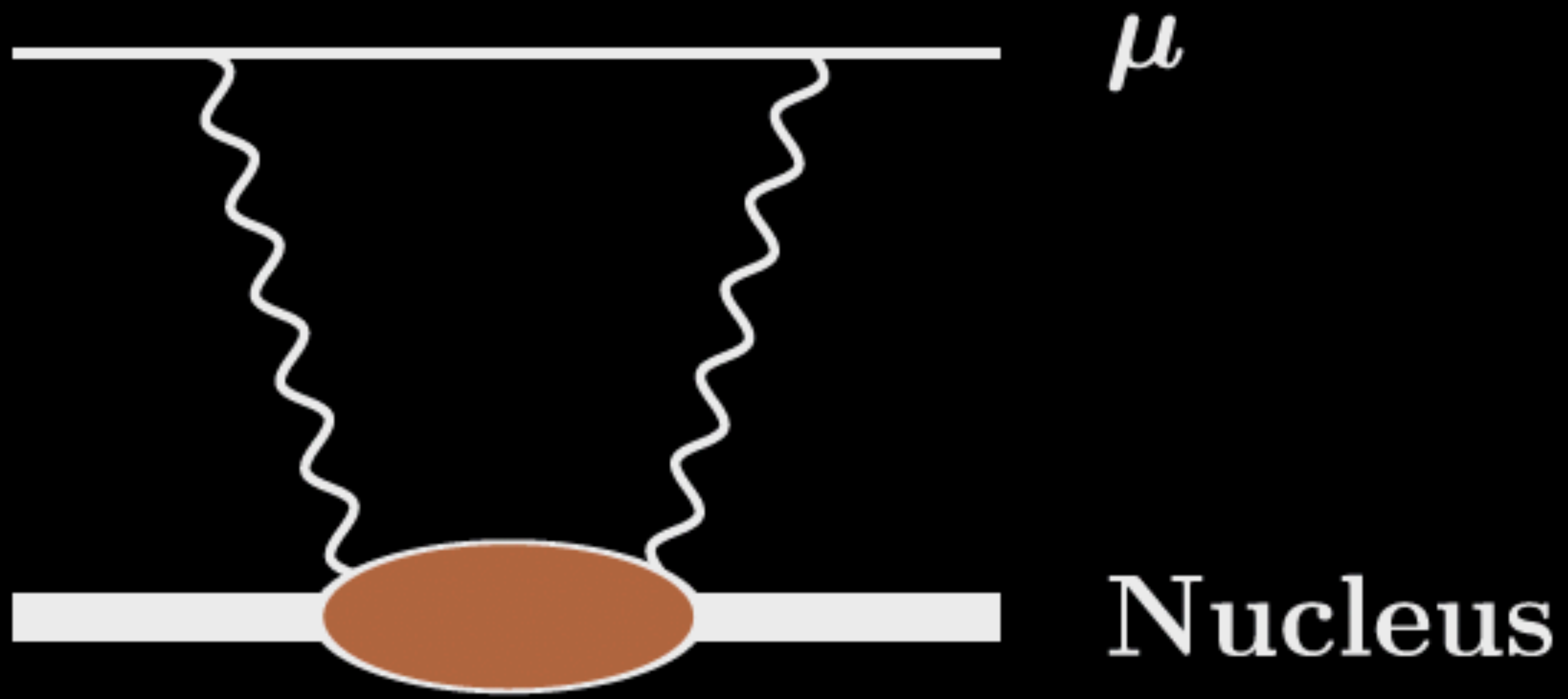
$$\delta_{LS} = \delta_{QED} + \mathscr{A}_{OPE} \cdot r^2_{nucl} + (\delta_{Zem} + \delta_{pol})$$

$$\delta_{pol} = \delta^A_{pol} + \delta^N_{pol}$$



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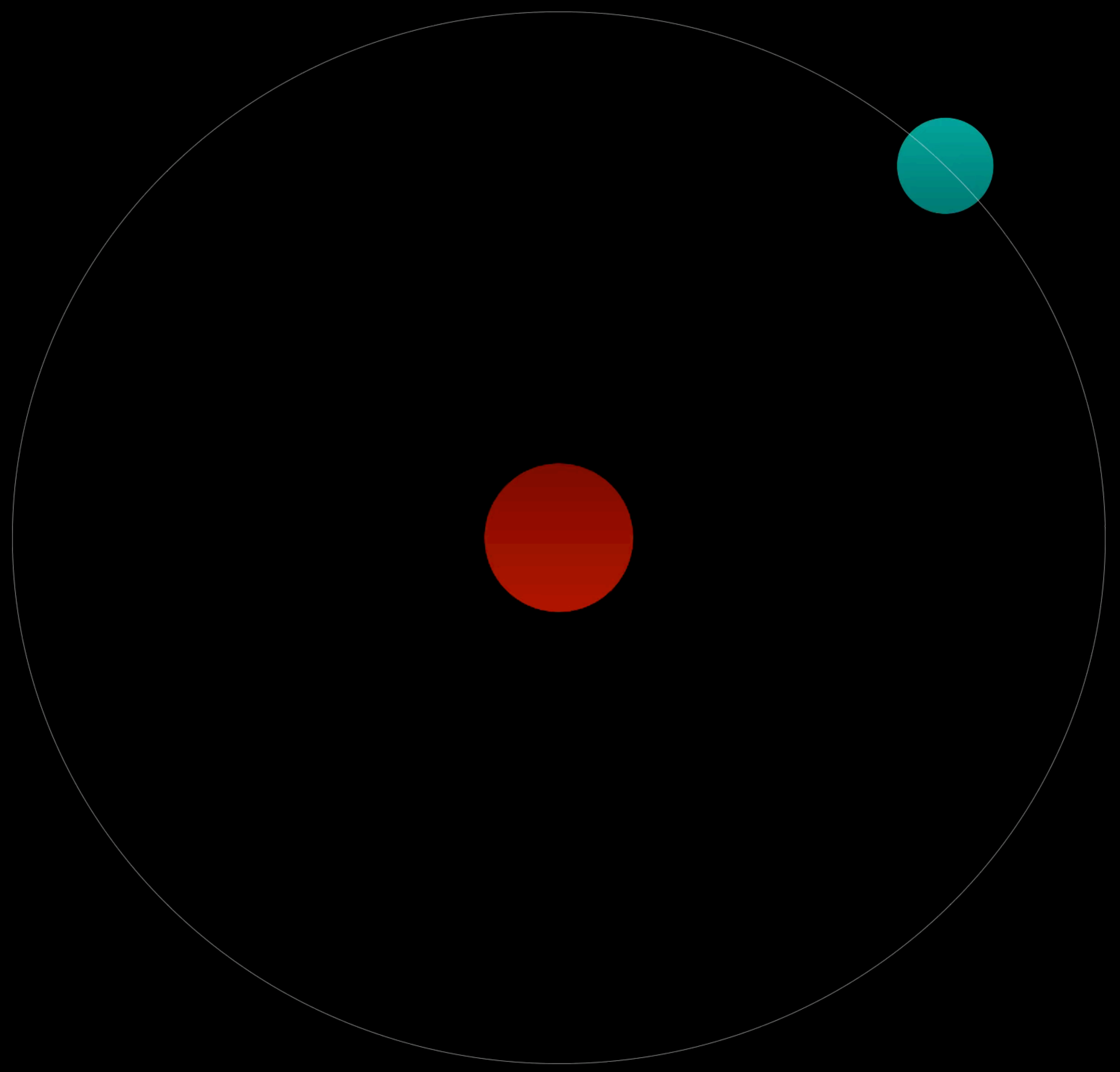

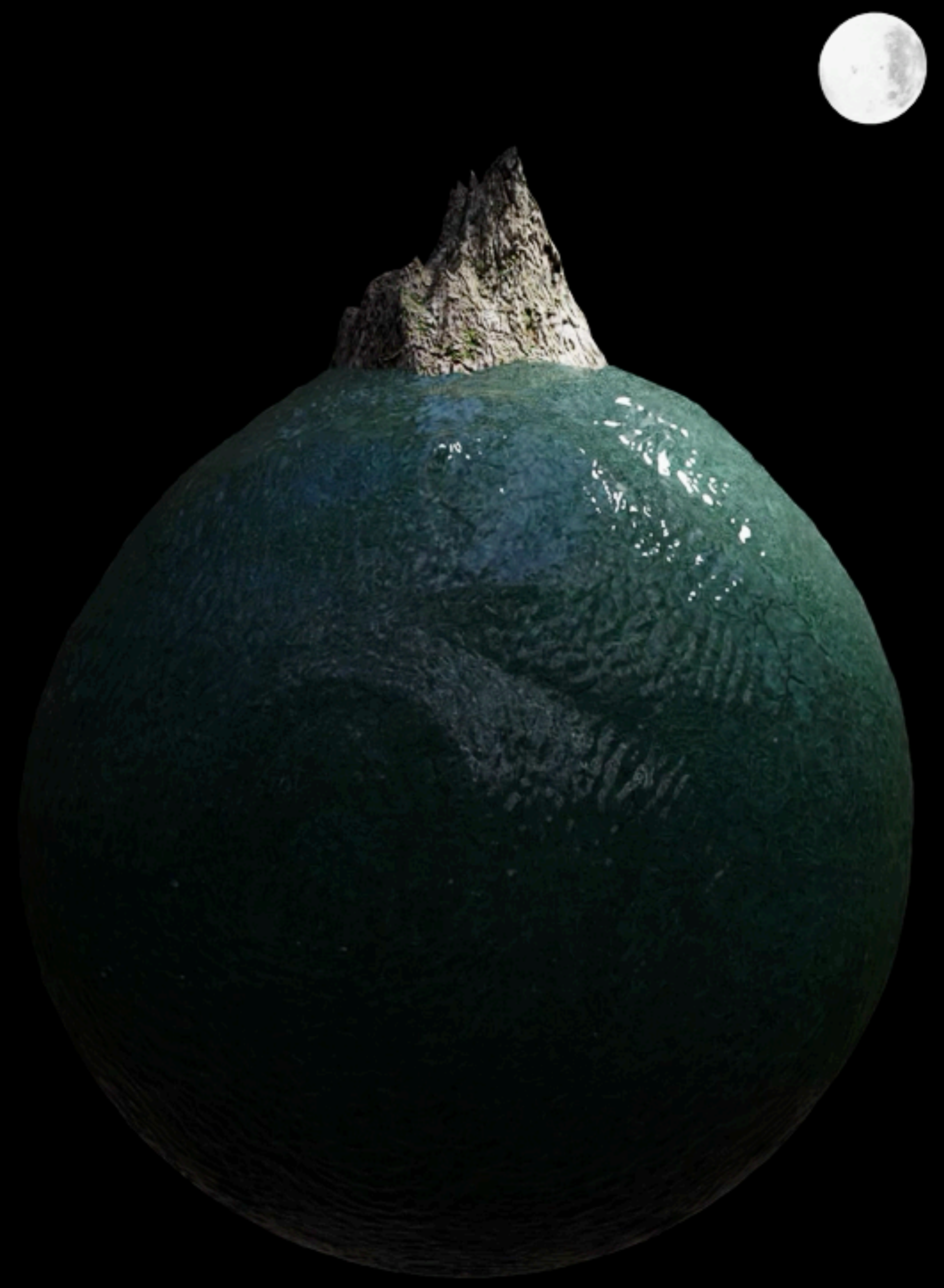

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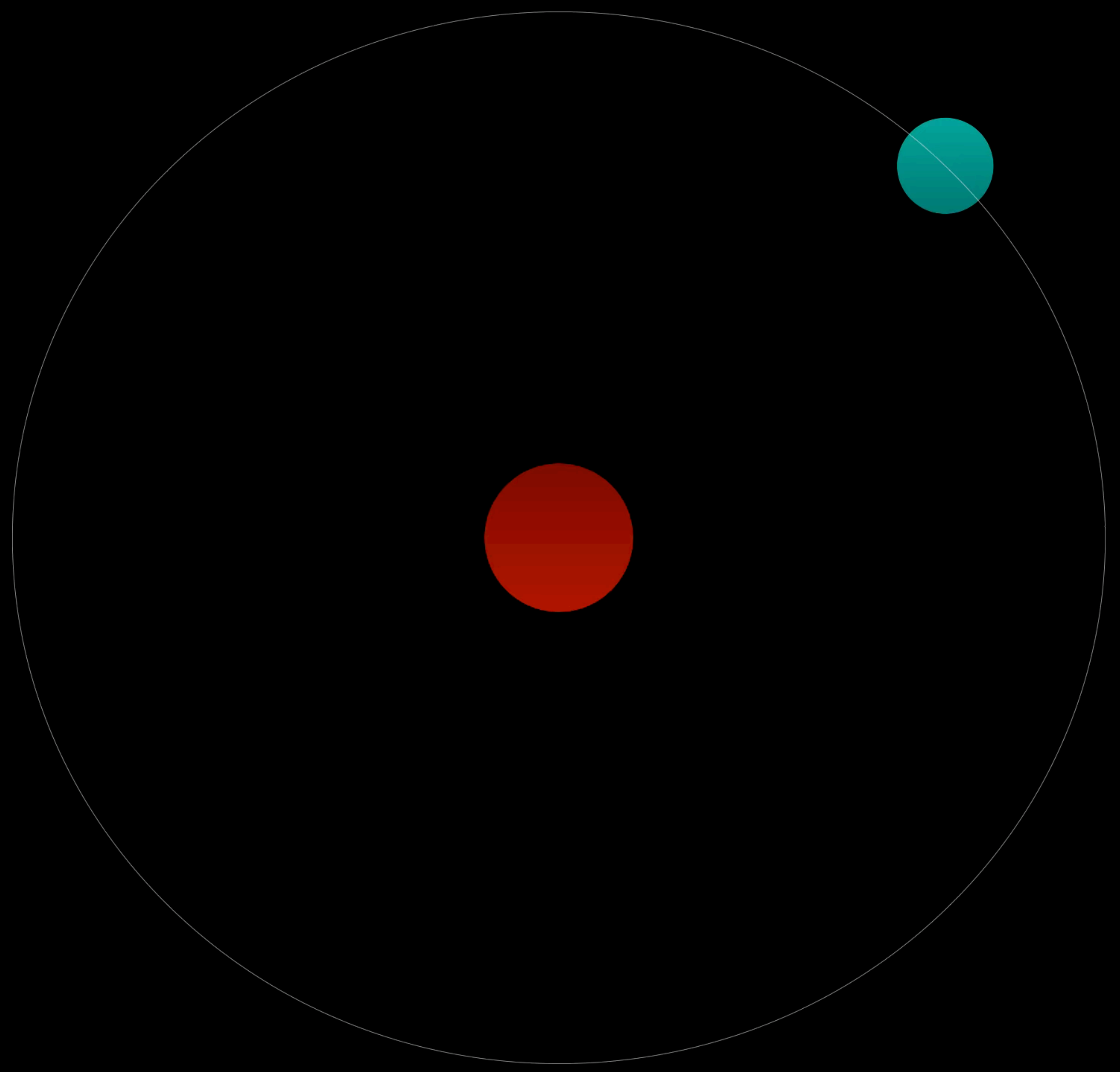

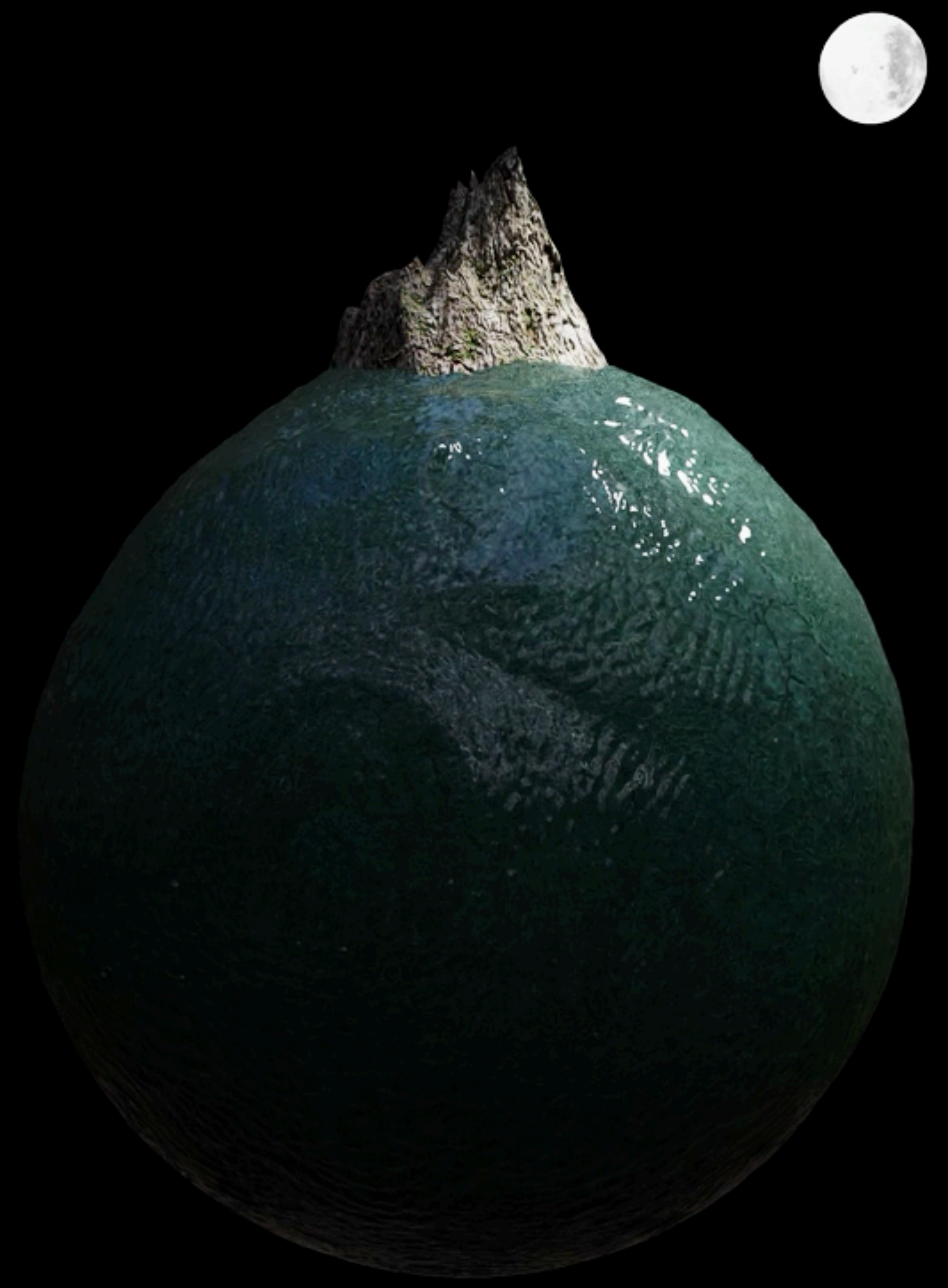

[Credit: Vinny Ravuri, https://www.doctormadnessfilms.com/]

Nuclear Structure Corrections

$$\delta^{A}_{pol} = \delta^{NR}_{pol} + \delta^{C}_{pol} + \delta^{R}_{pol} + \delta^{NS}_{pol}$$

$$= \delta^{(0)}_{D1} + \delta^{(1)}_{R3} + \delta^{(1)}_{Z3} + \delta^{(2)}_{R^2} + \delta^{(2)}_{Q} + \delta^{(2)}_{D1D3} + \delta^{(0)}_{C}$$

$$+\delta^{(0)}_{L} + \delta^{(0)}_{T} + \delta^{(0)}_{M} + \delta^{(1)}_{R1} + \delta^{(1)}_{Z1} + \delta^{(2)}_{\mathrm{NS}}$$

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Larger contributions accessible via dipole strength only

Calculate Dipole Strength

Theory and Reality

$$\delta_{D1}^{(0)} = -\frac{16\pi^2}{9}(Z\alpha)^2\phi^2(0)\int_0^\infty \mathrm{d}\omega \sqrt{\frac{2m_r}{\omega}}\, S_{D1}(\omega)$$

$$\delta_{C}^{(0)} = -\frac{16\pi^2}{9}(Z\alpha)^3\phi^2(0)\int_0^\infty \mathrm{d}\omega \,\frac{m_r}{\omega} \ln\left(\frac{2(Z\alpha)^2 m_r}{\omega}\right) S_{D1}(\omega)$$

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If we need these terms, why not just calculate?

