POTENTIAL ENERGY SURFACES WITH ACTIVE LEARNING

NPAC COMPUTER PROJECT

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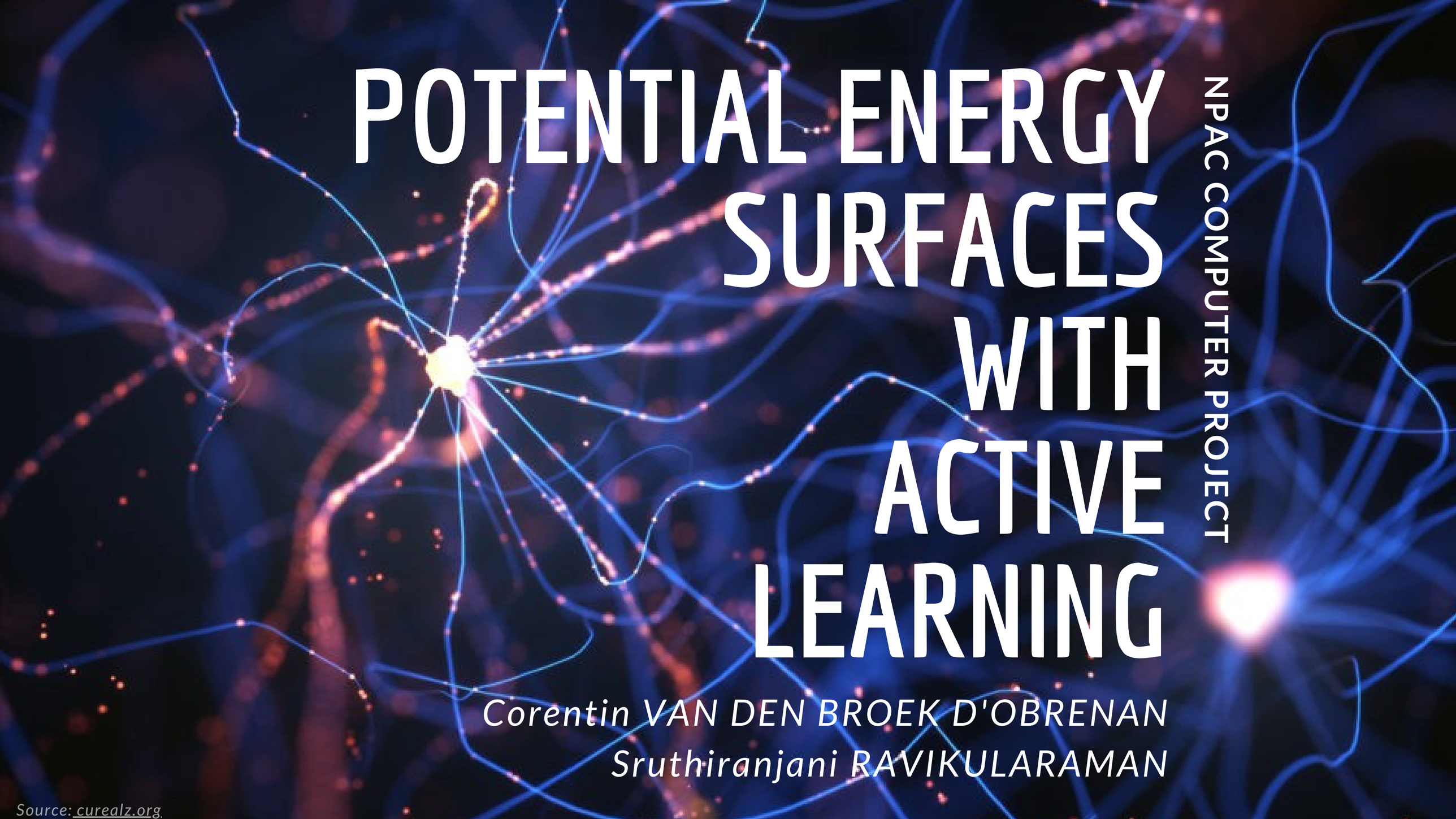
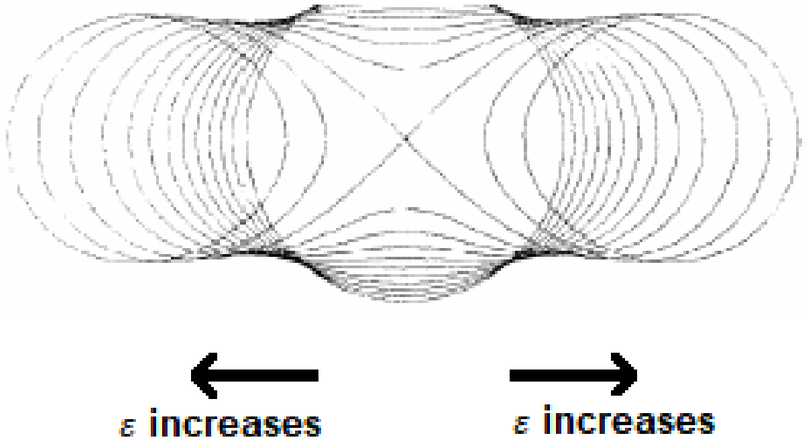