[Ji, Bacca, Barnea, Hernandez and Dinur, J: Phys. G: Nucl. Part. Phys. 45 (2018)]

Calculate Dipole Strength

Theory and Reality

Calculate Dipole Strength

Theory and Reality

$$S_{D1}(\omega) \sim \sum\!\!\!\!\!\!\int |\langle \Psi_f | \hat{D} | \Psi_0 \rangle|^2 \delta(E_f - E_0 - \omega)$$

Calculate Dipole Strength

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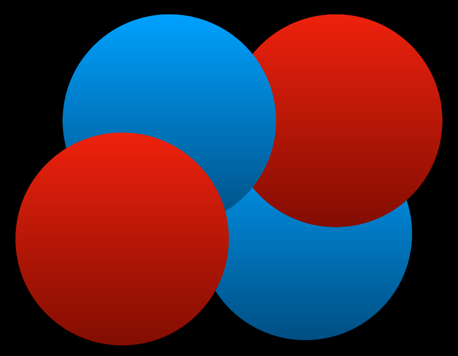

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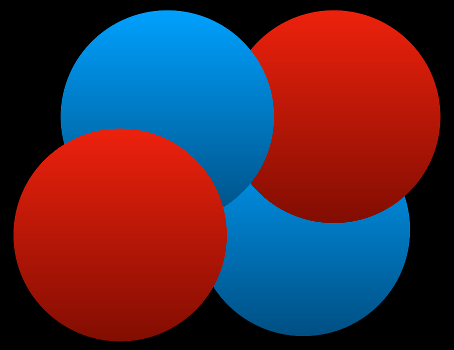

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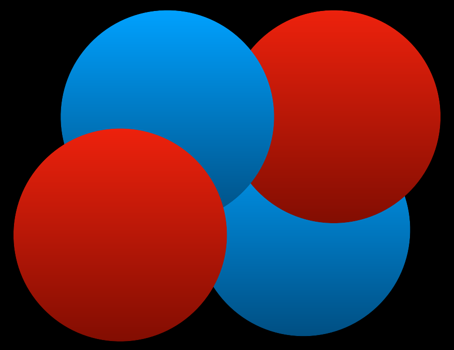

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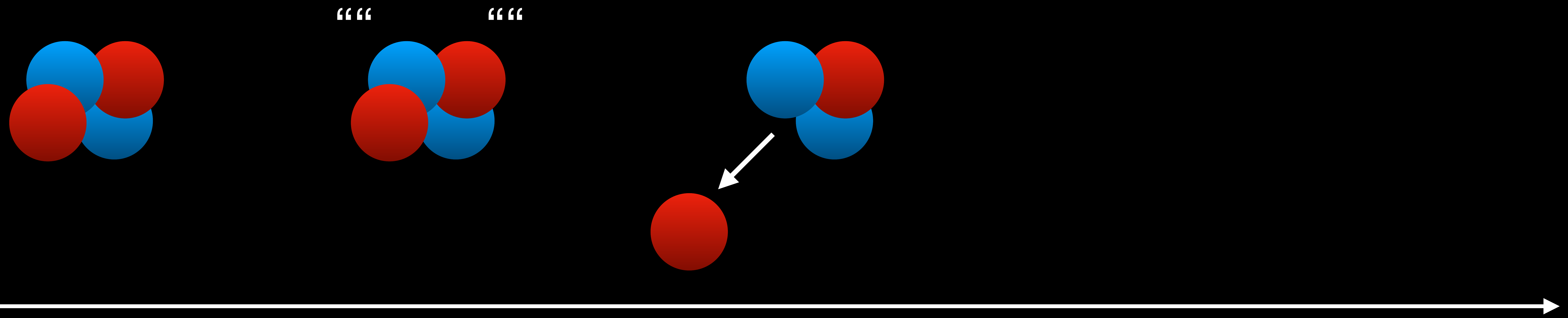

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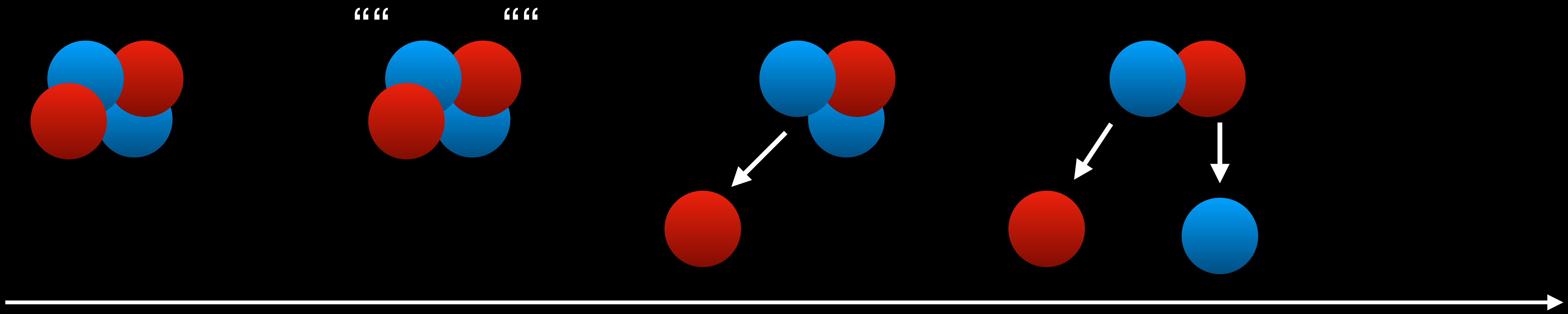

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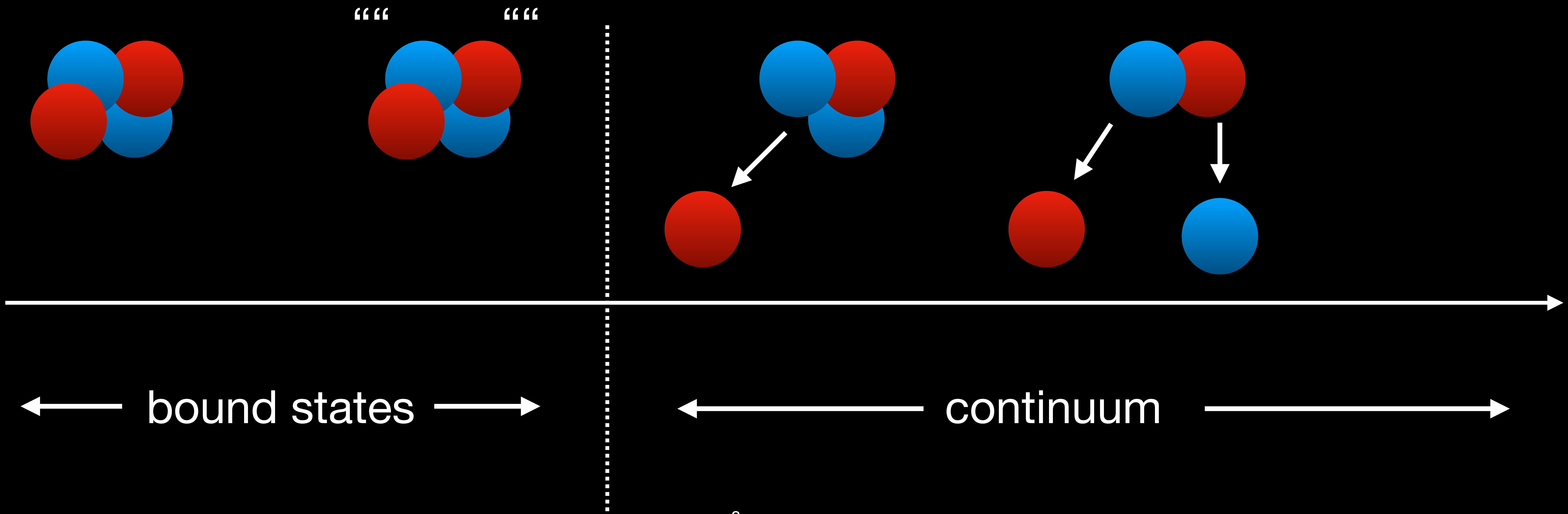

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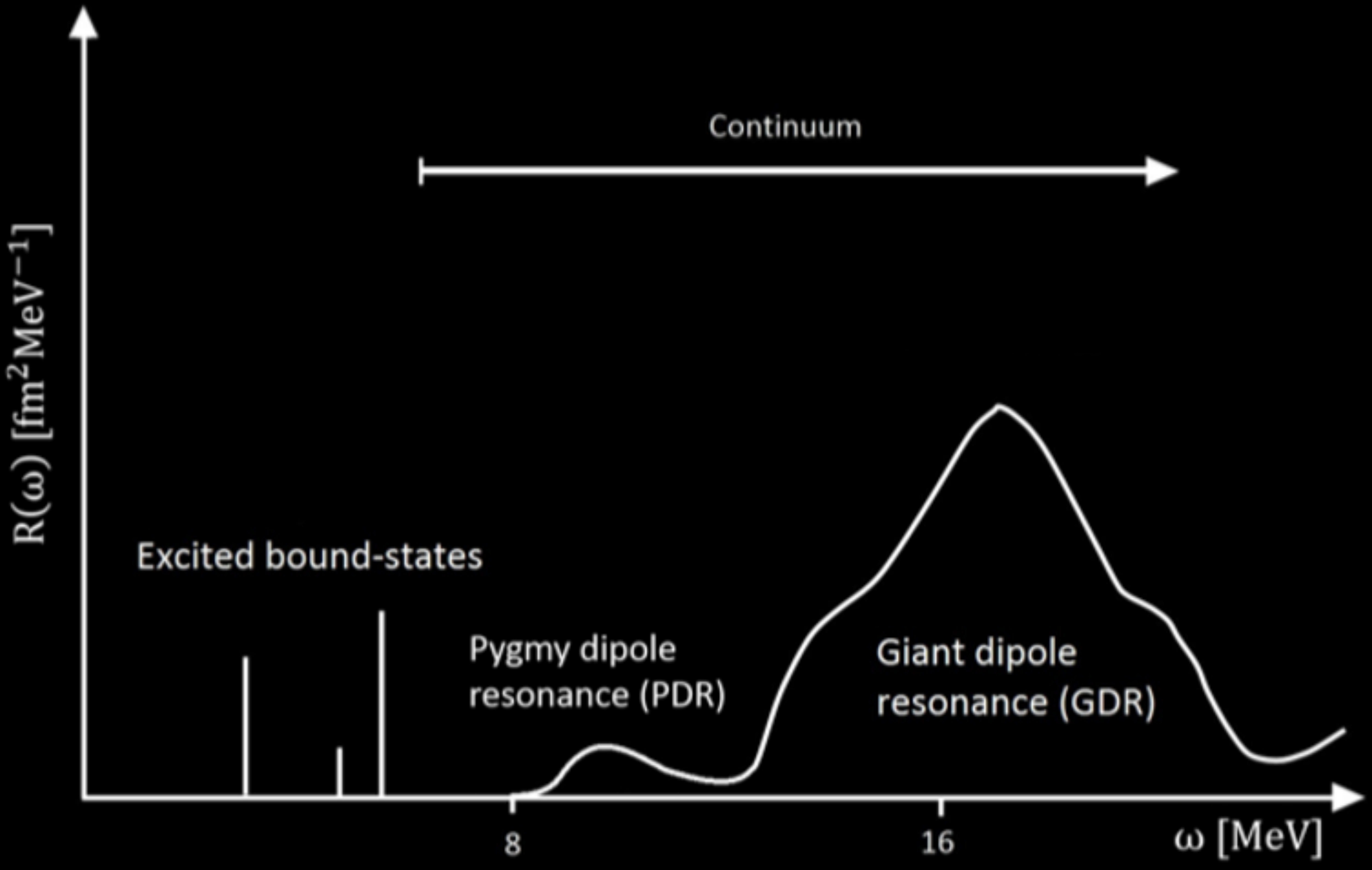


The Idea

$$S_{D1}(\omega)$$

or

$$\sigma(\omega)$$

[SORA]

The Idea

$S_{D1}(\omega)$

or

$\sigma(\omega)$

Disclaimer

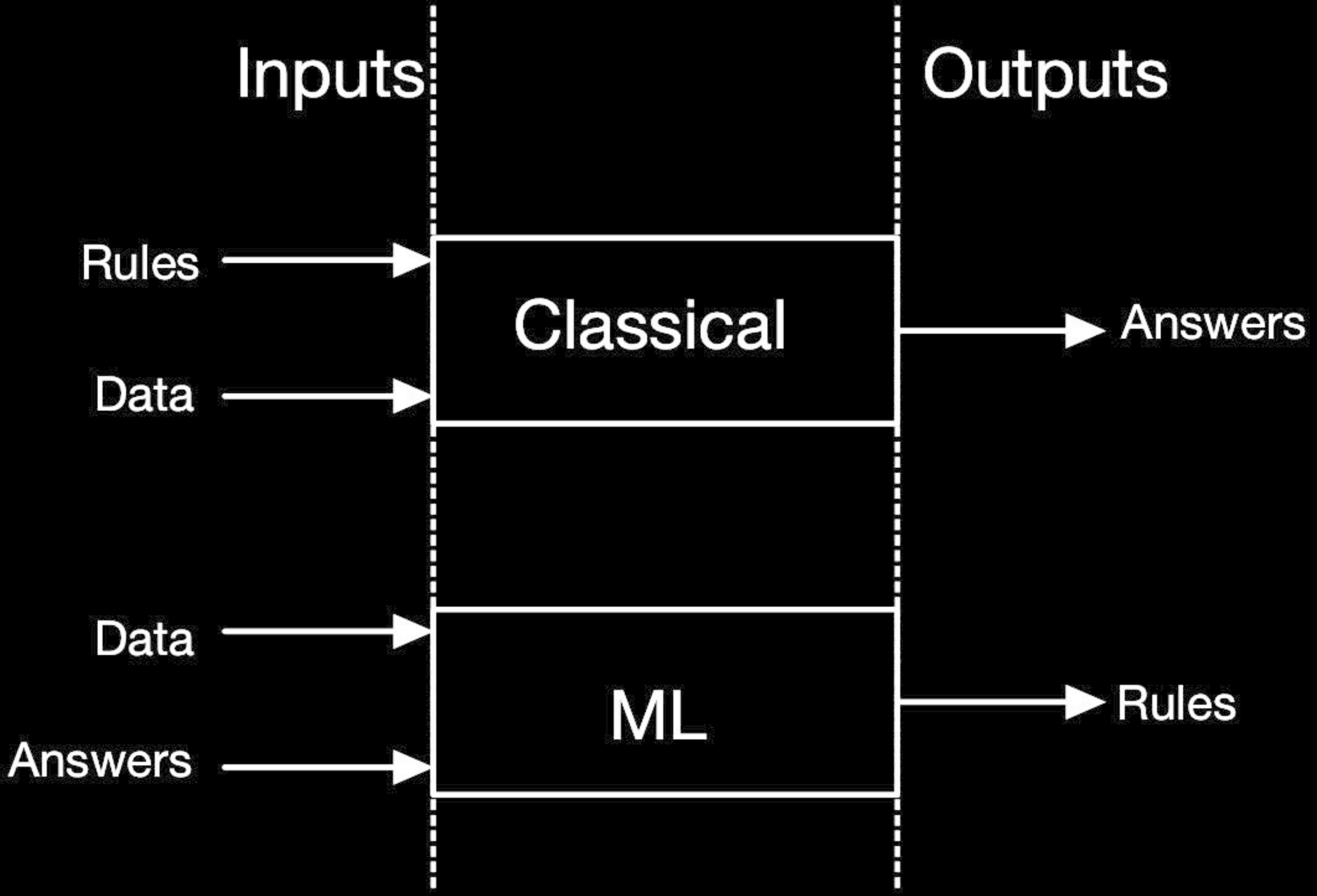
$$S_{D_1} \sim f_1 \sim \frac{\sigma(\omega)}{\omega}$$

In the unretarded dipole approximation

What is an ANN

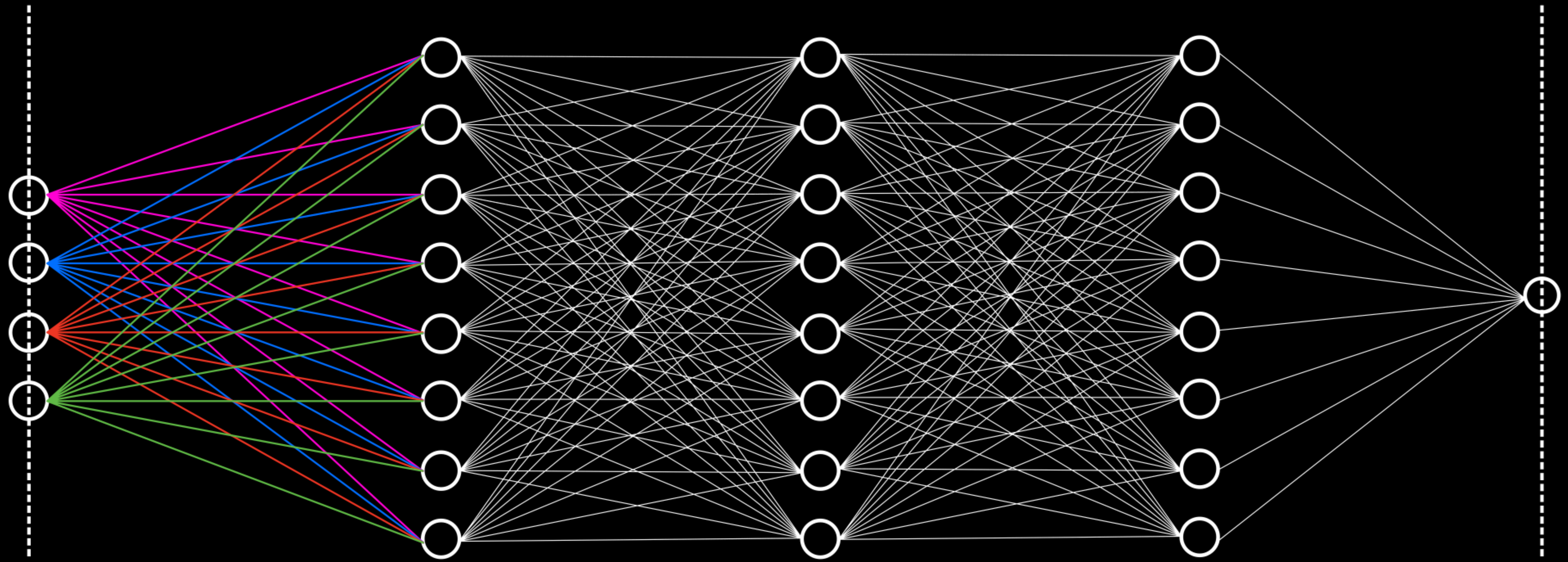
Difference in classical programming and ML

- Classical = outputs answers
- ML = outputs models



What is an ANN

Structure



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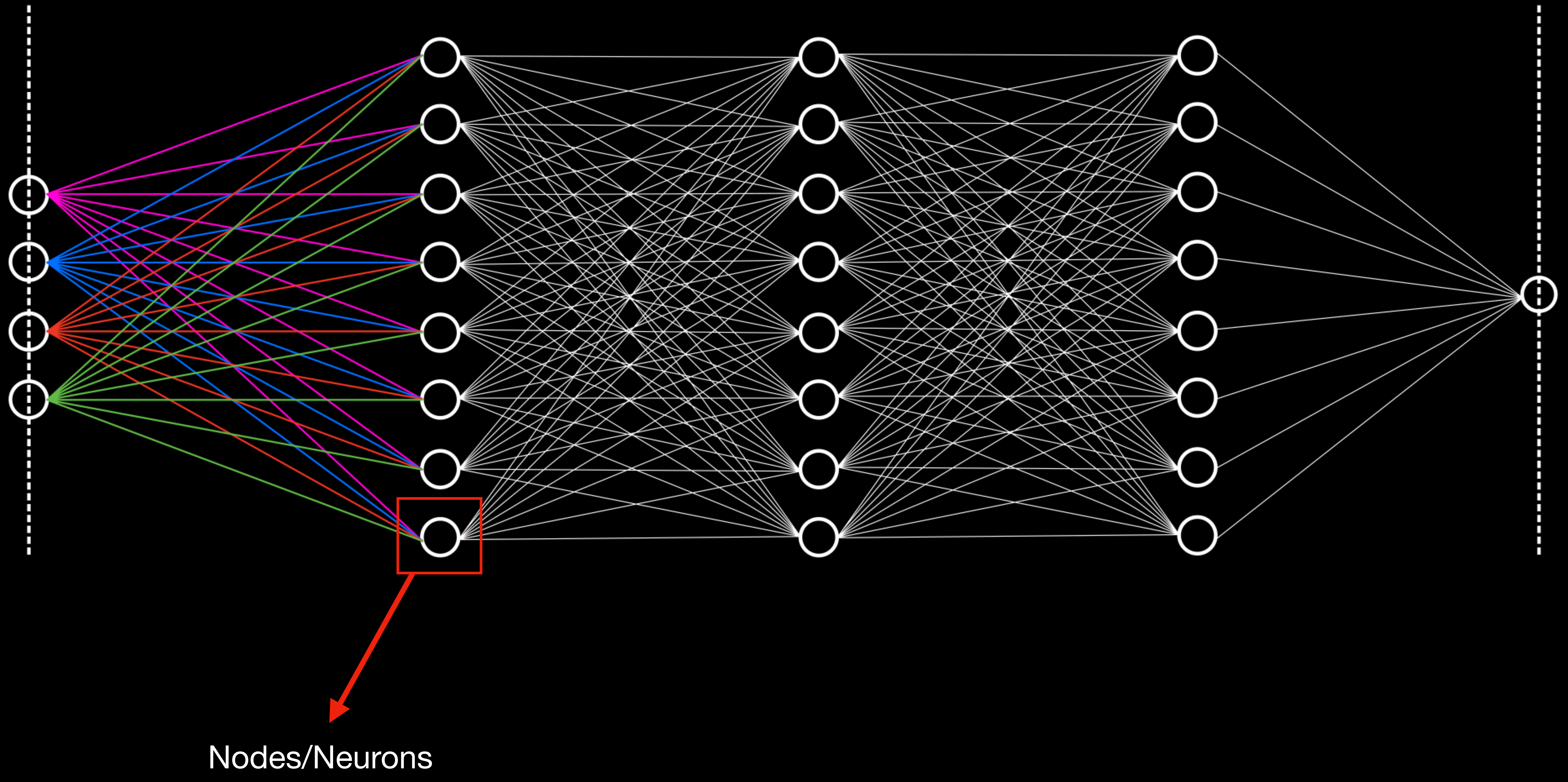

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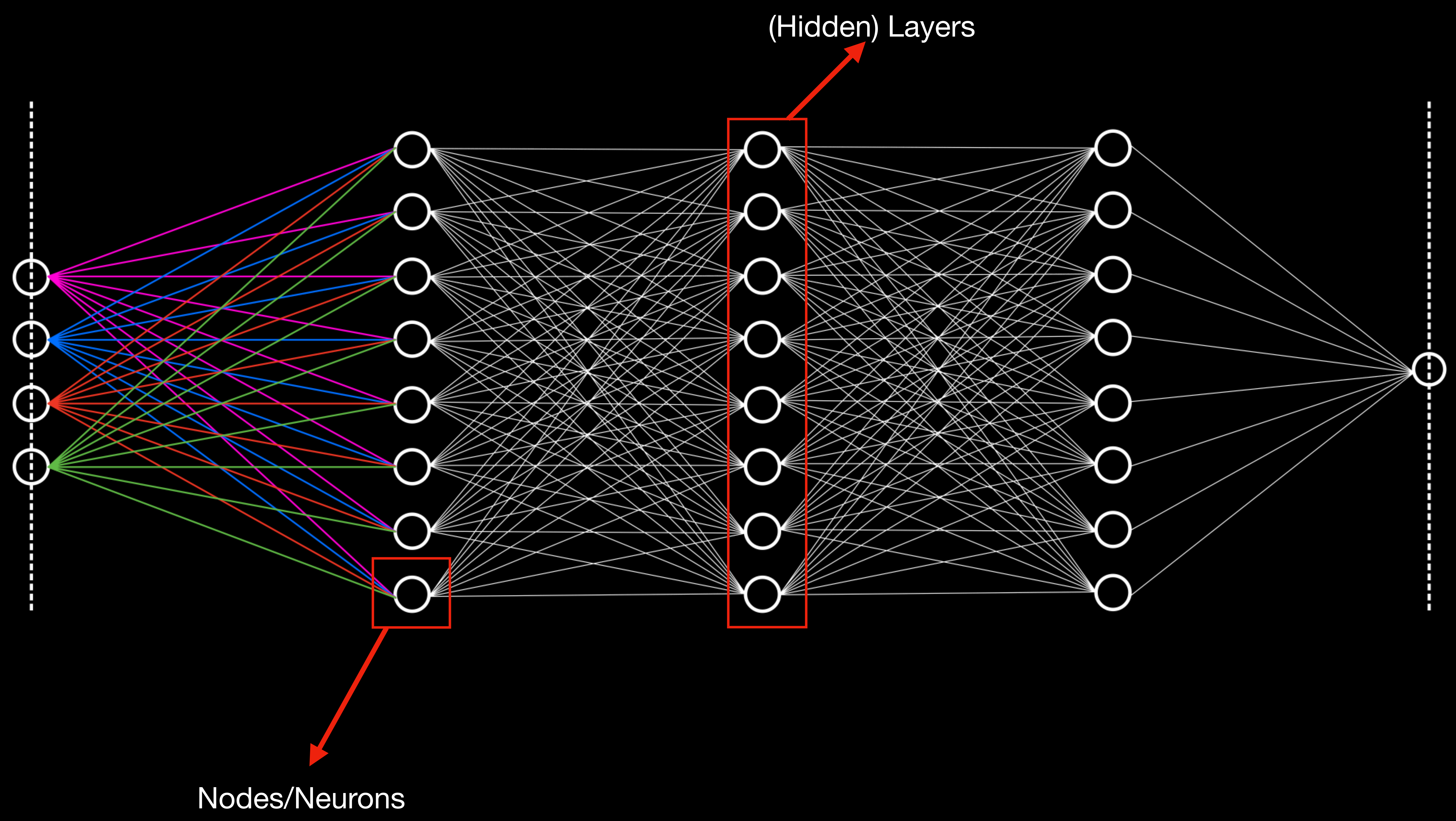