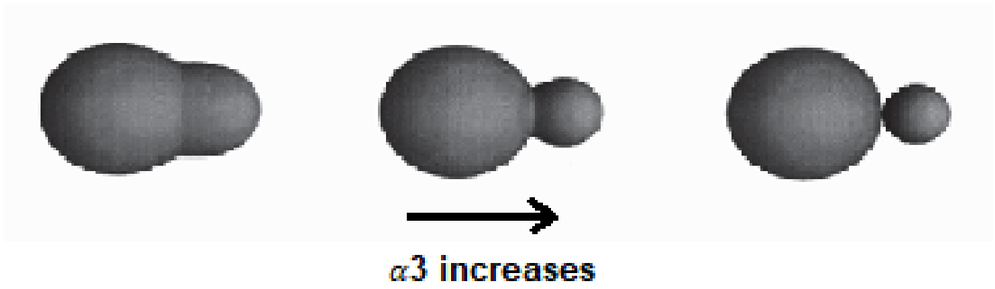
Source: curealz.org

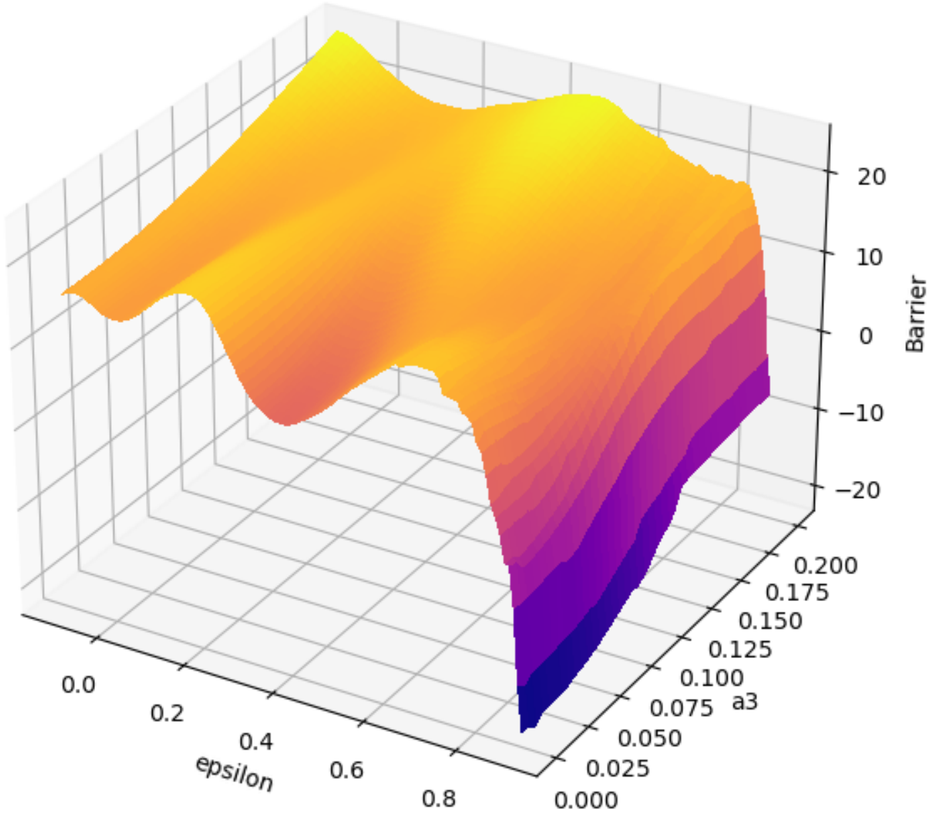
POTENTIAL ENERGY SURFACES

Fission barrier : activation energy required for a nucleus to undergo fission

2D PES: Nucleus energy as a function of elongation ε and left/right asymmetry $\alpha 3$