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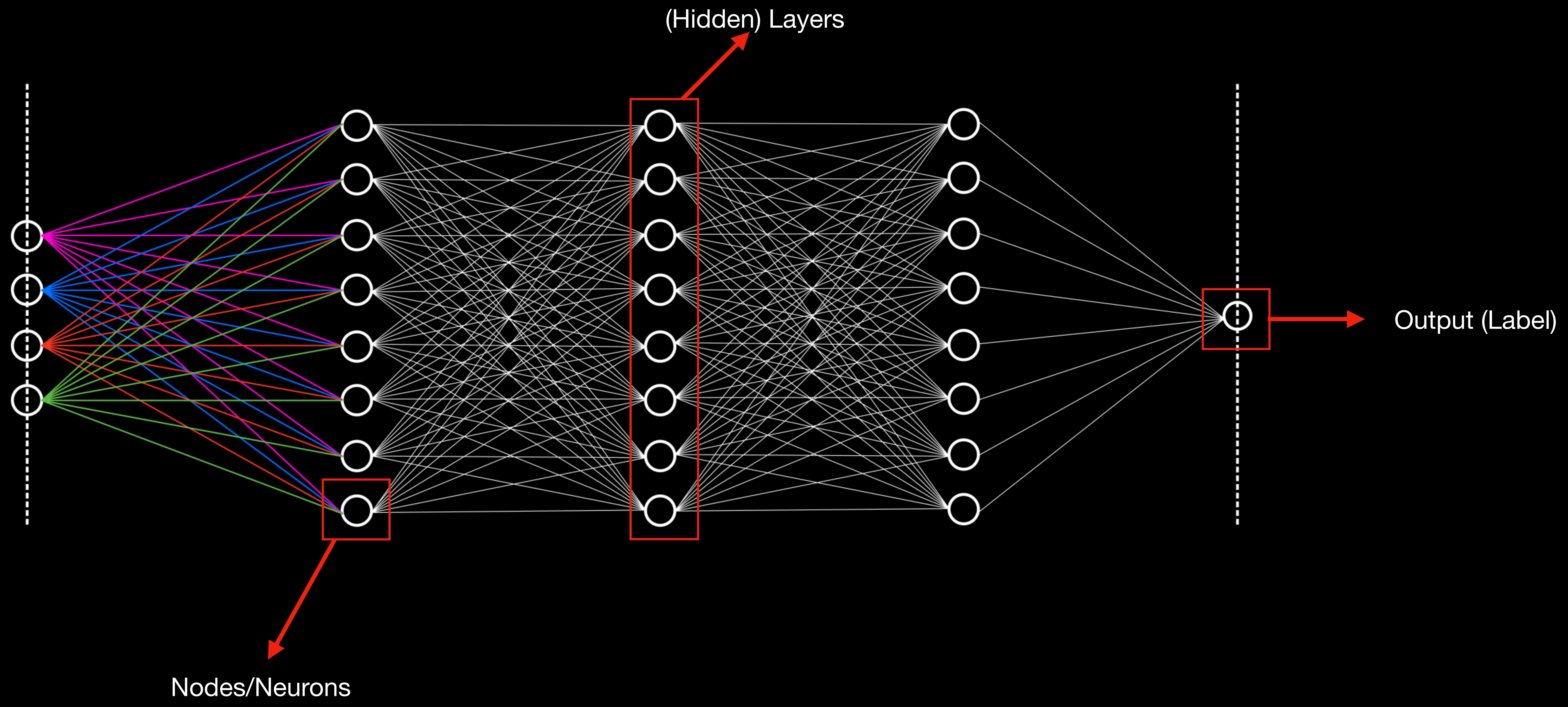

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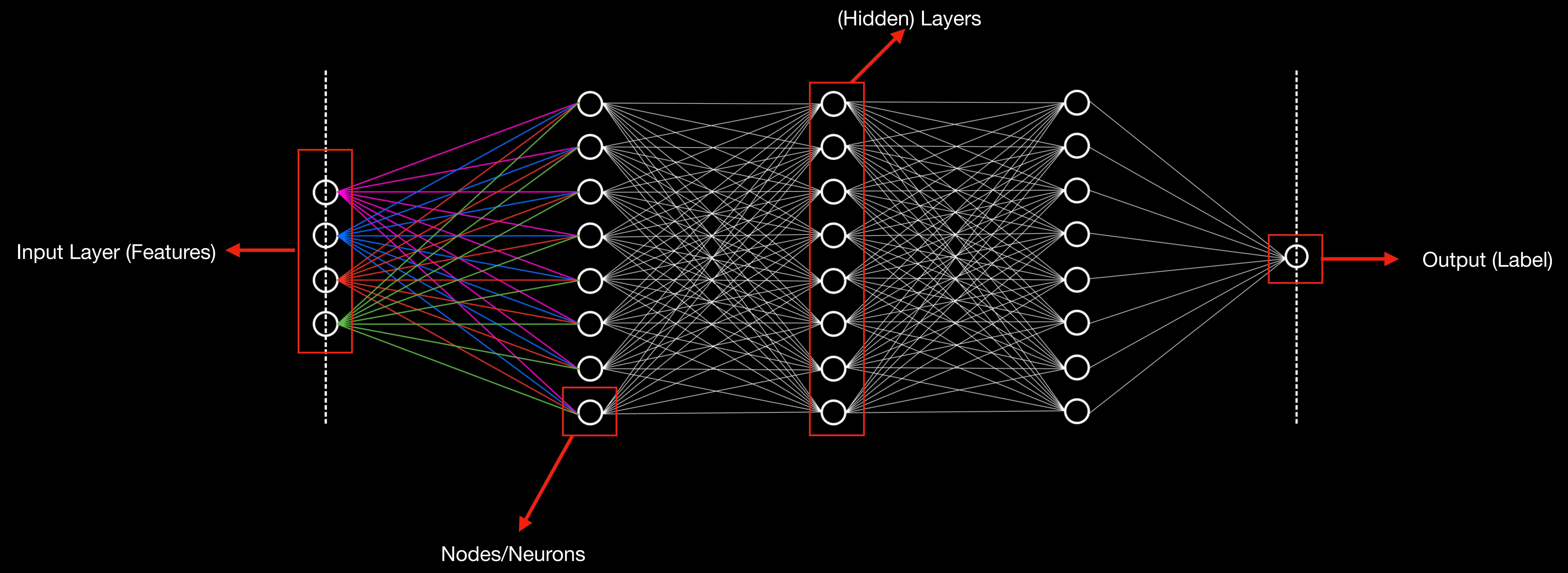

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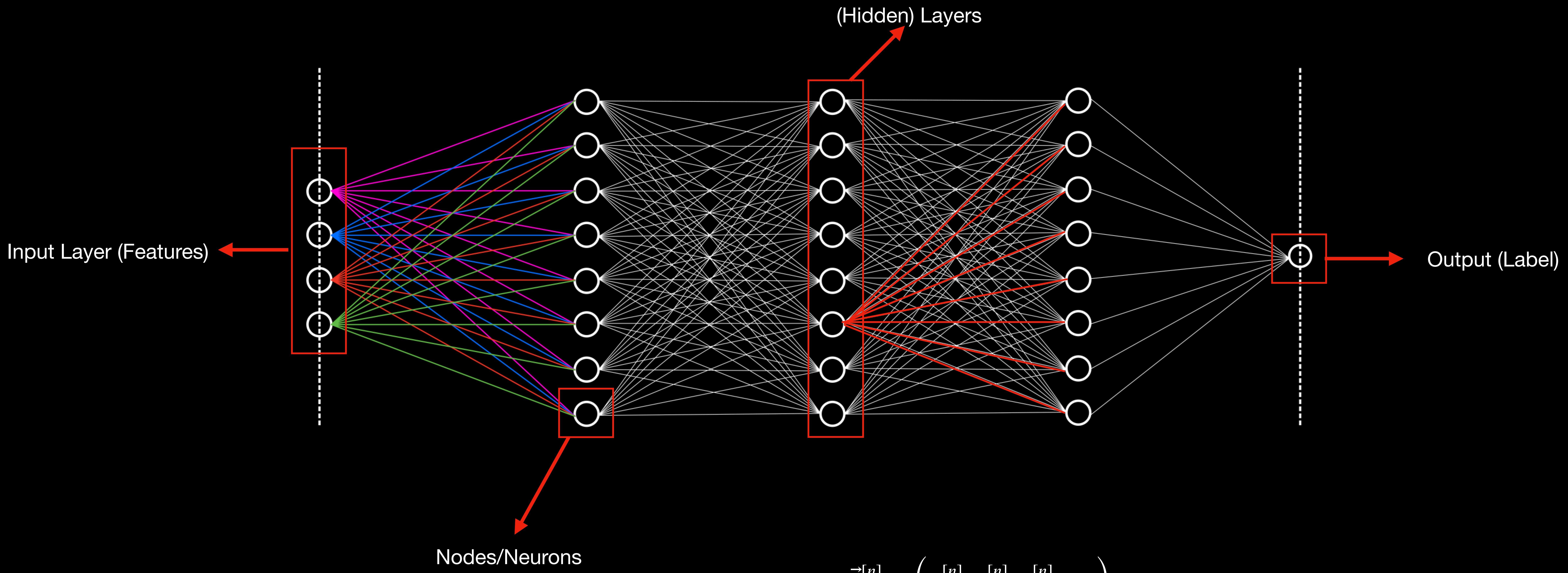


$$\vec{a}^{[n]} = \left(a_1^{[n]}, a_2^{[n]}, a_3^{[n]}, \ldots\right)$$

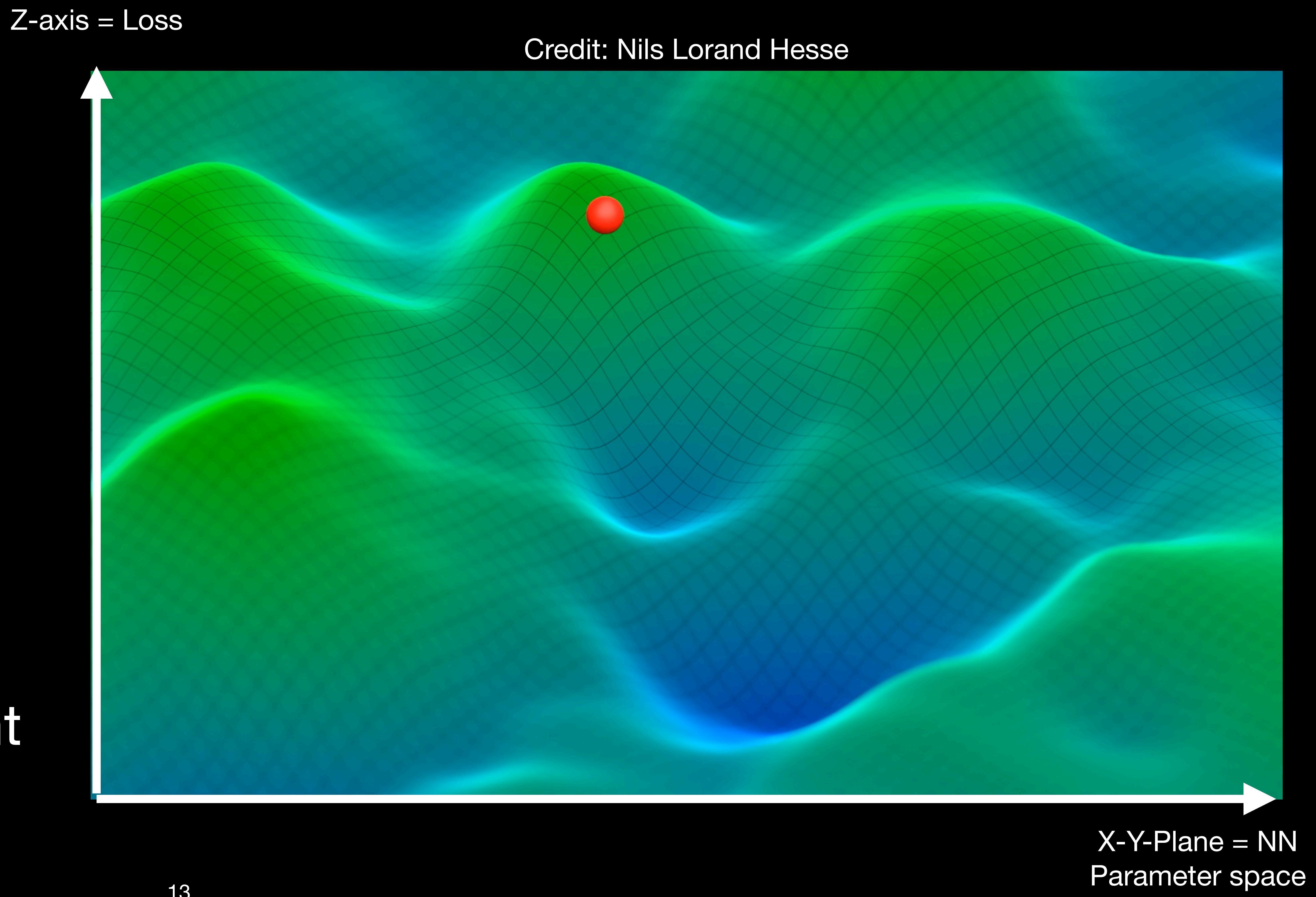
What is an ANN

Training

- Loss as quantity for NN performance (e.g. MSE)
- In this project:

$$\mathscr{L}_{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - g(x_i))^2$$

- Training = $\min_{g} \mathscr{L}$
- The optimizer (adam) finds the lowest loss via gradient descent



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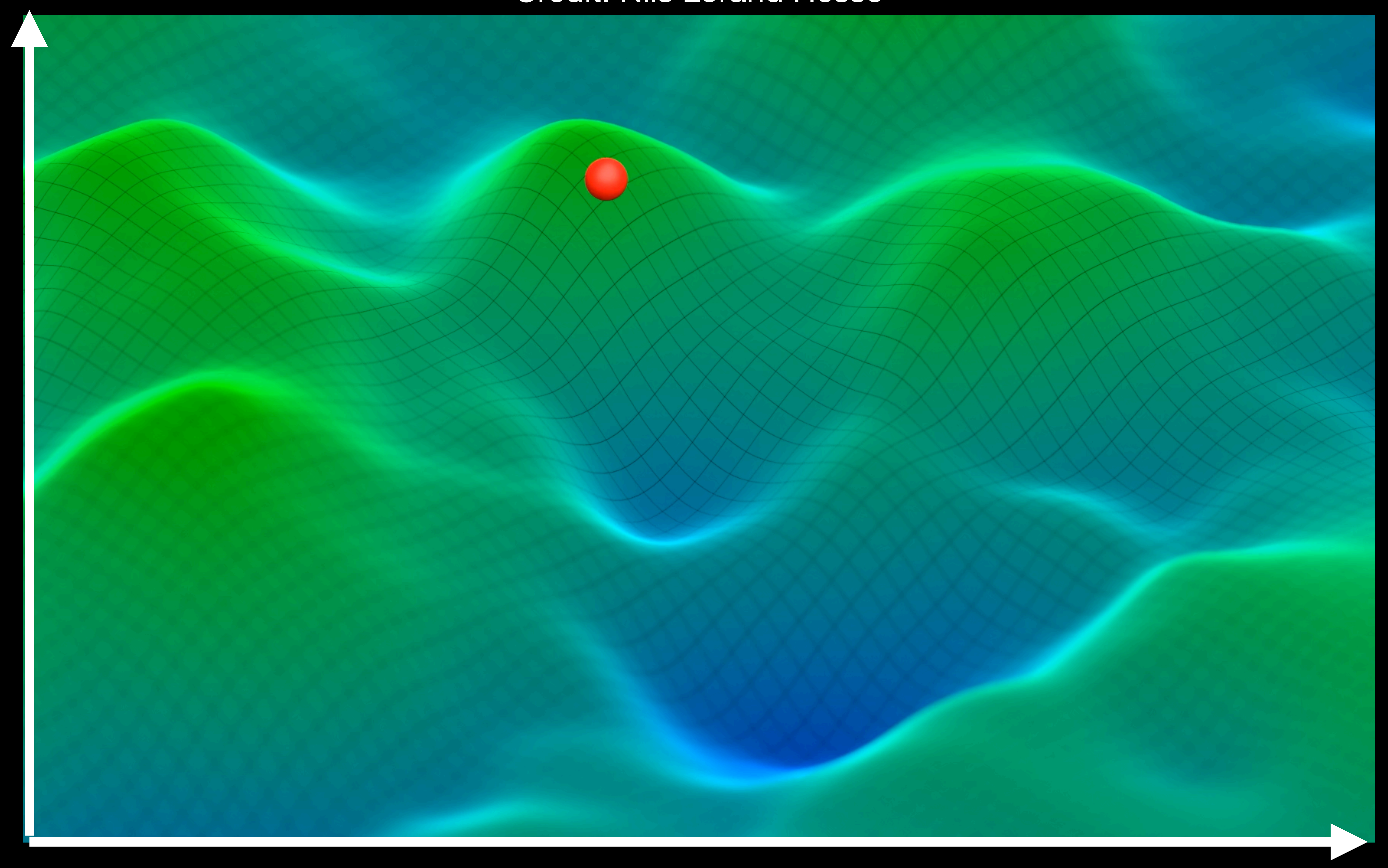

Evolution of Networks We Used

Evolution of Networks We Used

B.Sc

- trained on other dataset with ~100 points
- dataset way too small
- Overfitting

  → What is overfitting?

Evolution of Networks We Used

Overfitting

- Divide data into train, validation and test sets

  → Trace of losses indicate generalization and optimization performance

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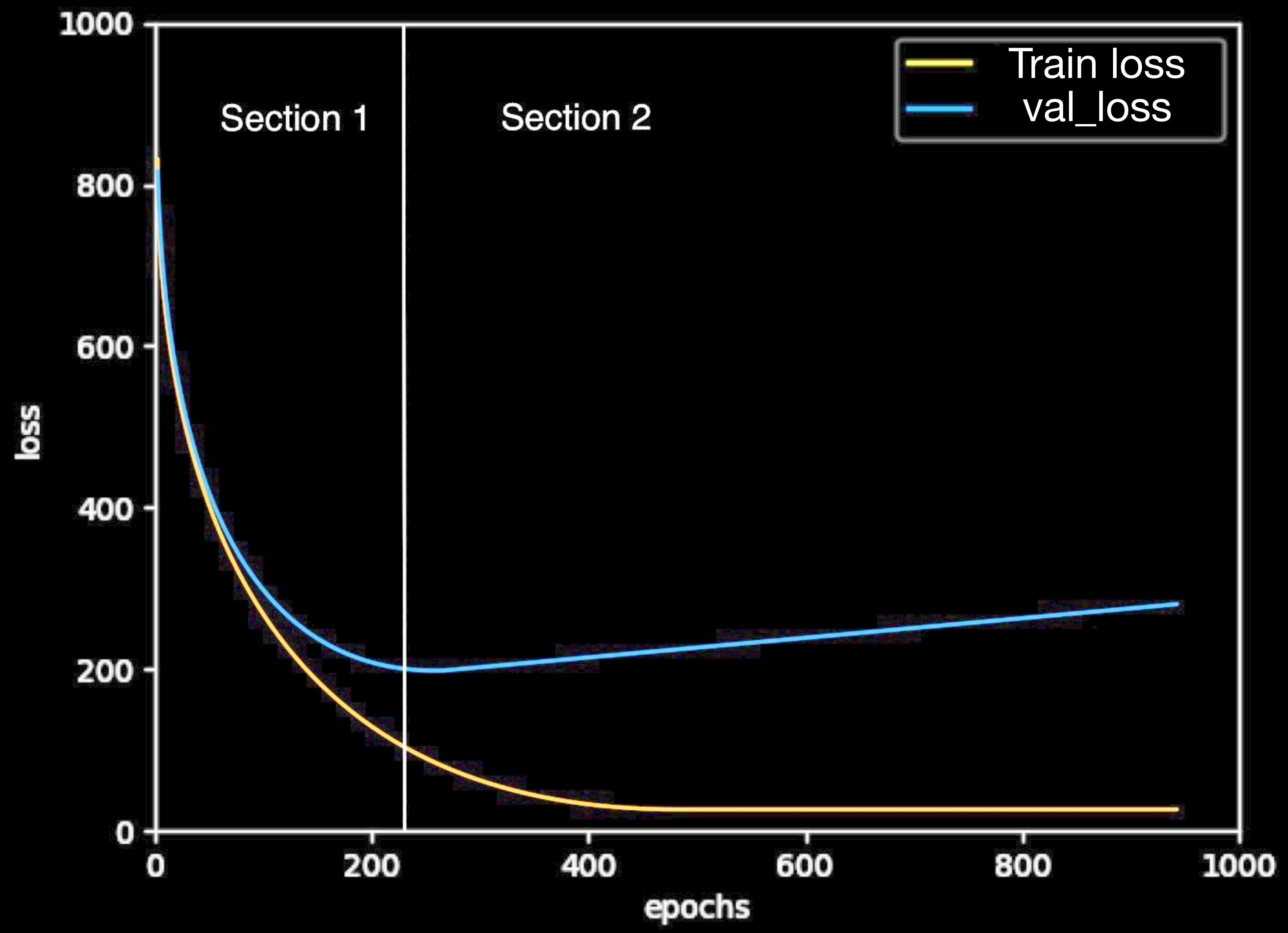

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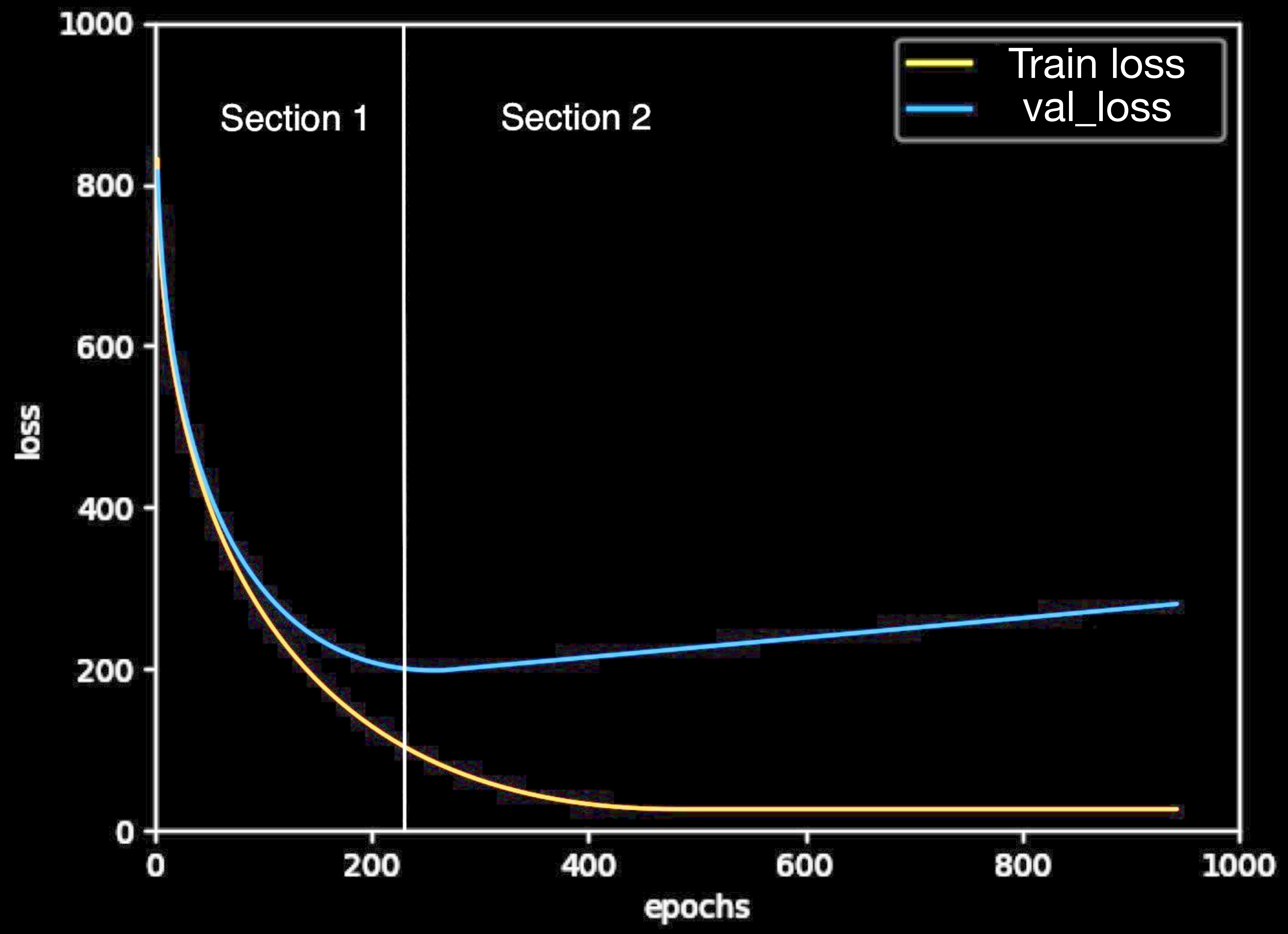

- Diverging validation loss

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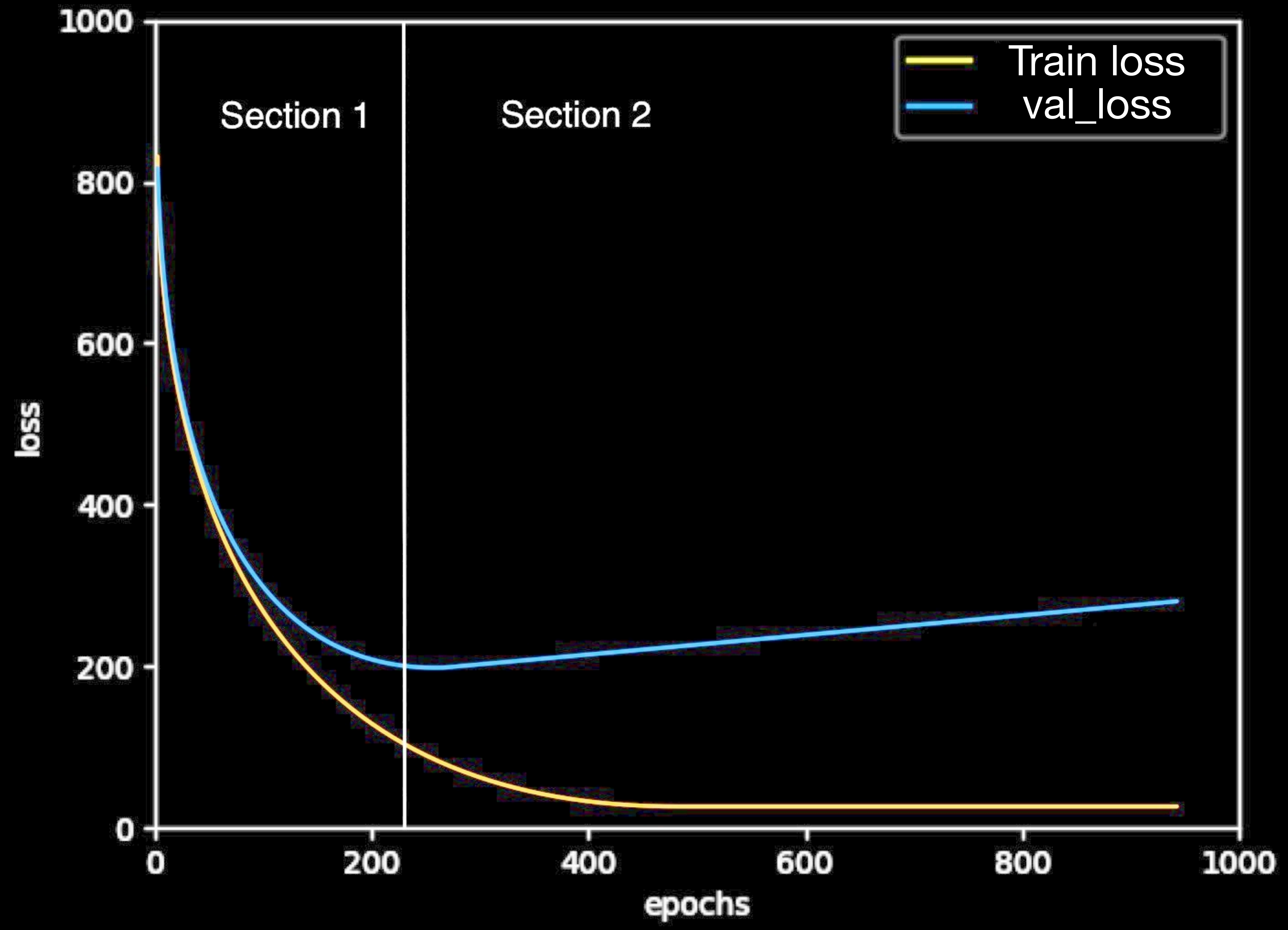

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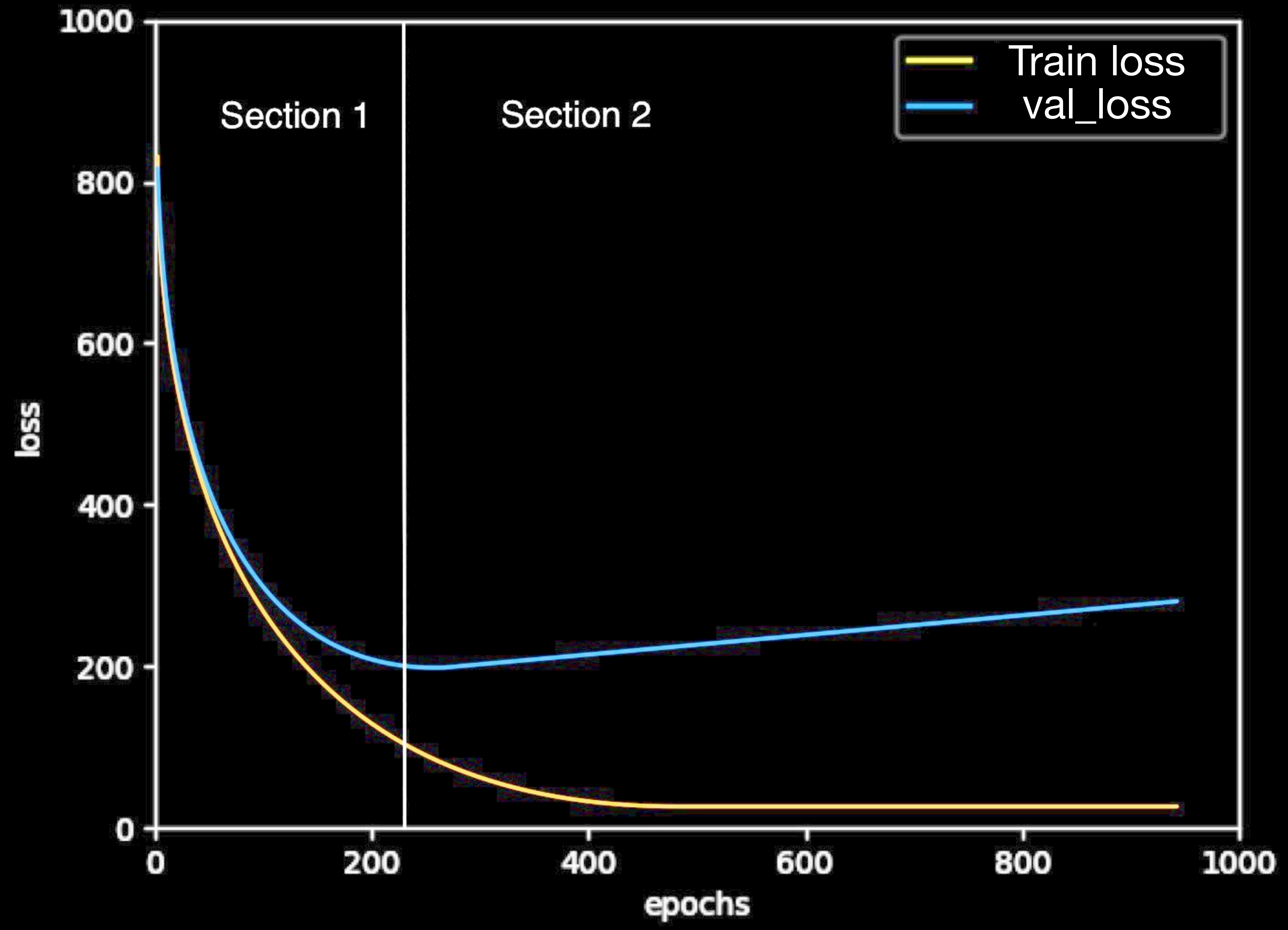


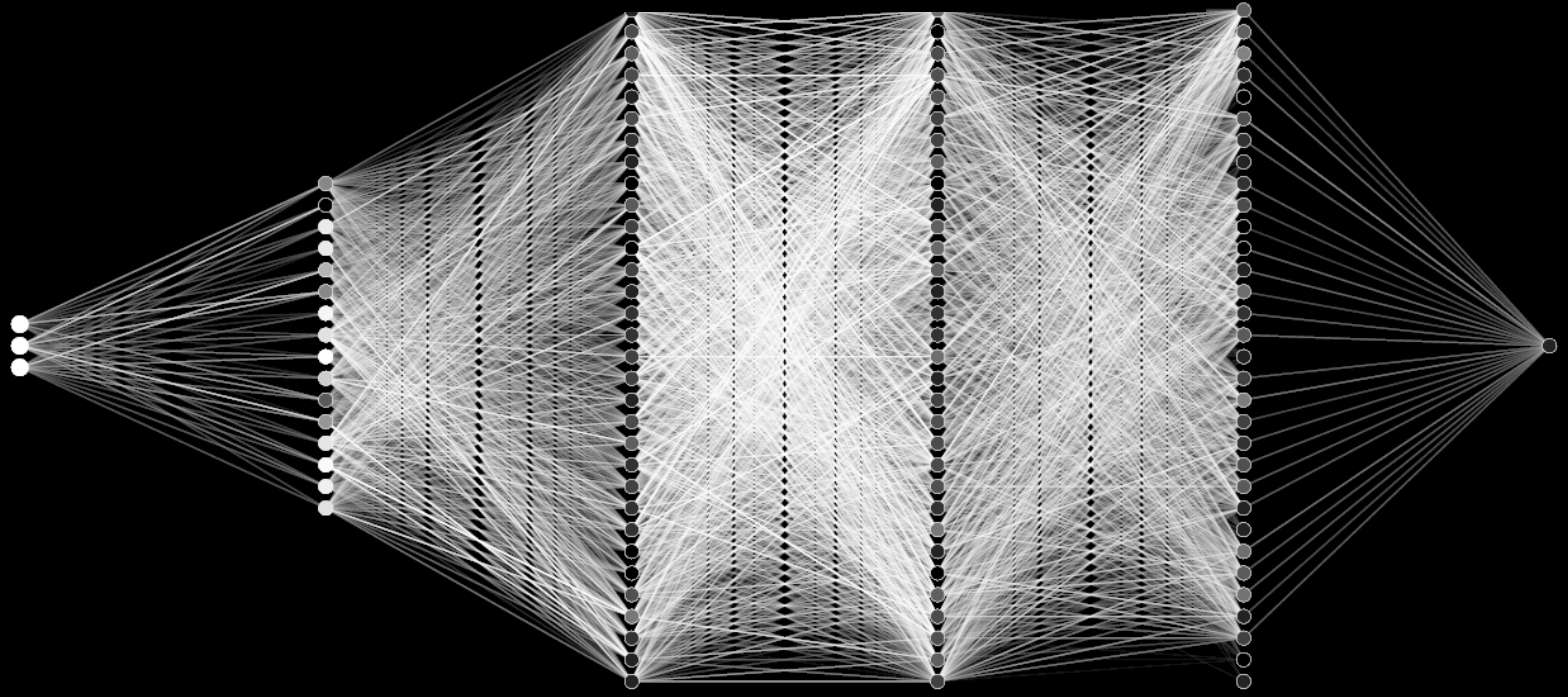
- Diverging validation loss
- Performance on test set much worse
- Prevent by: Dropout, reducing size, more data, regularizer

Evolution of Networks We Used

LETTER

Data-driven analysis of dipole strength functions using artificial neural networks

W. G. Jiang[1,*], T. Egert[1], S. Bacca[1,2], F. Bonaiti[1,3,4], and P. von Neumann-Cosel[5]



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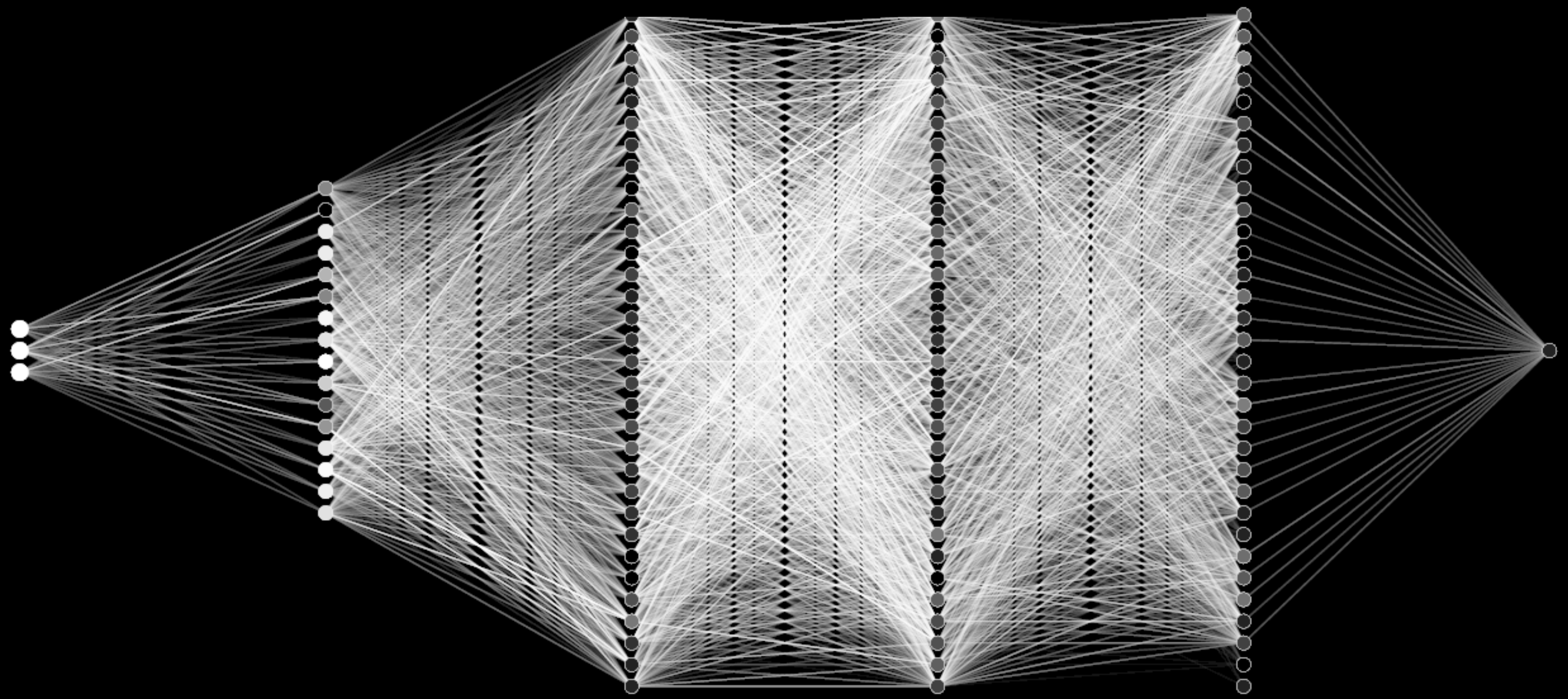

[W. Jiang, T. Egert, S. Bacca, F. Bonaiti, P. Von Neumann Cosel, Phys. Rev. C **111**, L051308]

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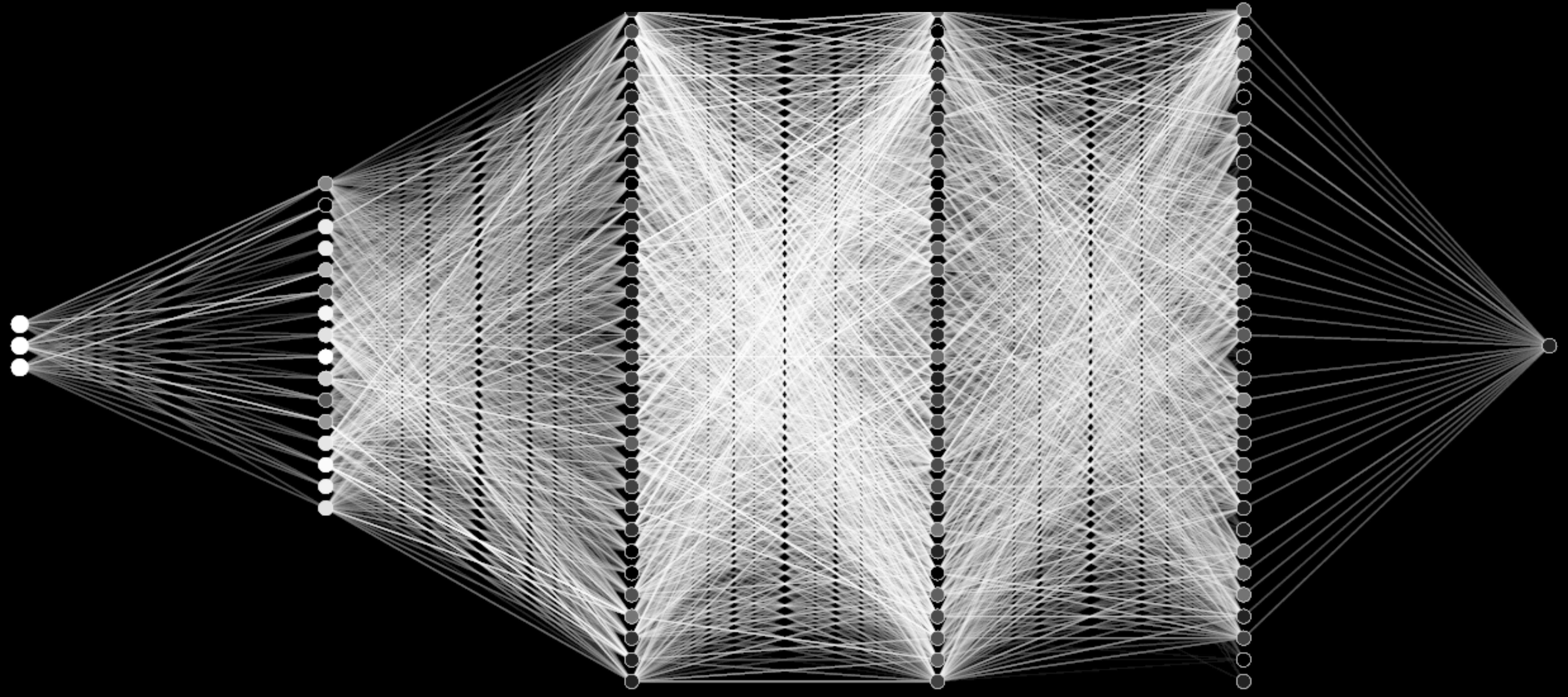