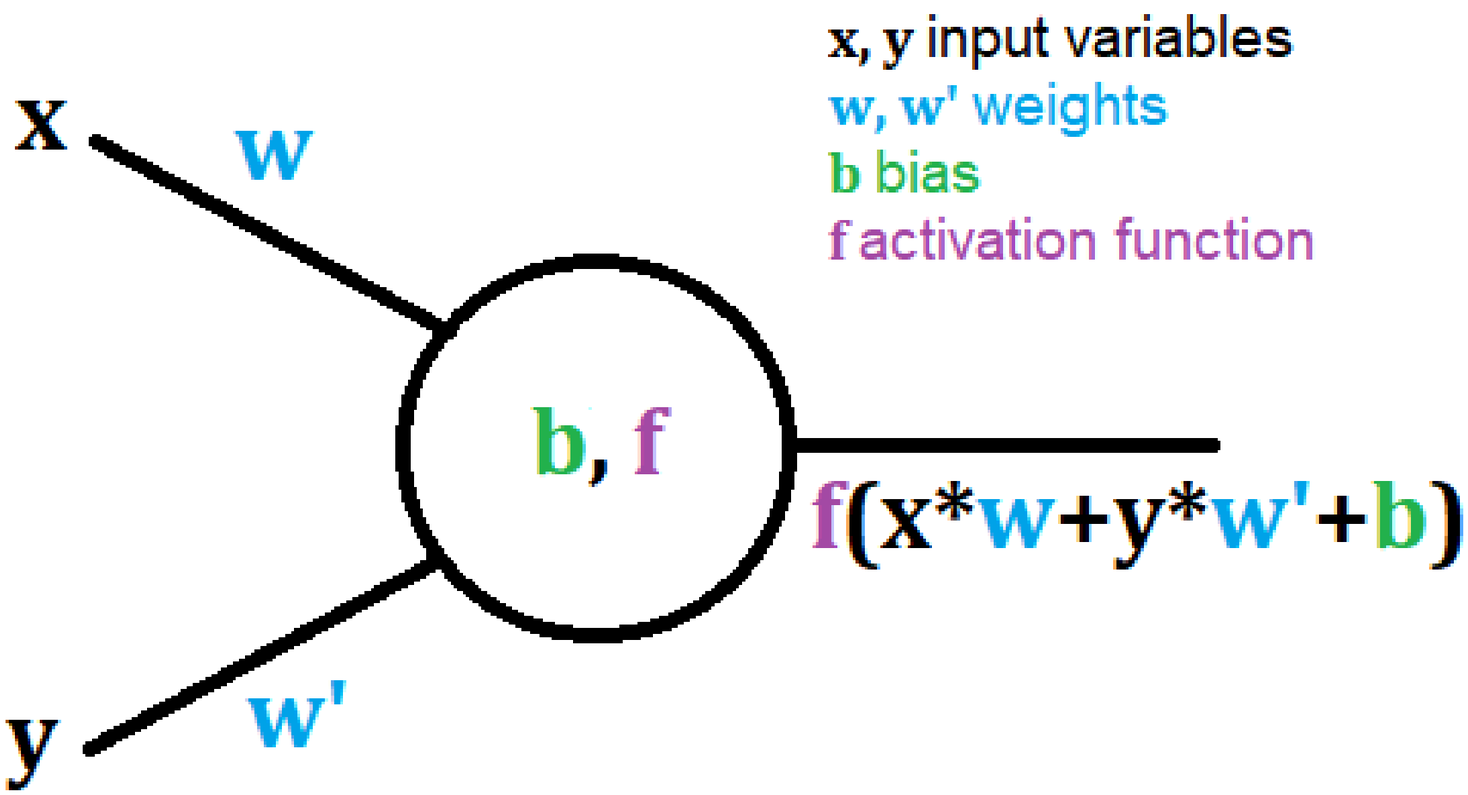




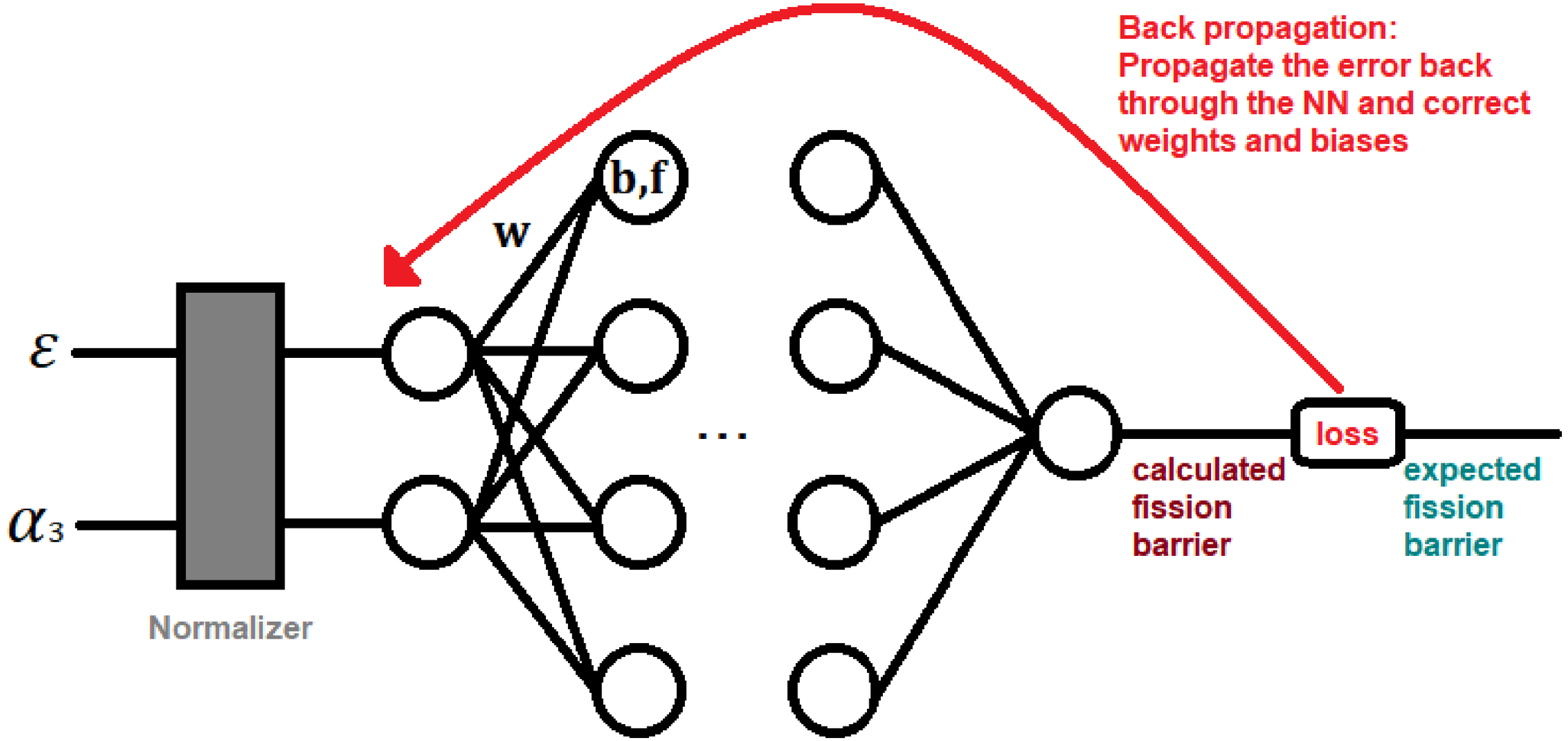
ε increase -> fission barrier falls

$\alpha 3$ tends to 0 -> fission barrier falls