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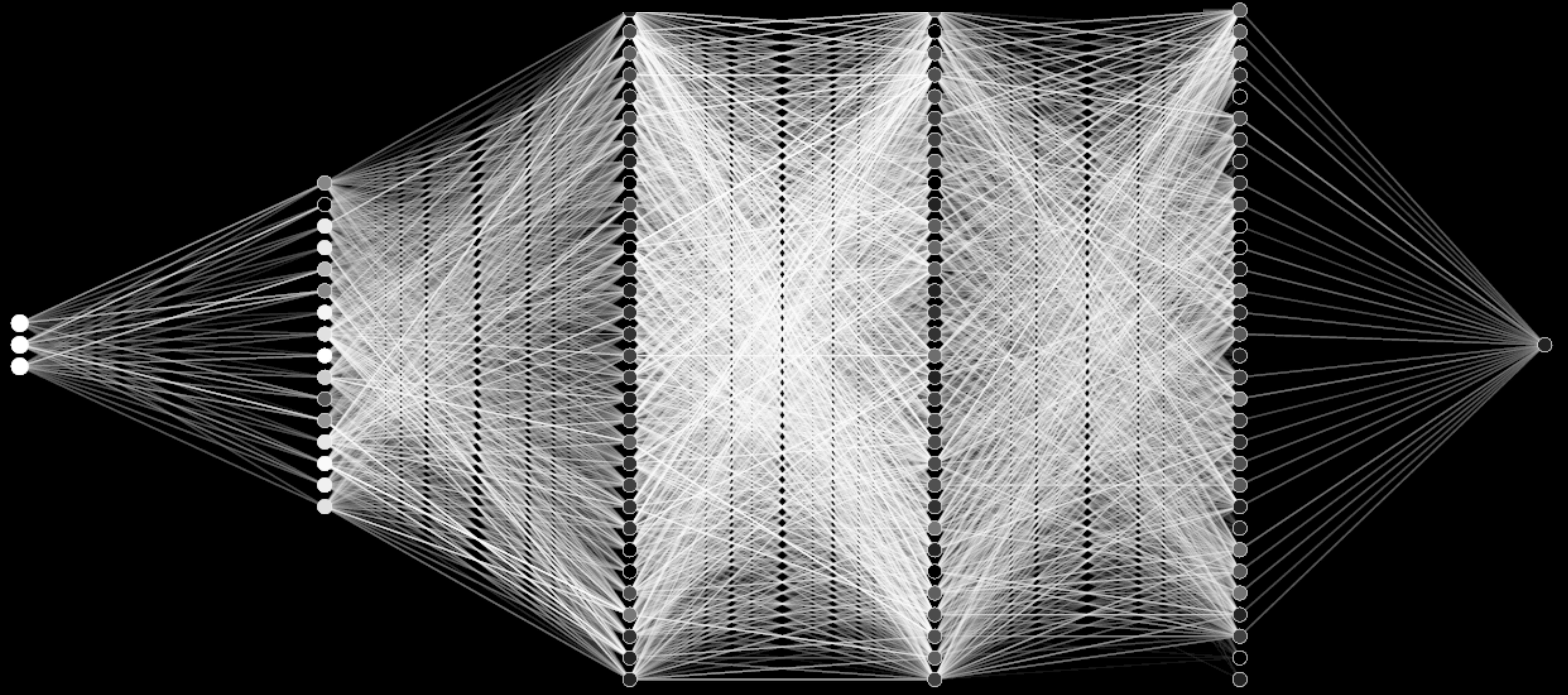

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[W. Jiang, T. Egert, S. Bacca, F. Bonaiti, P. Von Neumann Cosel, Phys. Rev. C **111**, L051308]

Evolution of Networks We Used

Results from PRC Paper

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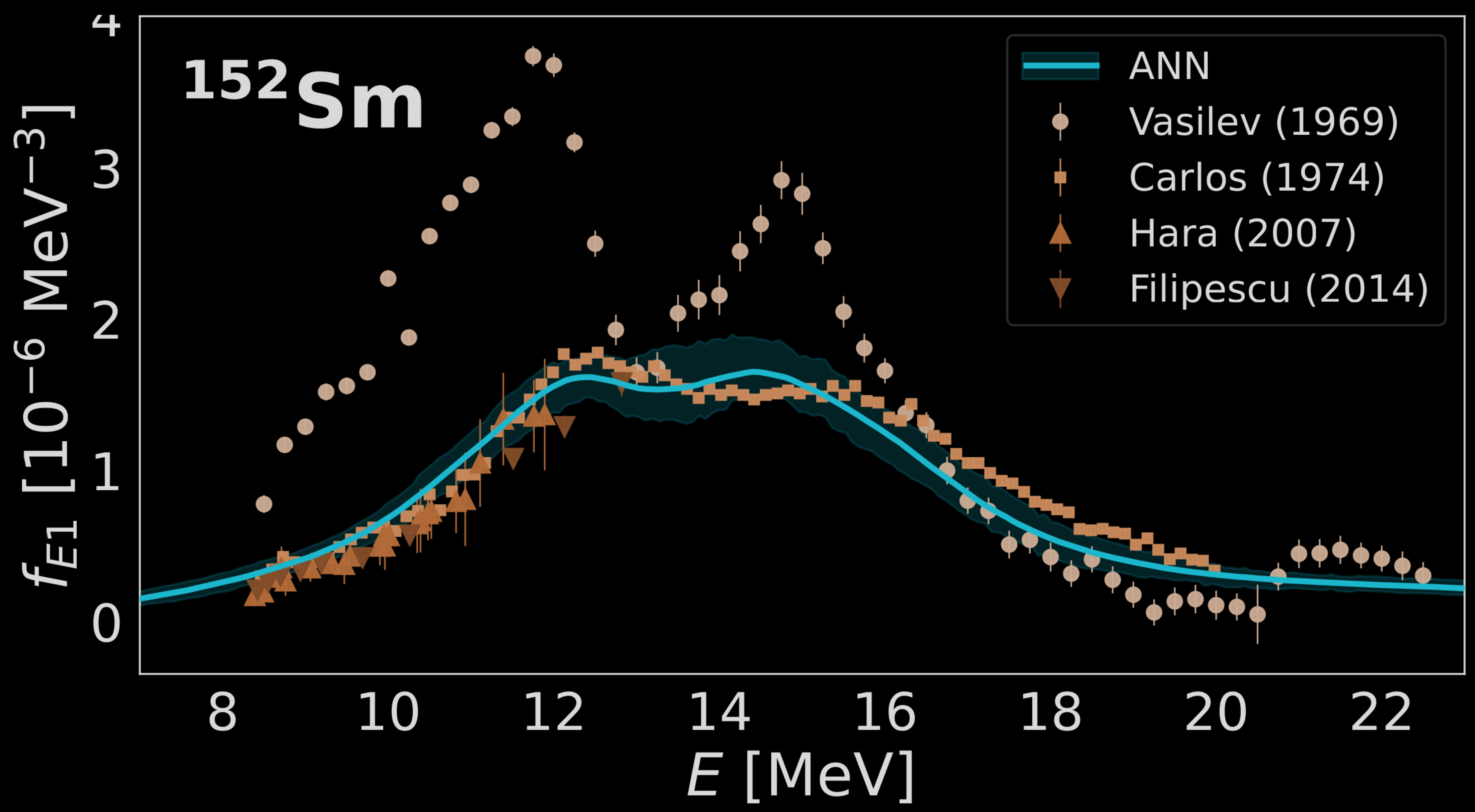

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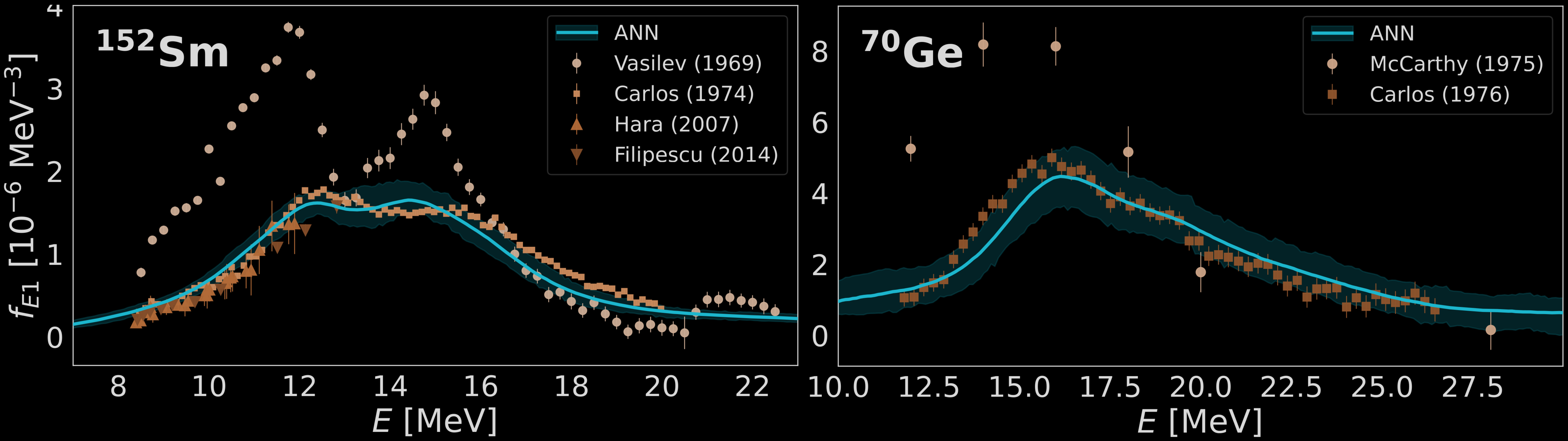

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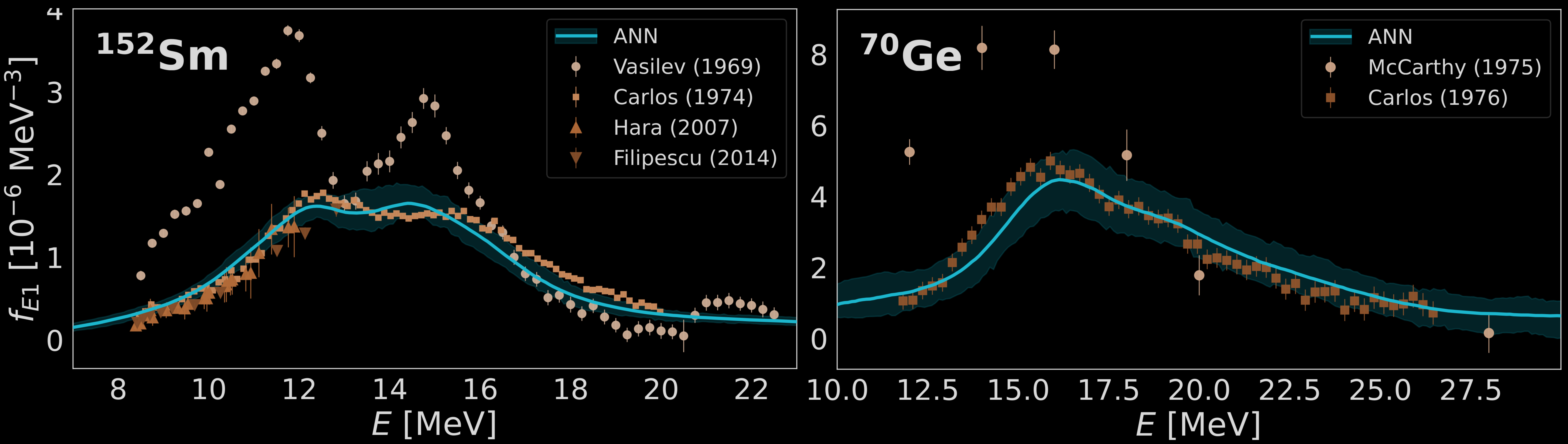

[W. Jiang, T. Egert, S. Bacca, F. Bonaiti, P. Von Neumann Cosel, Phys. Rev. C **111**, L051308]

- Use ANN to discard datasets (if ambiguous)

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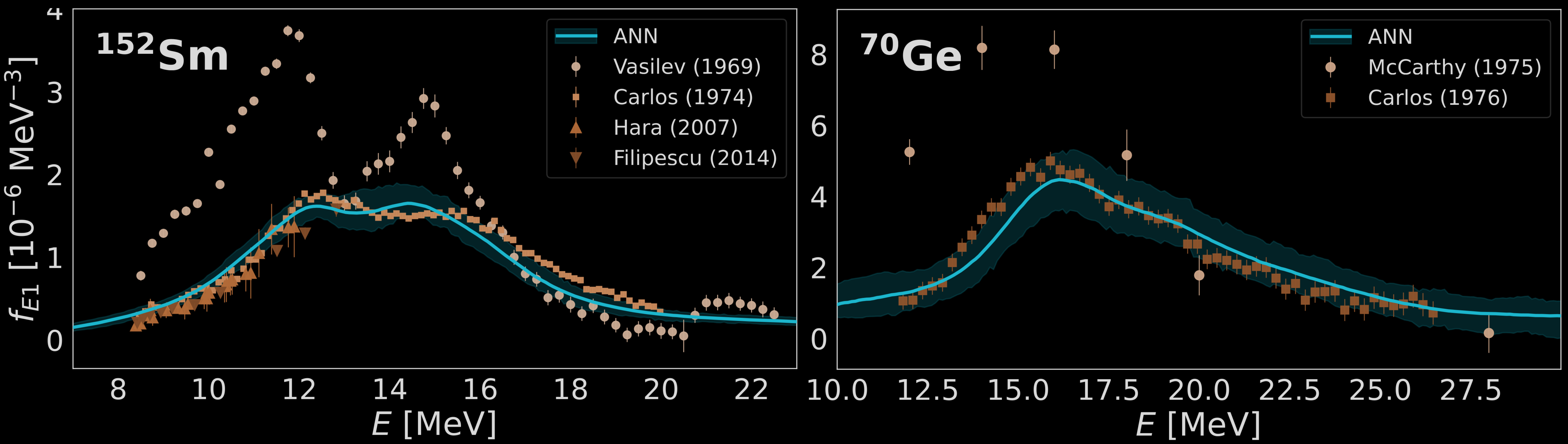

[W. Jiang, T. Egert, S. Bacca, F. Bonaiti, P. Von Neumann Cosel, Phys. Rev. C **111**, L051308]

- Use ANN to discard datasets (if ambiguous)
- Generate dipole strength for nuclei that have no experimental data

Evolution of Networks We Used

How to generate uncertainties

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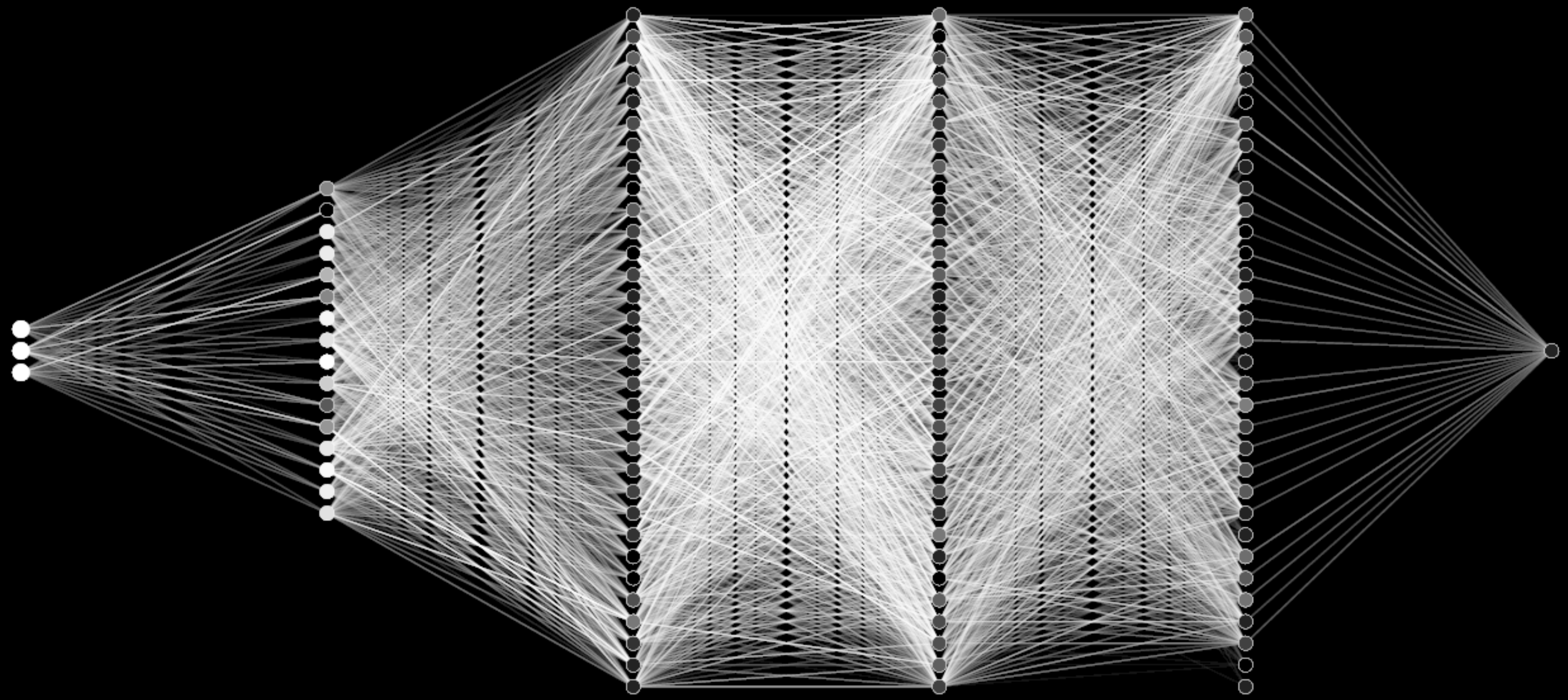
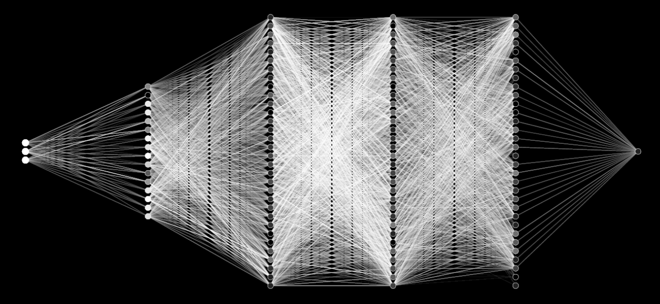


Evolution of Networks We Used

How to generate uncertainties



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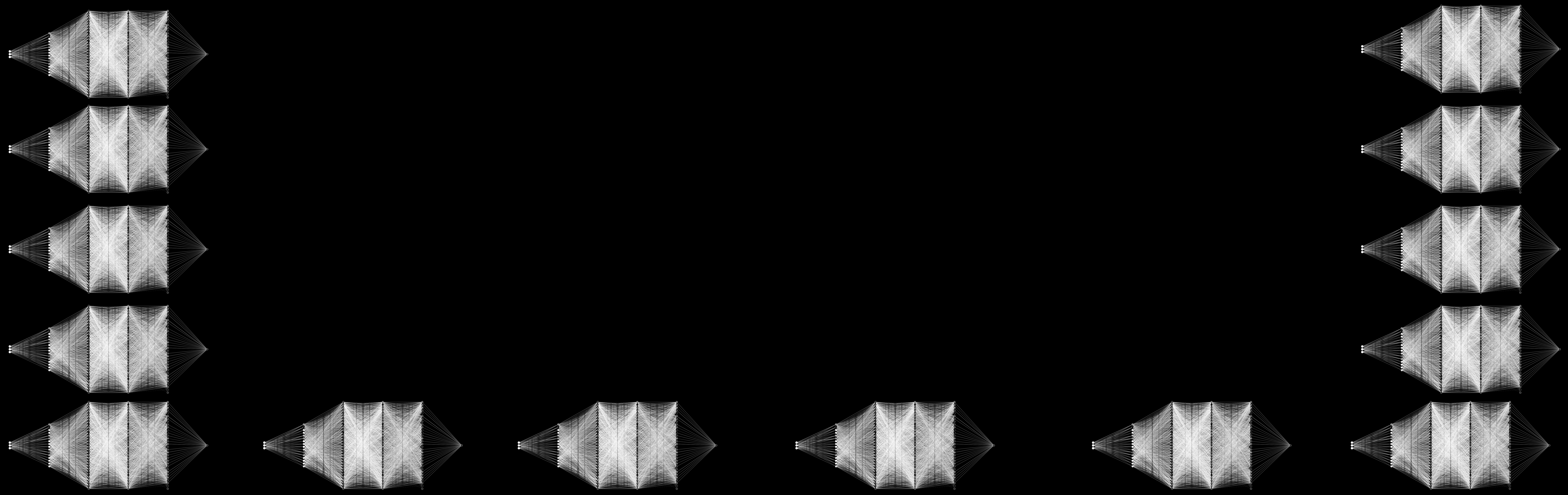

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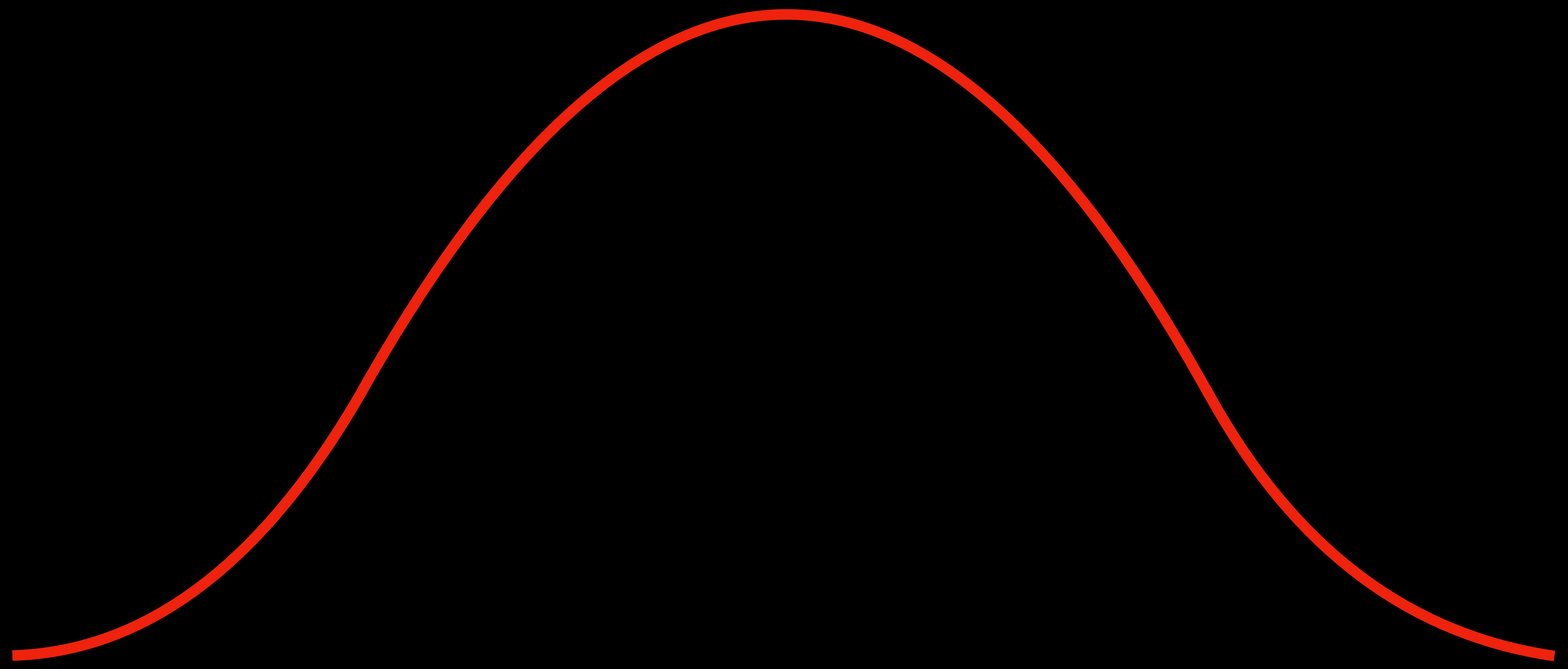
How to generate uncertainties



Evolution of Networks We Used

Muonic atoms - what’s new?

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- Embedding space

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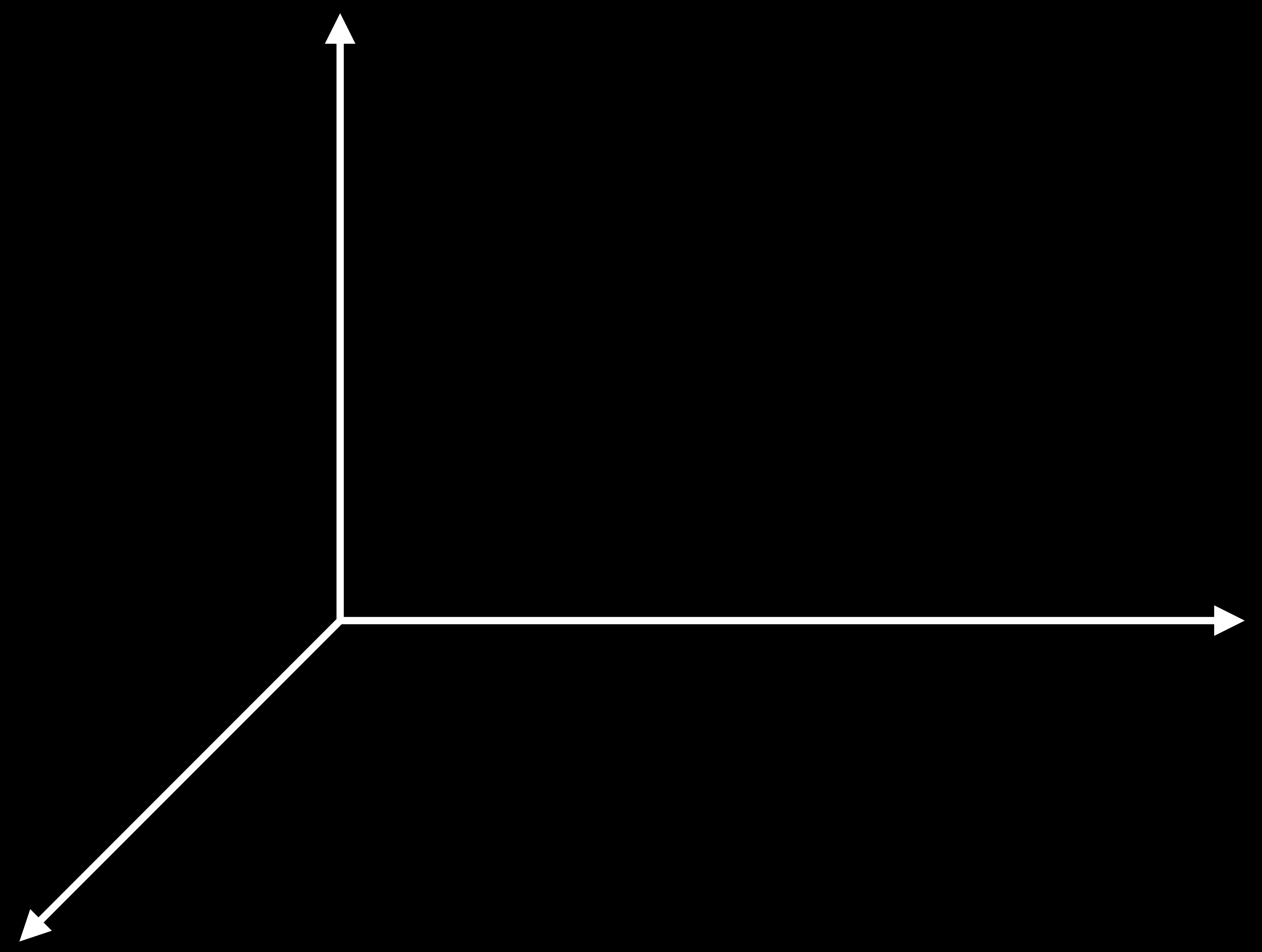

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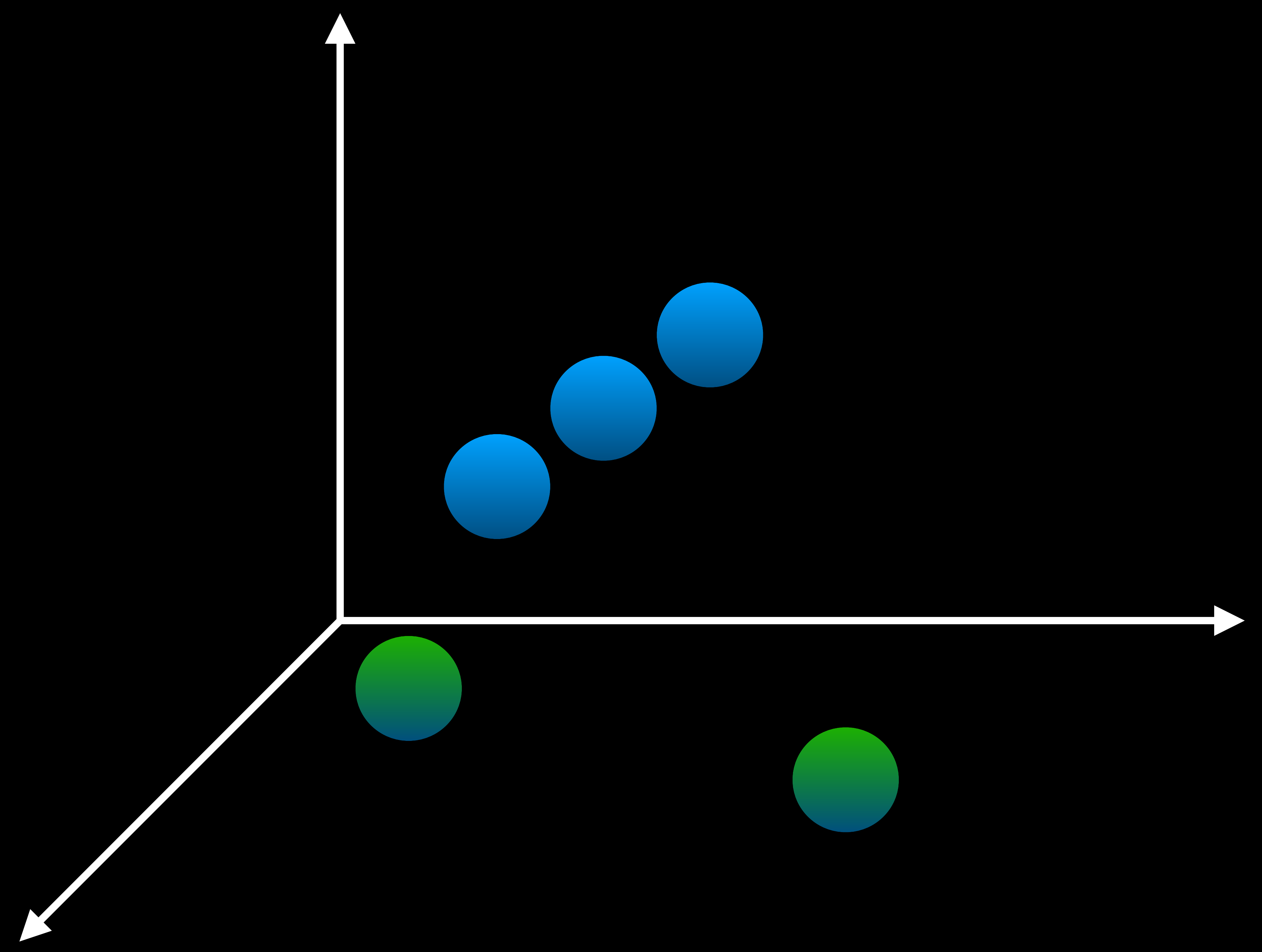

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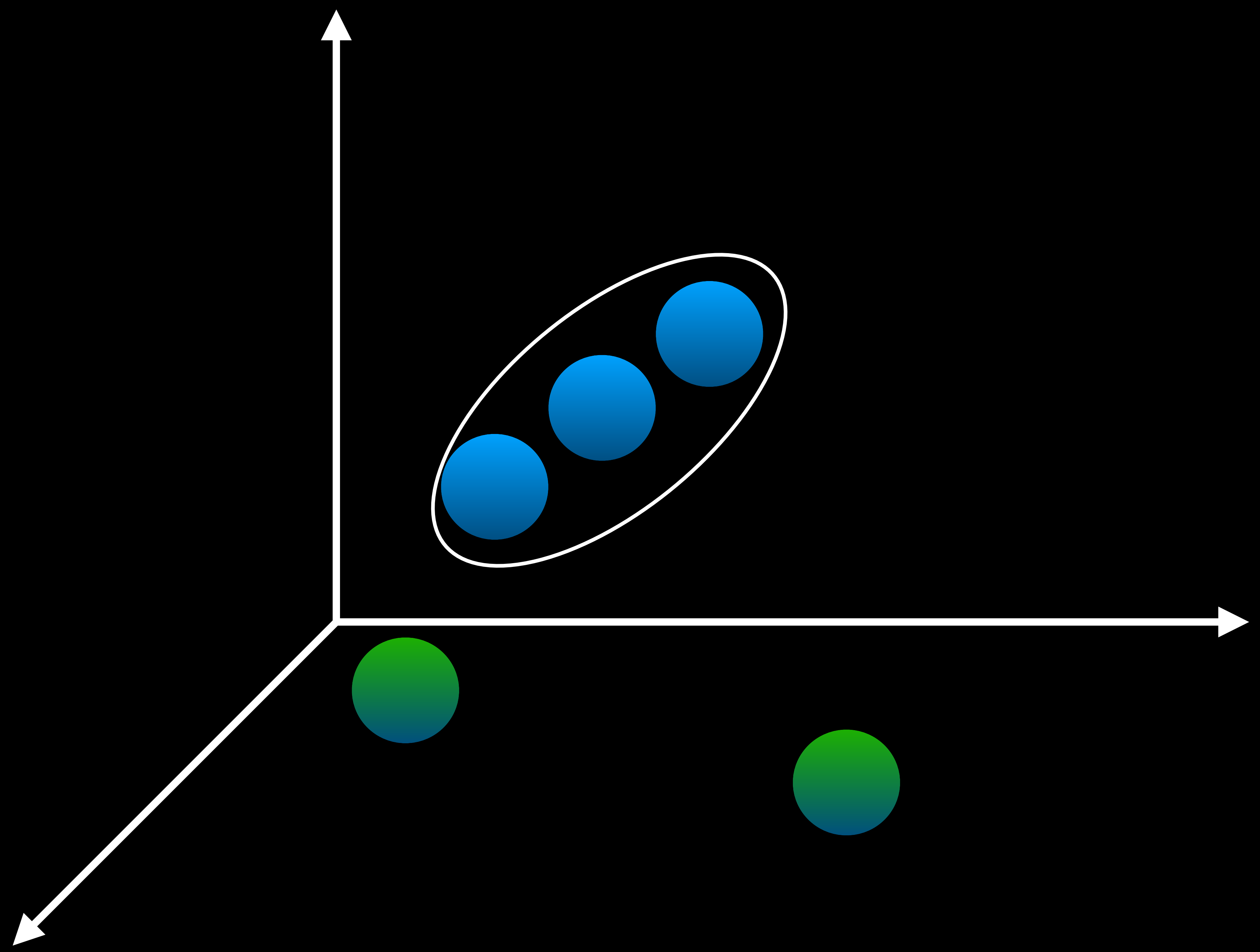

Evolution of Networks We Used

Muonic atoms - what's new?

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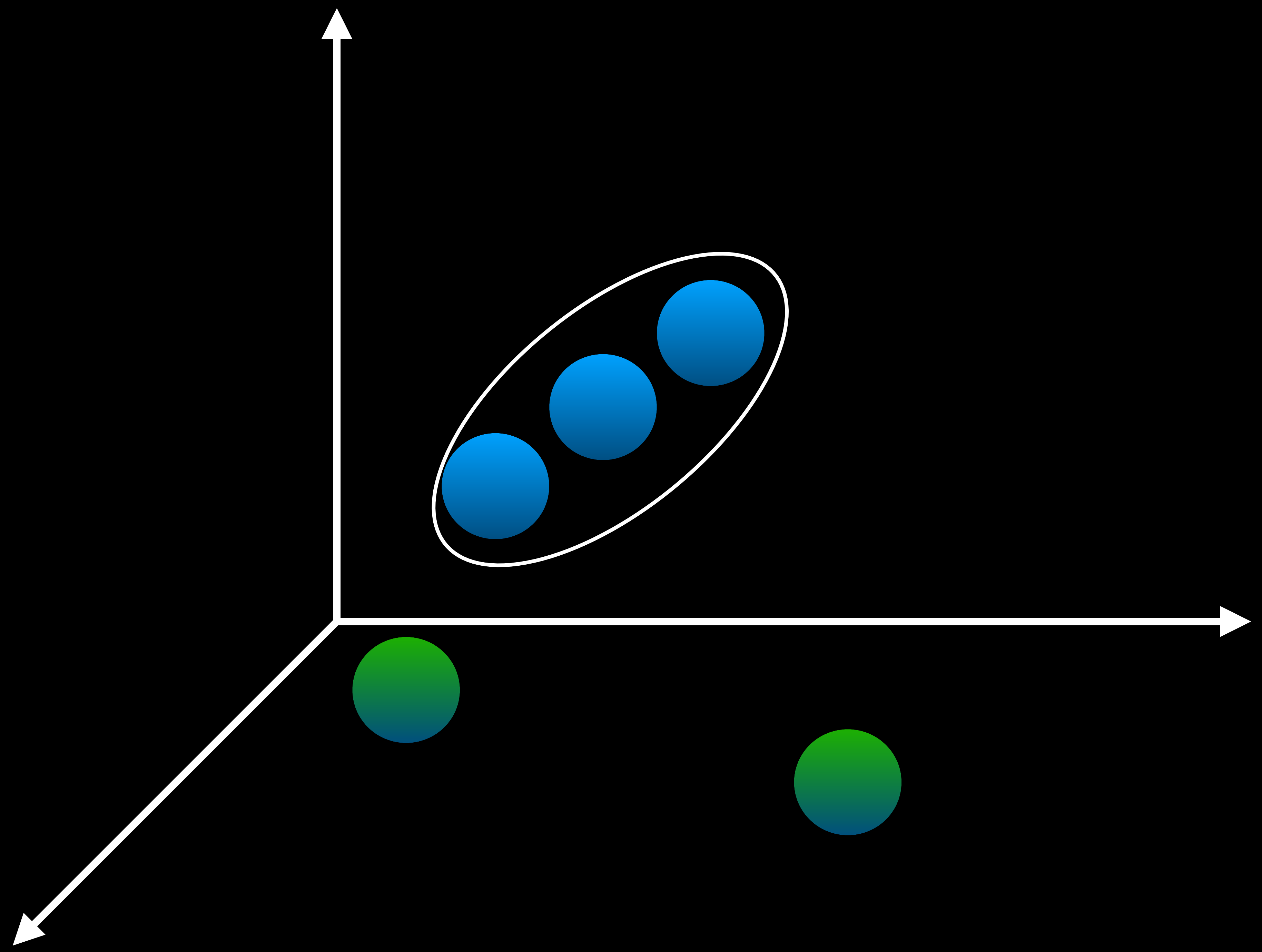
- custom loss



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ANN Loss

$$\mathscr{L}_{\text{tail}} = \lambda \left\langle \Theta(E - E_0) \left(f_{\text{pred}} \cdot \frac{E^n}{E_0^n} - \left\langle f_{\text{pred}} \cdot \frac{E^n}{E_0^n} \right\rangle \right)^2 \right\rangle_E$$

Evolution of Networks We Used

Muonic atoms - what's new?

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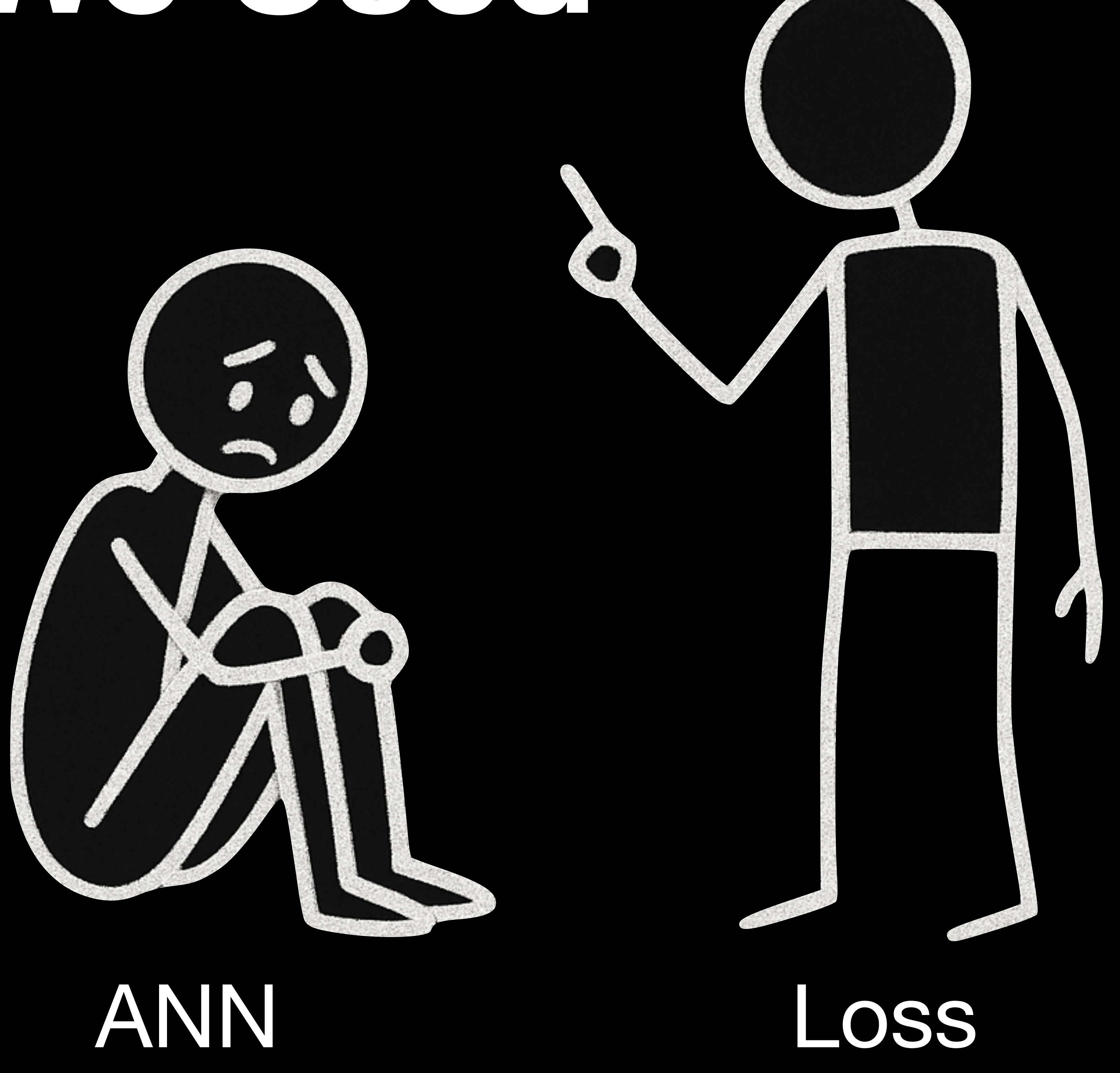
- cutoff at A = 50



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Evolution of Networks We Used

Muonic atoms - what's new?