REGRESSION WITH A NEURAL NETWORK - A NEURON



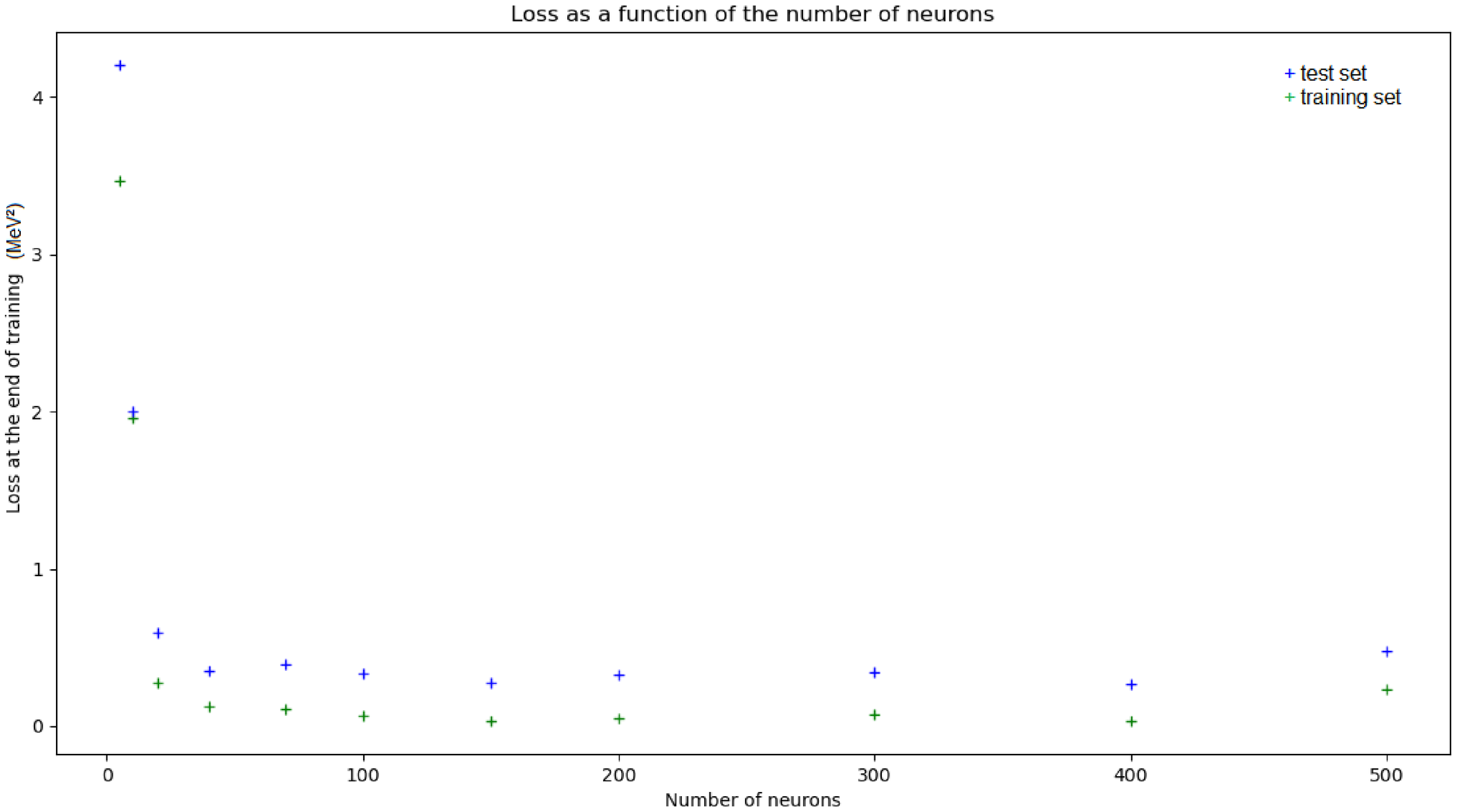
REGRESSION WITH A NEURAL NETWORK - NEURAL NETWORK