- Embedding space
- custom loss
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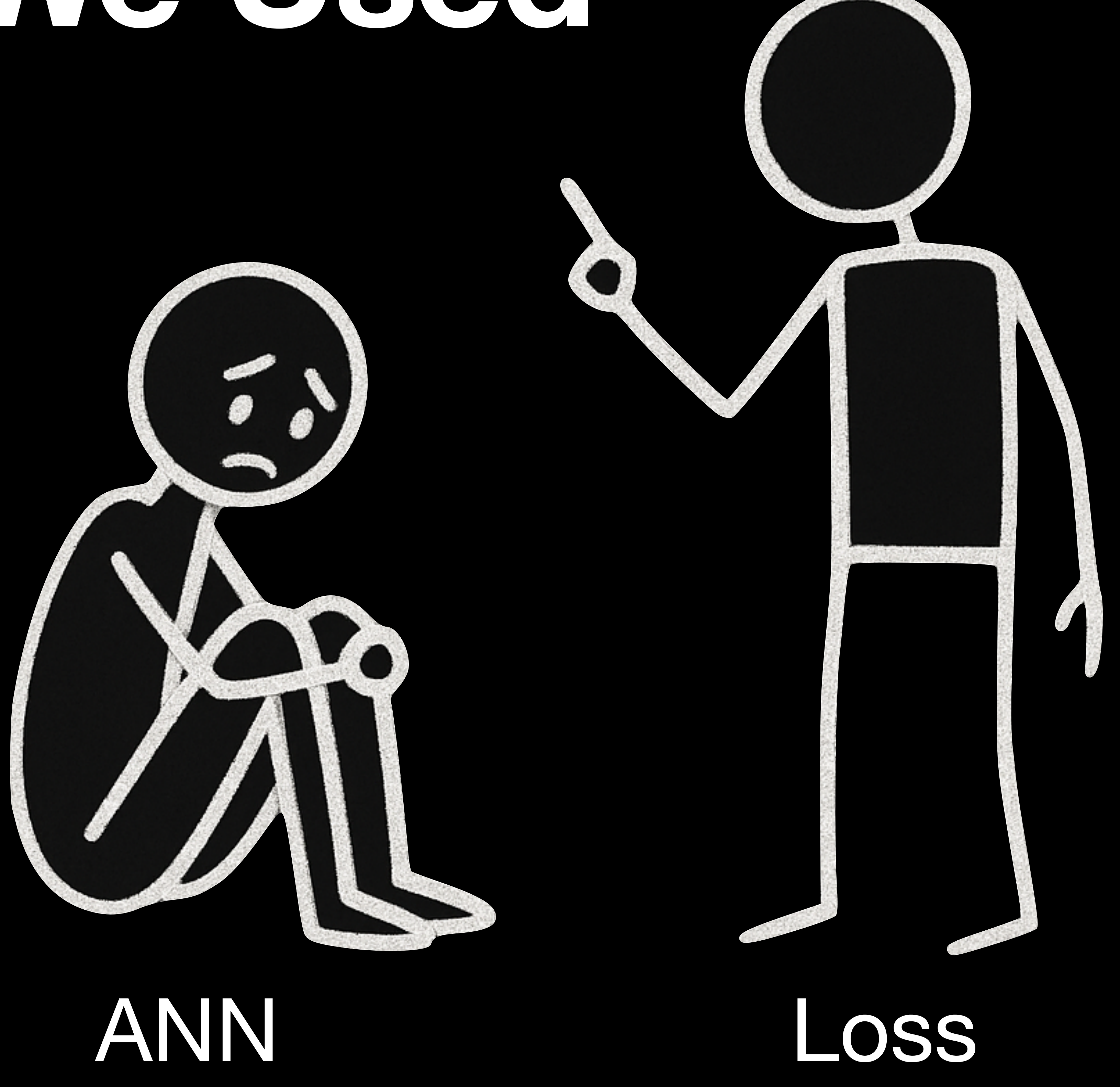
- sample weights = uncertainties



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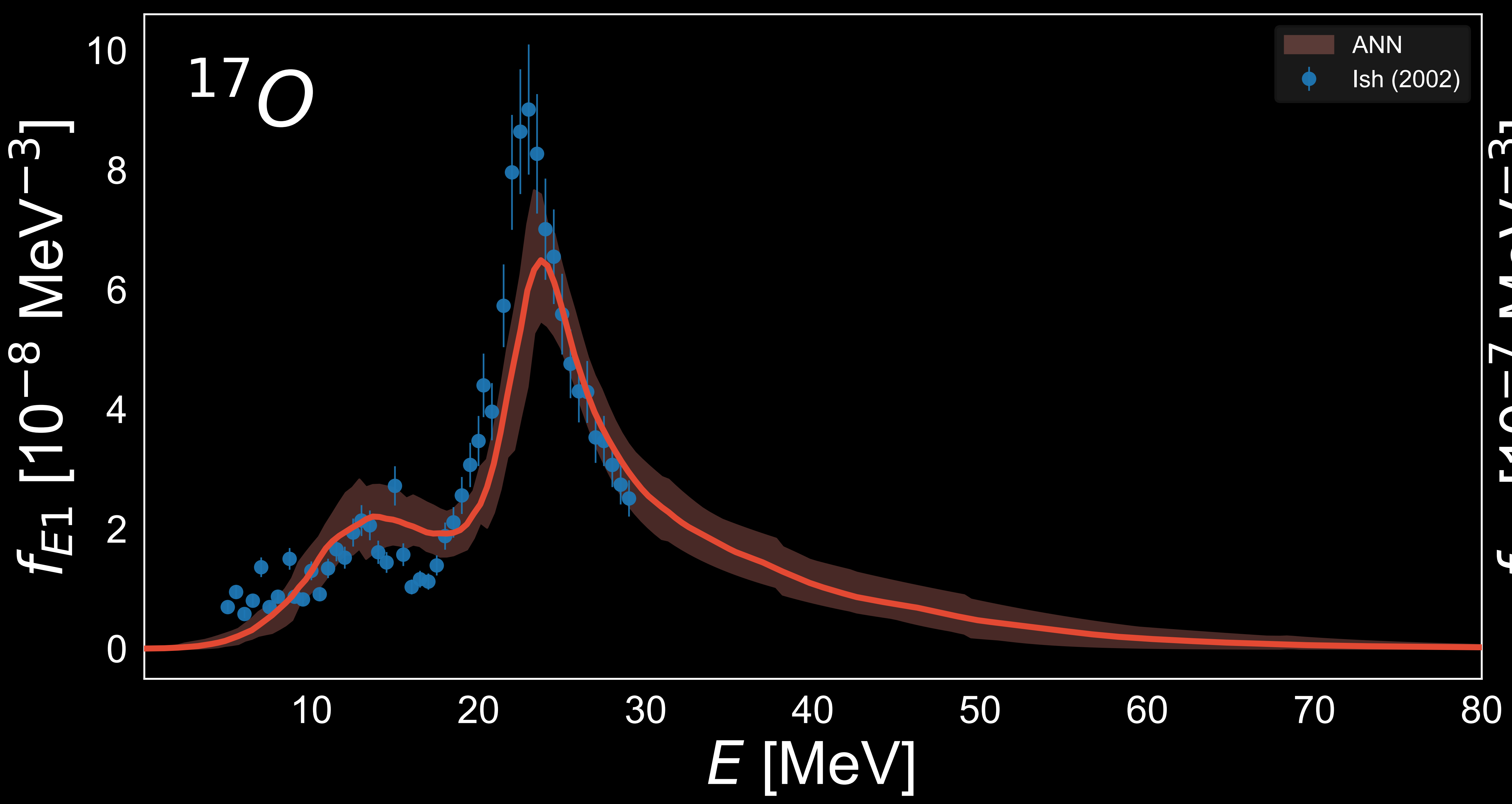
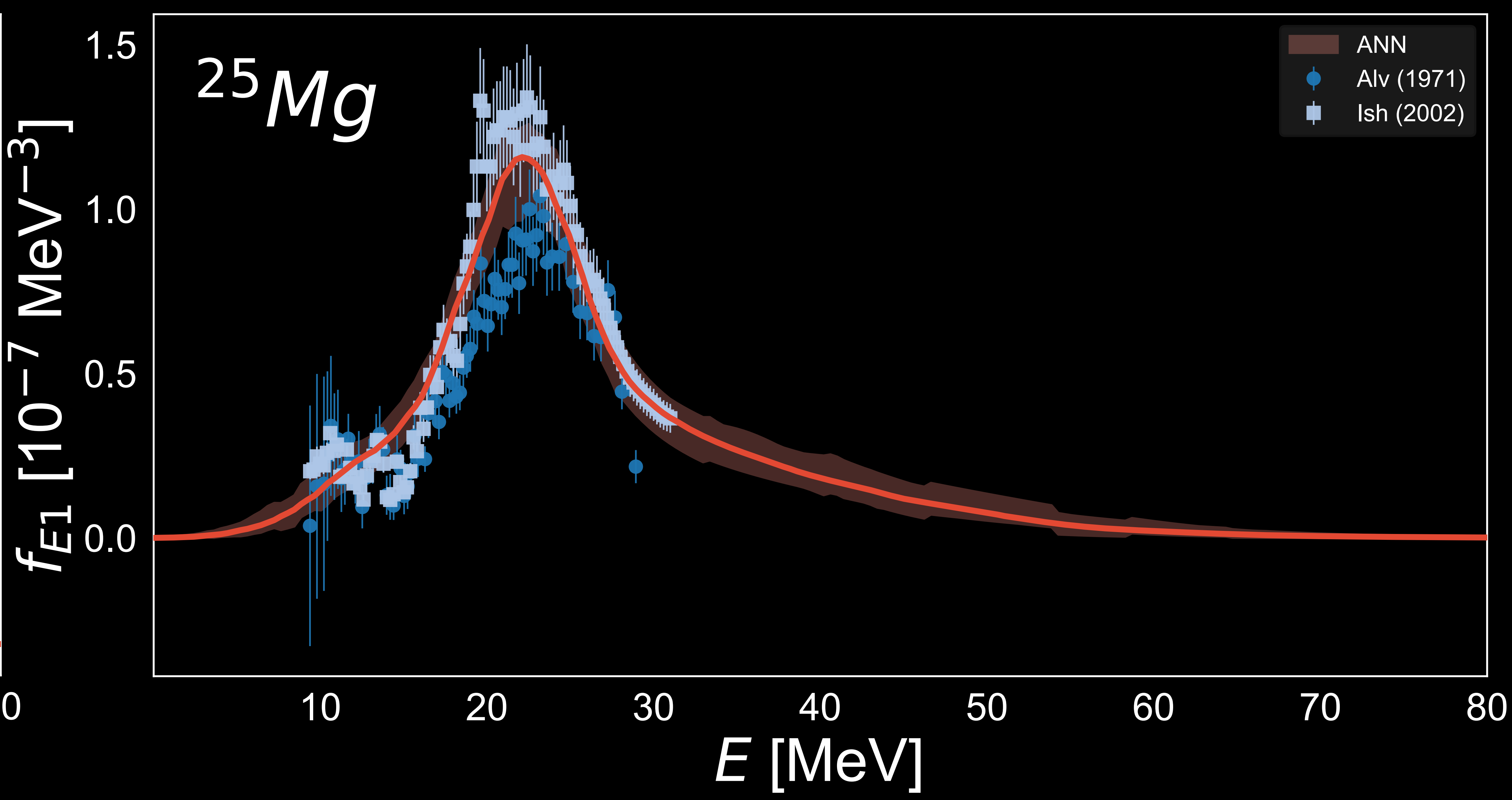
Evolution of Networks We Used

Muonic atoms - predictive power within isotope chains

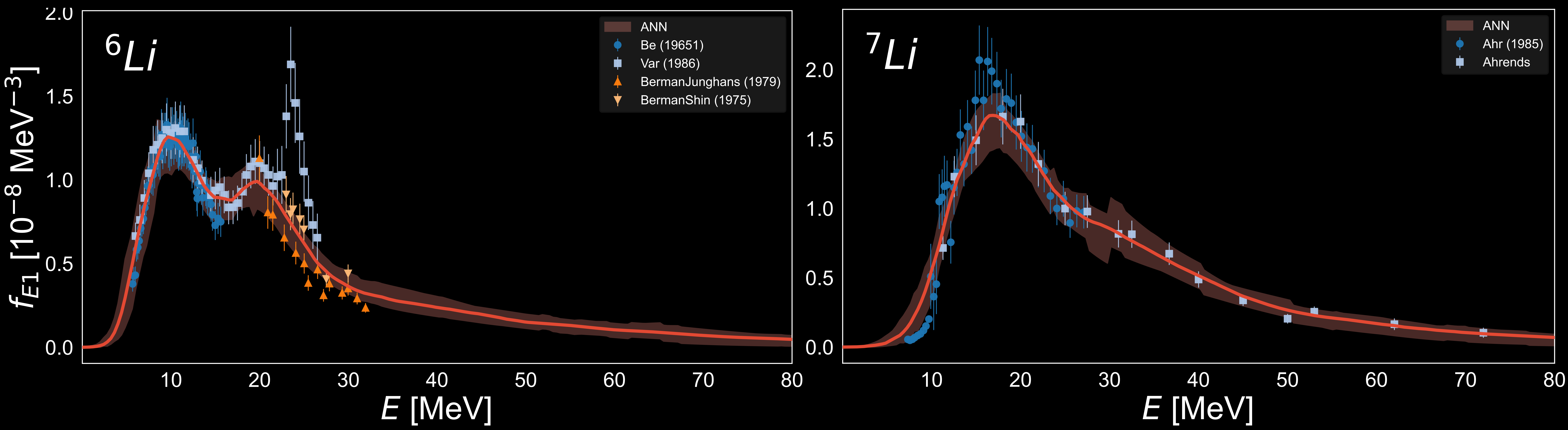




What can we do from here?

Evolution of Networks We Used

Muonic atoms - results for lithium



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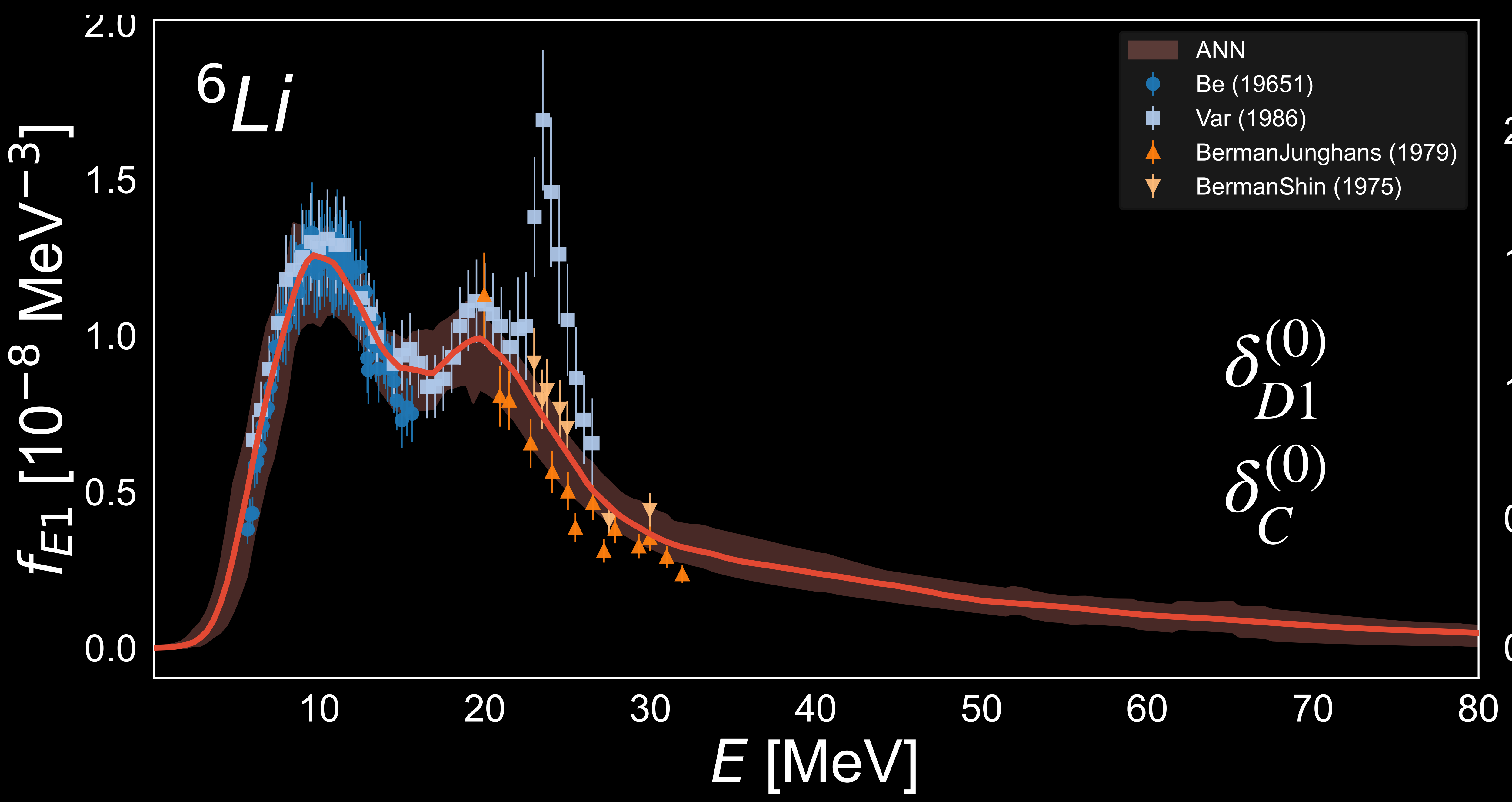

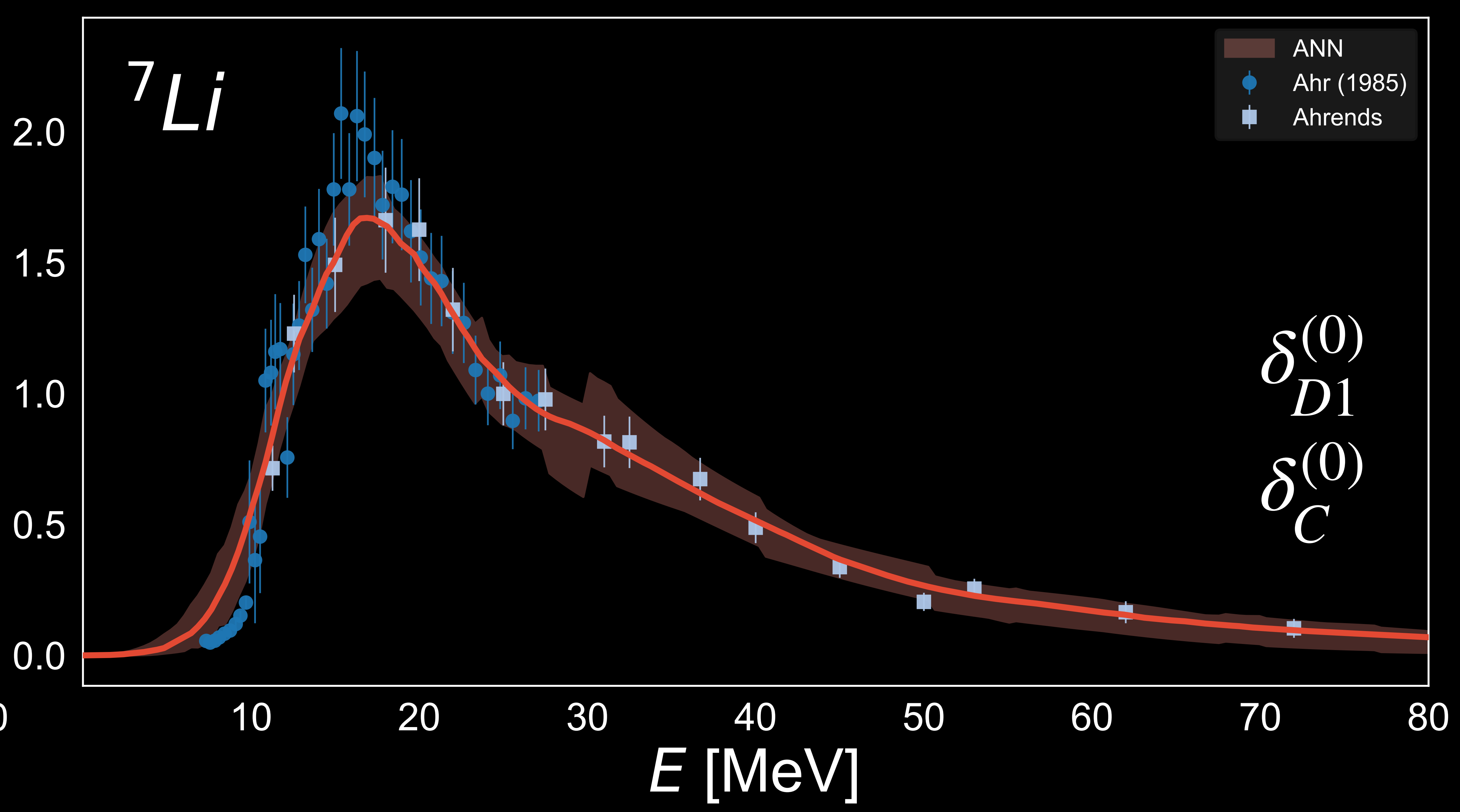

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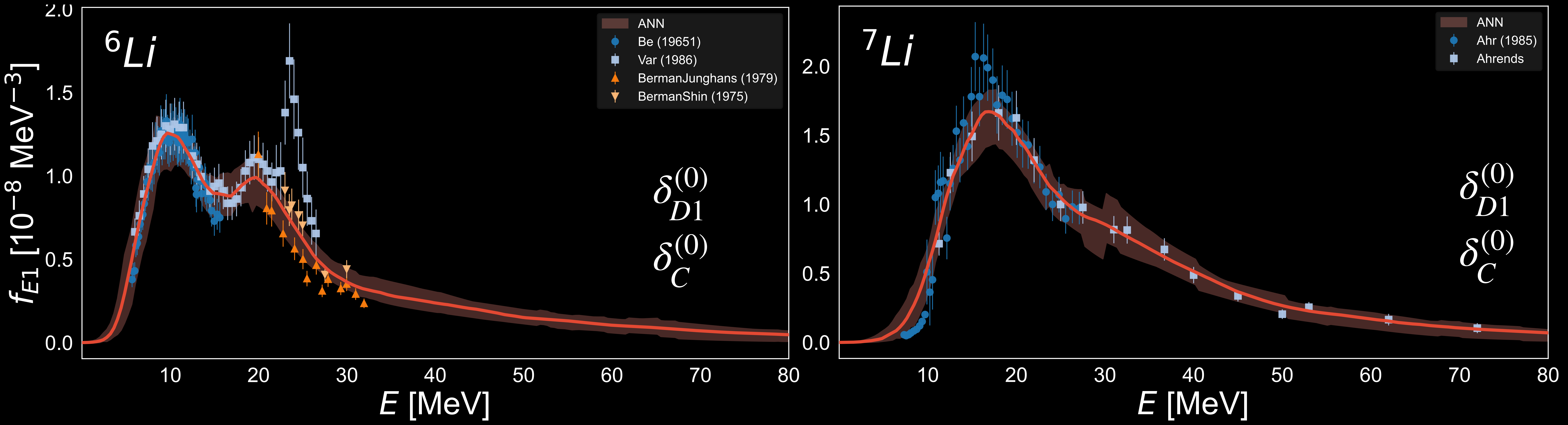

$$\delta^{(0)}_{D1} = -\frac{16\pi^2}{9}(Z\alpha)^2\phi^2(0)\int_0^\infty \mathrm{d}\omega\sqrt{\frac{2m_r}{\omega}}S_{D1}(\omega)$$