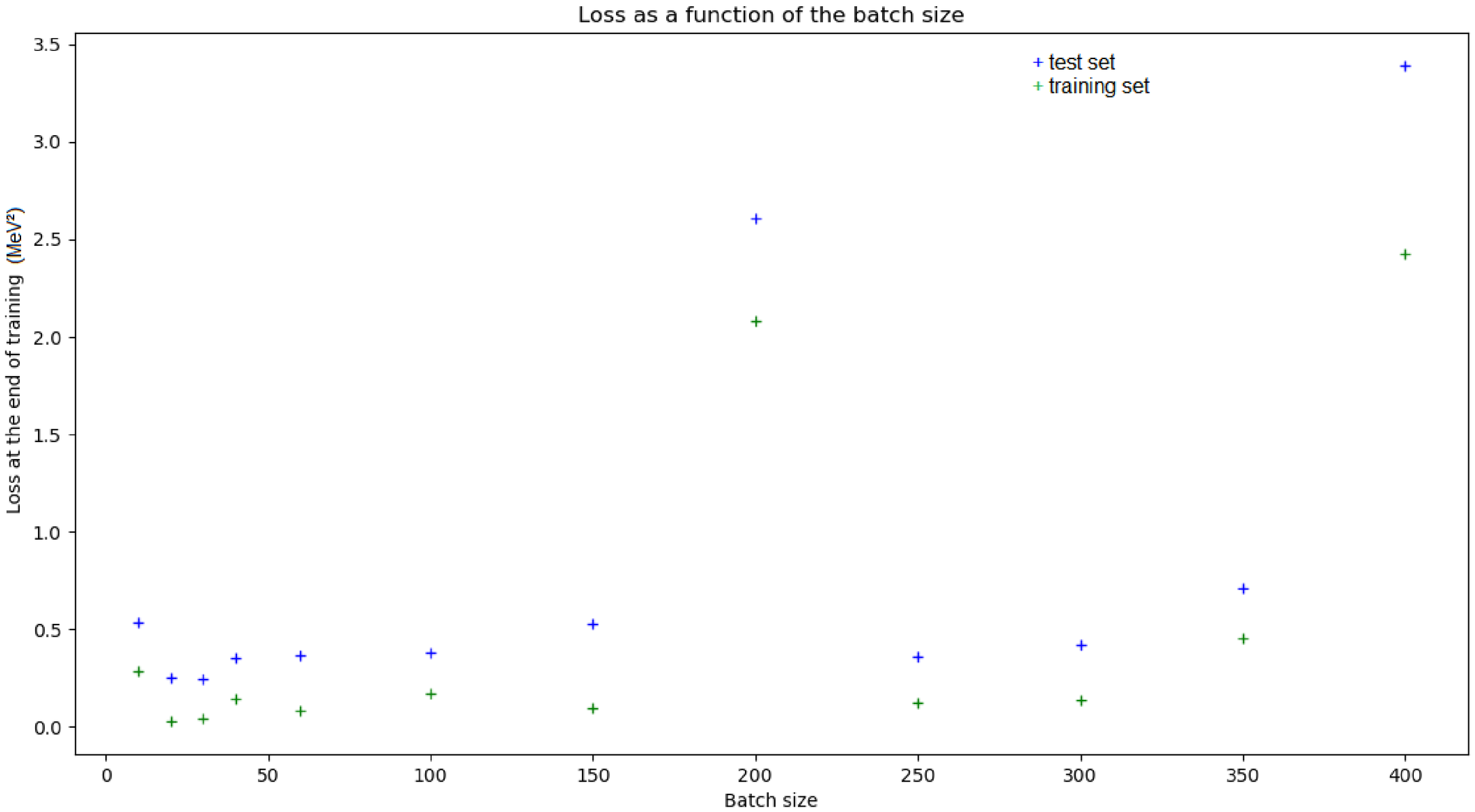
OPTIMIZATION OF HYPERPARAMETERS

1. **The number of hidden layers**
2. **The number of neurons per layer**
3. **The batch size**
4. **The number of epochs**
5. **The activation function**
6. **The loss optimizer**
7. **The loss function**

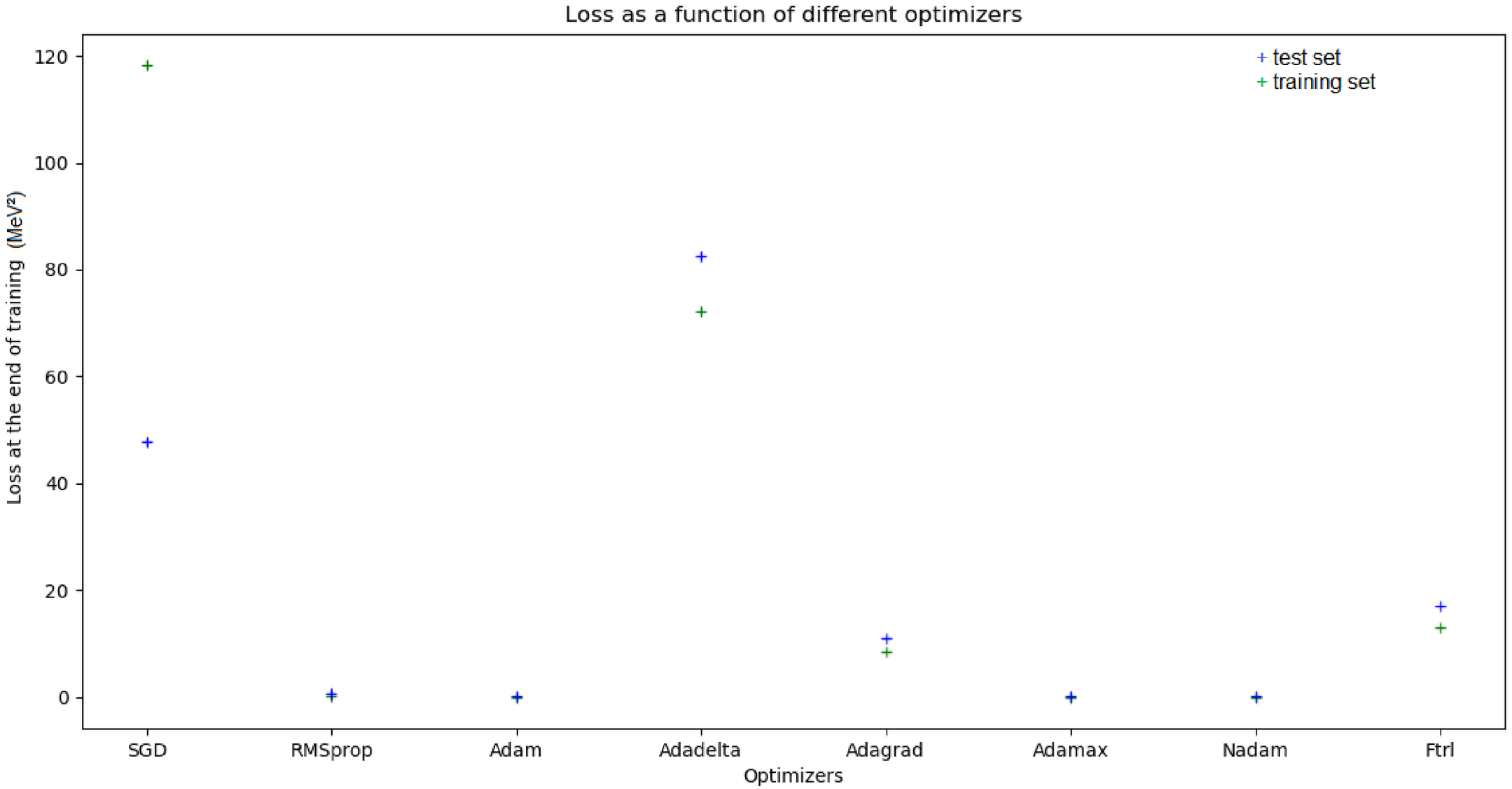
OPTIMIZATION OF HYPERPARAMETERS - NUMBER OF NEURONS



OPTIMIZATION OF HYPERPARAMETERS - BATCH SIZE



OPTIMIZATION OF HYPERPARAMETERS - OPTIMIZER

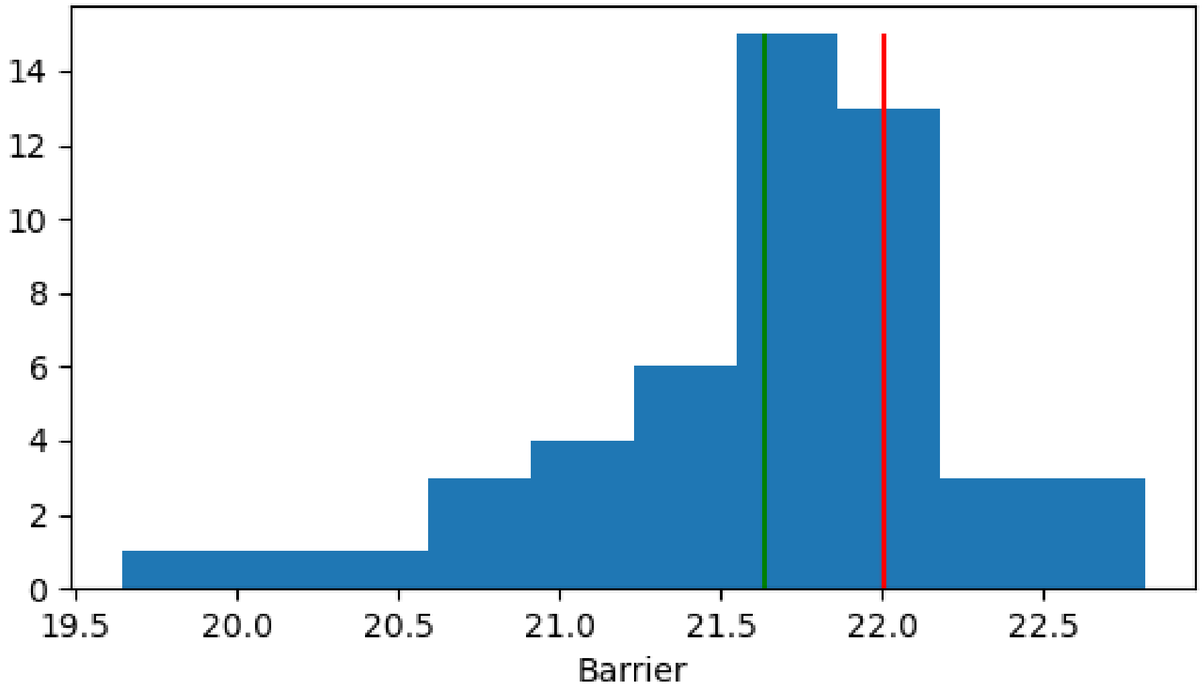


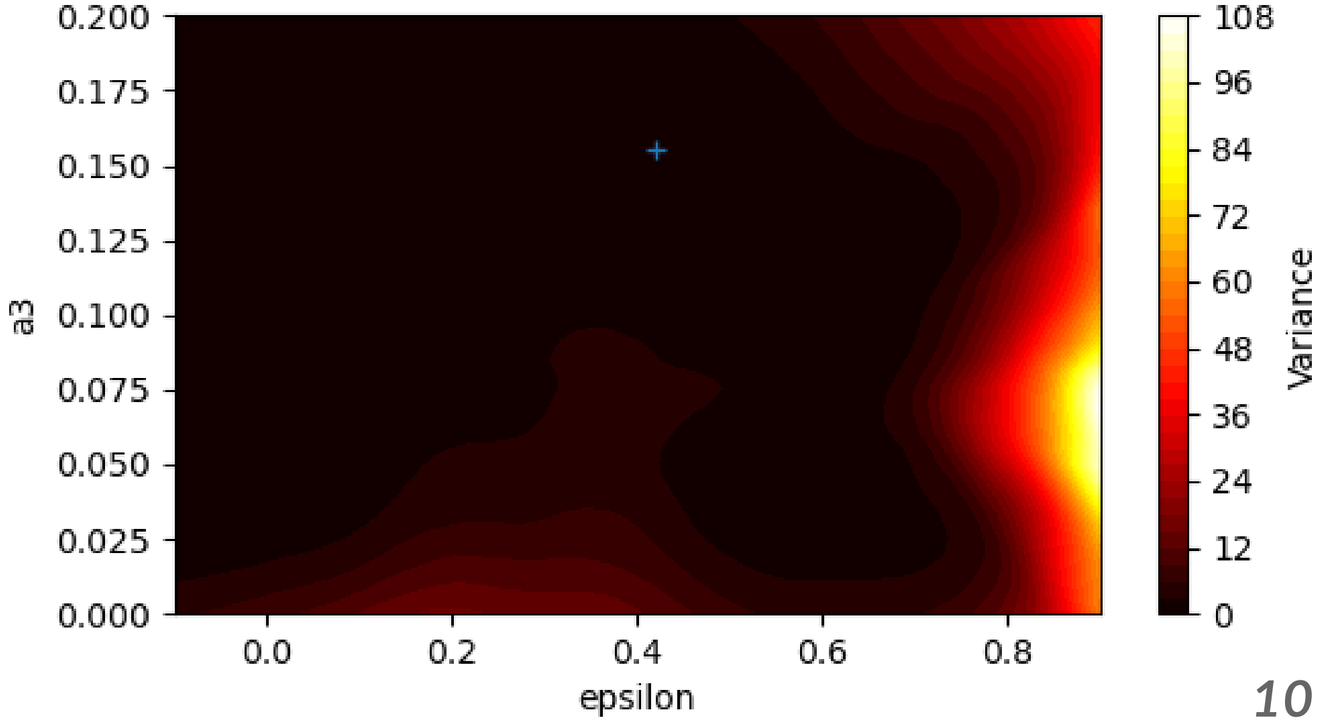
OPTIMIZATION OF HYPERPARAMETERS

1. **The number of hidden layers**	***3 - 6***	
2. **The number of neurons per layer**	***150***	
3. **The batch size**	***10 - 60***	***< len(train_set)***
4. **The number of epochs**	***2000***	
5. **The activation function**	***'relu'***	
6. **The loss optimizer**	***'Adamax'***	
7. **The loss function**	***'mean_squared_error'***	