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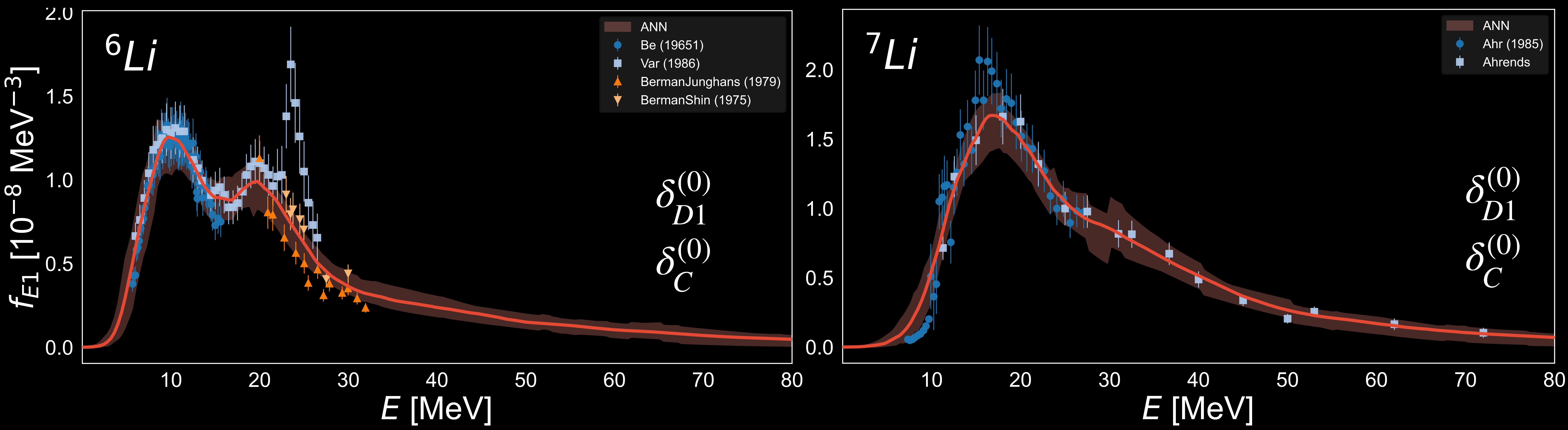

$$\delta^{(0)}_{D1} = -\frac{16\pi^2}{9}(Z\alpha)^2\phi^2(0)\int_0^\infty \mathrm{d}\omega \sqrt{\frac{2m_r}{\omega}}\, S_{D1}(\omega)$$

$$\delta^{(0)}_{C} = -\frac{16\pi^2}{9}(Z\alpha)^3\phi^2(0)\int_0^\infty \mathrm{d}\omega \frac{m_r}{\omega} \ln\left(\frac{2(Z\alpha)^2 m_r}{\omega}\right) S_{D1}(\omega)$$

Nuclear Structure Corrections

From ANN predictions

Preliminary

Nucleus/energy correction	$\delta_{D1}^{(0)}$ [meV]	$\delta_{C}^{(0)}$ [meV]
^{6}Li	(-29.21, -32.12, -34.92)	(5.82, 6.49, 7.03)
^{7}Li	(-34.39, -42.80, -39.18)	(6.29, 7.08, 7.64)

Nuclear Structure Corrections

Mikhail Gorchtein: „A hitchhiker's guide to nuclear polarization in muonic atoms“

[M. Gorchtein, arXiv:2501.15274v1]

$$\Delta E_{1S}^{NP,corr} = \Delta E_{1S}^{NP} F_R(\epsilon_1) K^{(1)}(\sqrt{\epsilon_2})$$

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leading nuclear polarization shift of nS level

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leading nuclear polarization shift of nS level

Coulomb distortion

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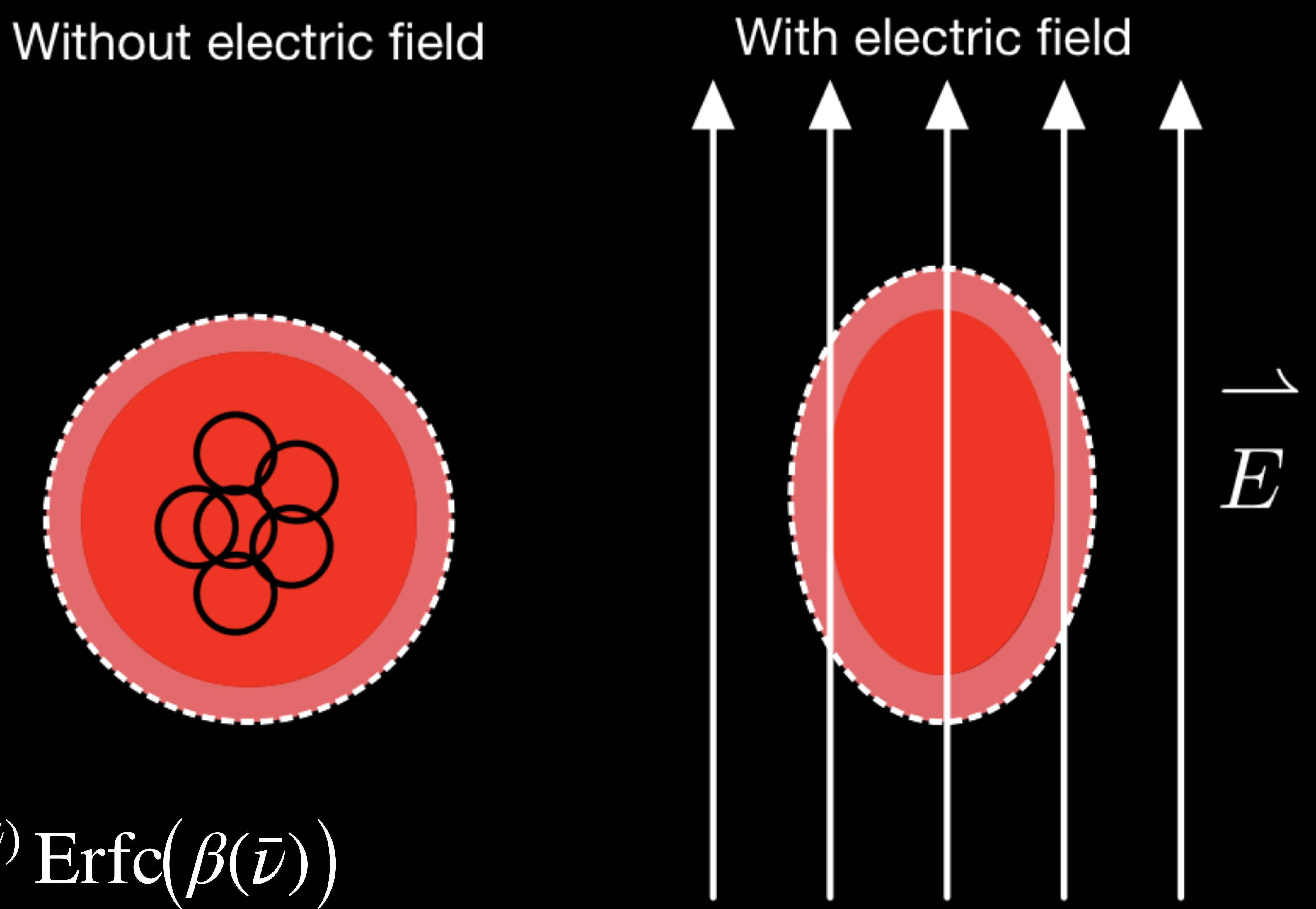
Polarization $\mathbf{P} = \alpha_D \mathbf{E}$



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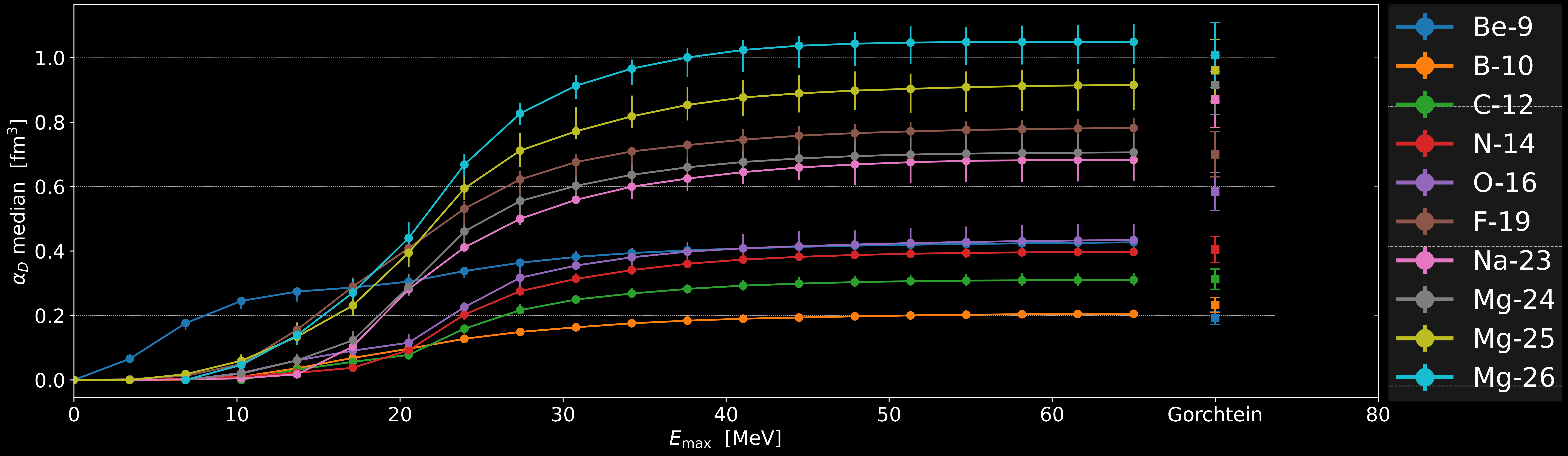

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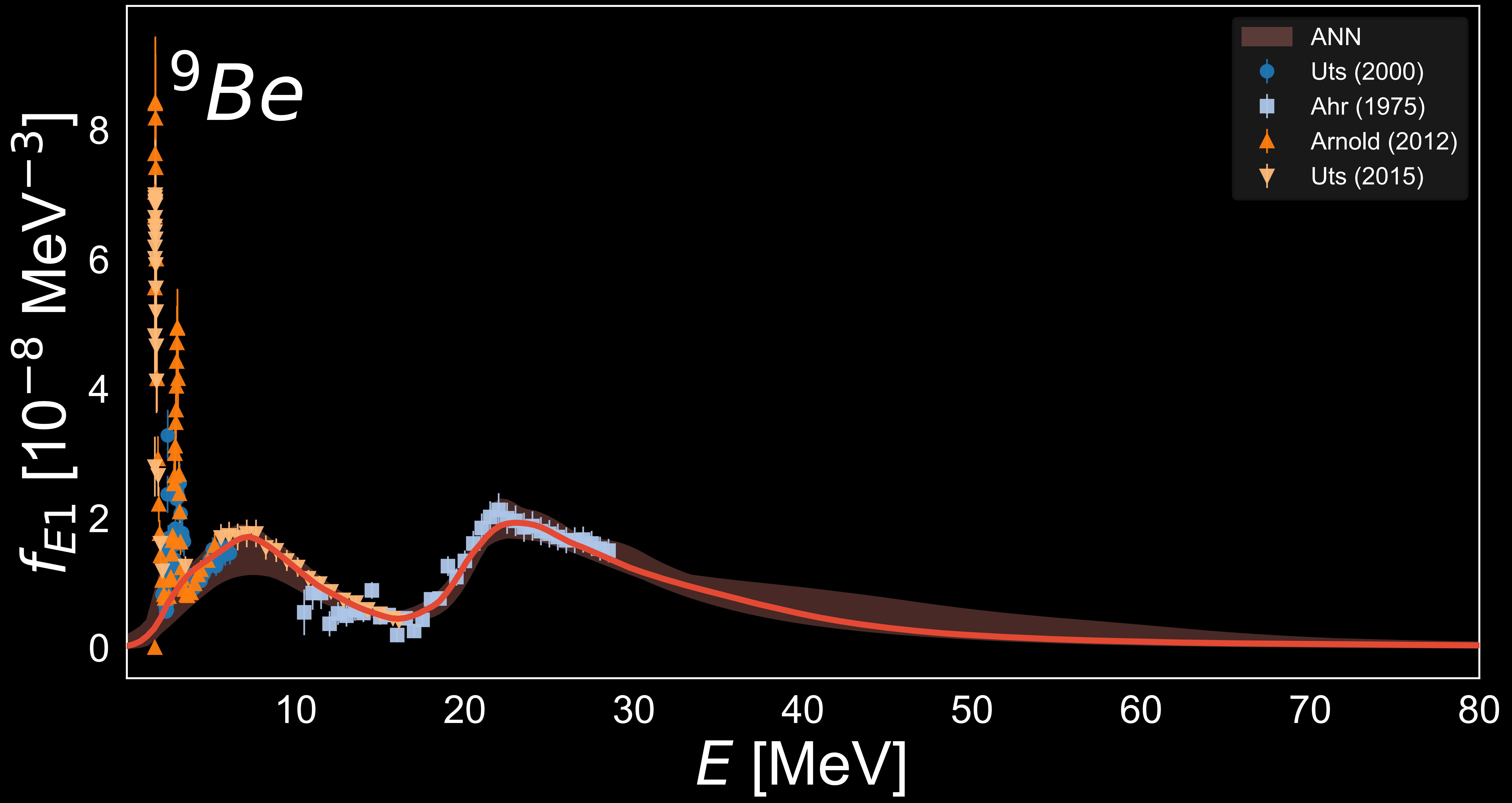
Nuclear Structure Corrections

Comparison ANN and Ahrens



Nuclear Structure Corrections

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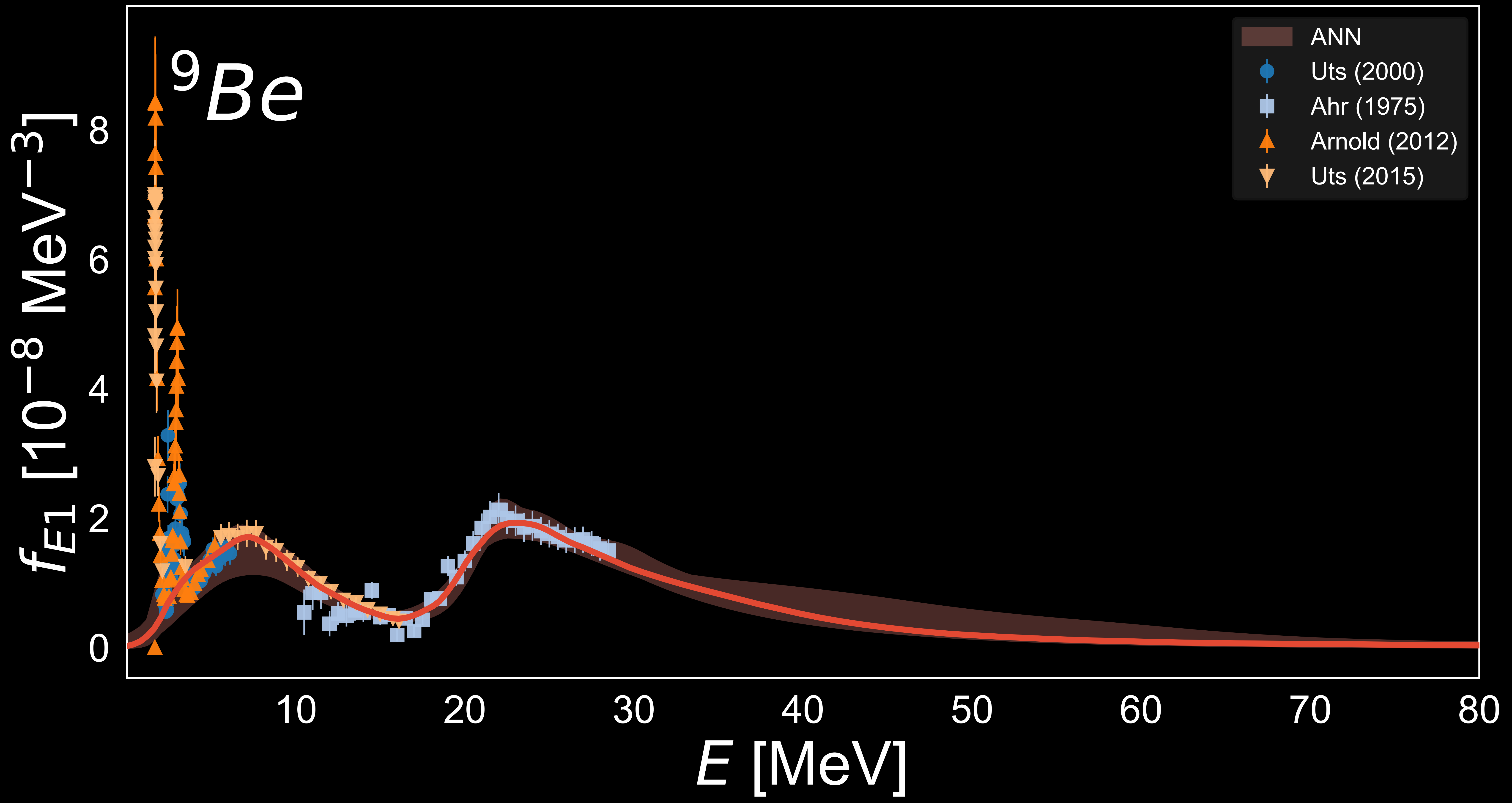

$\alpha_D(\text{Ahrens}) = 0.192\ \text{fm}^3$

Nuclear Structure Corrections

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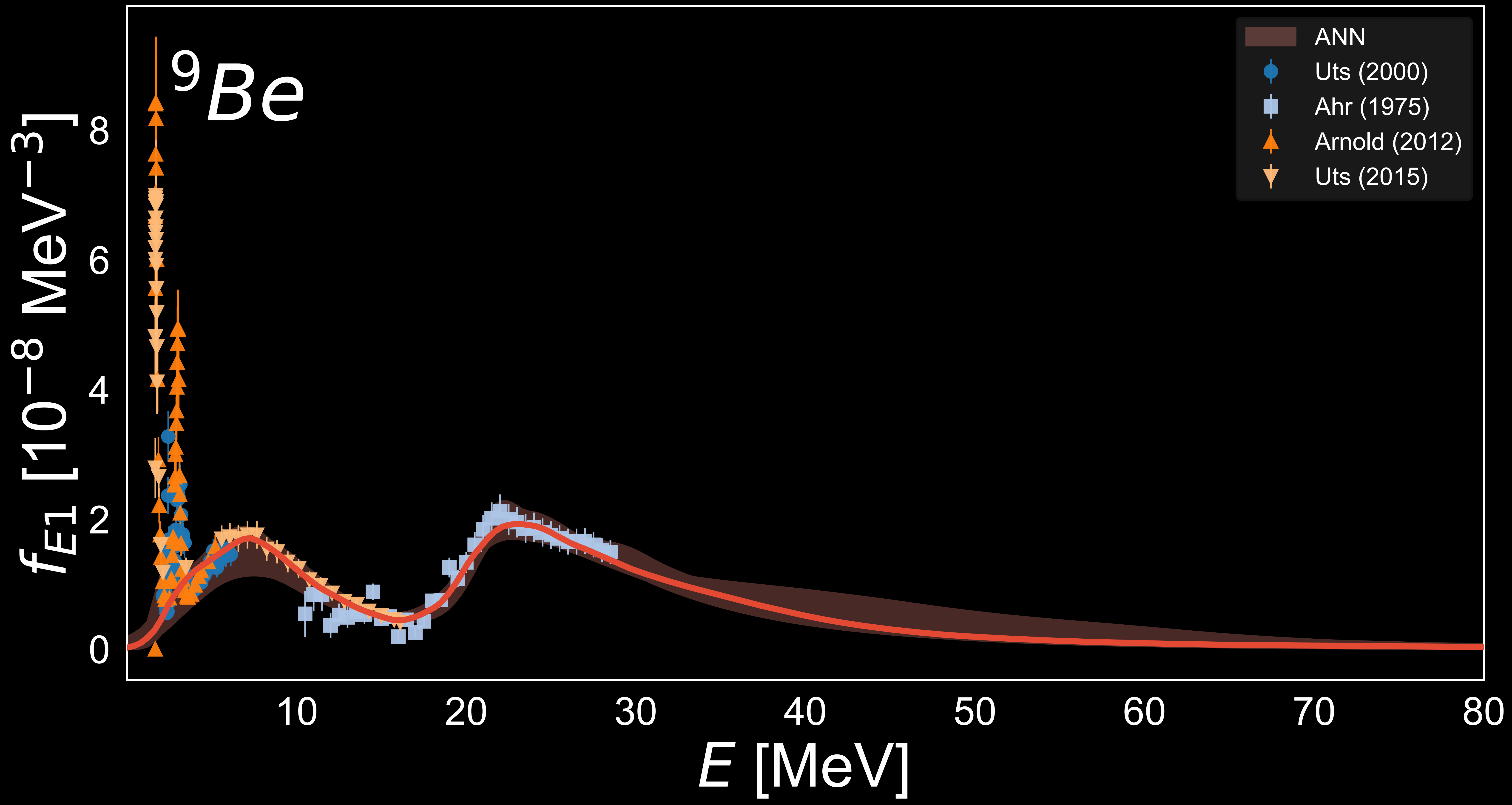

$\alpha_D(\text{Ahrens}) = 0.192\ \text{fm}^3$

$\alpha_D(\text{ANN}) = 0.415^{+0.07}_{-0.017}\ \text{fm}^3$

Summary

- An ANN can predict dipole strength function/cross sections
- Can be optimized for light nuclei with more physics information
- Predictions can be used to calculate nuclear structure corrections in muonic atoms while also providing uncertainty bands based on statistics

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- Where to go from here?

Thank you!

Collaborators:

Weiguang Jiang

Sonia Bacca

Francesca Bonaiti

Peter von Neumann Cosel

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