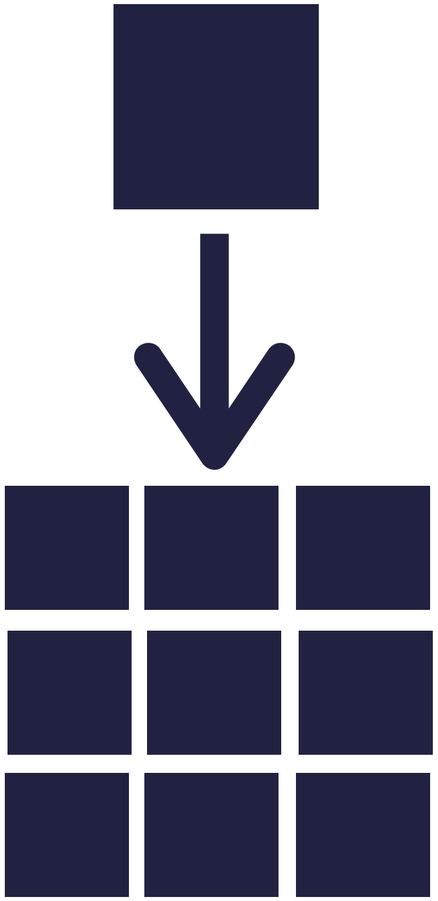
COMMITTEE - IDEA

A single neural network is initialized randomly and can converge to different minima of the loss function. These fluctuations can be removed when using a committee of models.
It also add a useful indicator: the variance.

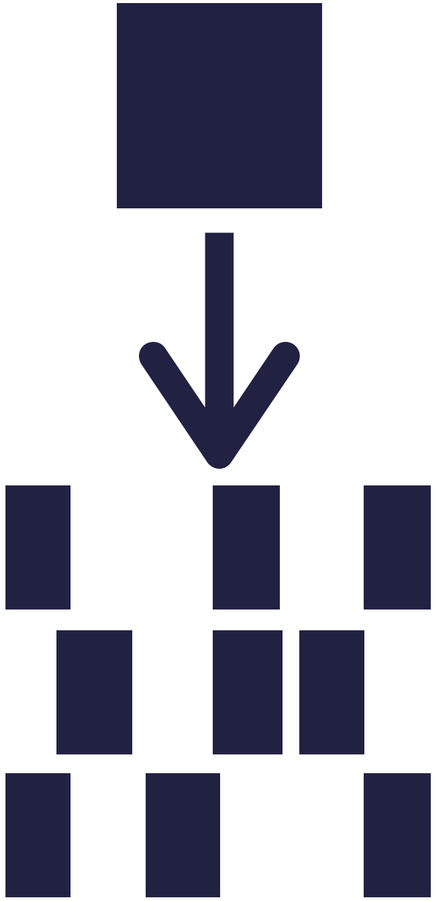




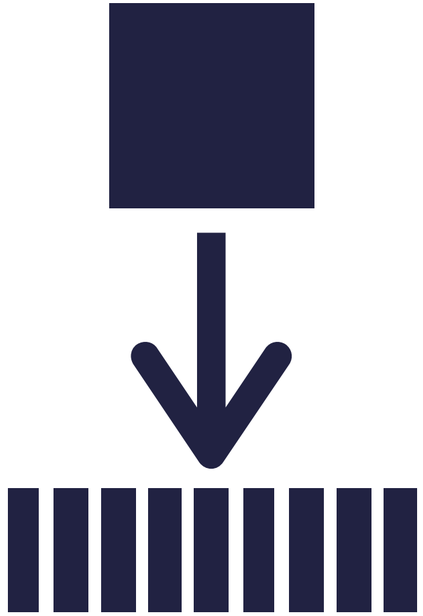
COMMITTEE - SHARING THE TRAINING SET



Sharing

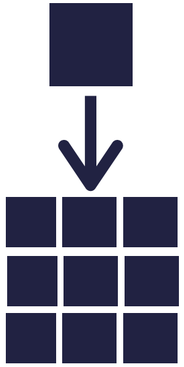


Bootstrapping



Splitting

COMMITTEE - SHARING THE TRAINING SET



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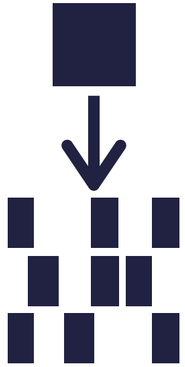
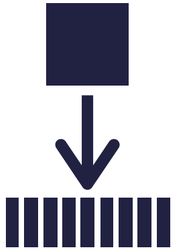


Bootstrapping



Splitting

More systematic errors ⟷ **Less systematic errors**

Need less data ⟷ **Need more data**

ACTIVE LEARNING - IDEA

Generating a PES without simulating a PES

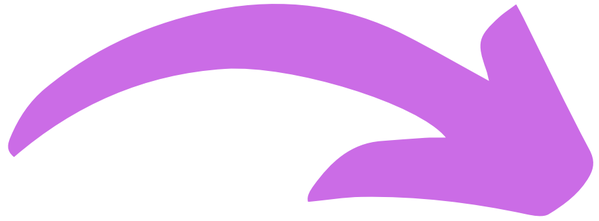
The Committee of models gets a an initial set of training points, fits and uses the variance to tell where to add more training data.

Goal : maximize the reconstruction accuracy

minimize the size of the training set.

ACTIVE LEARNING - ALGORITHM

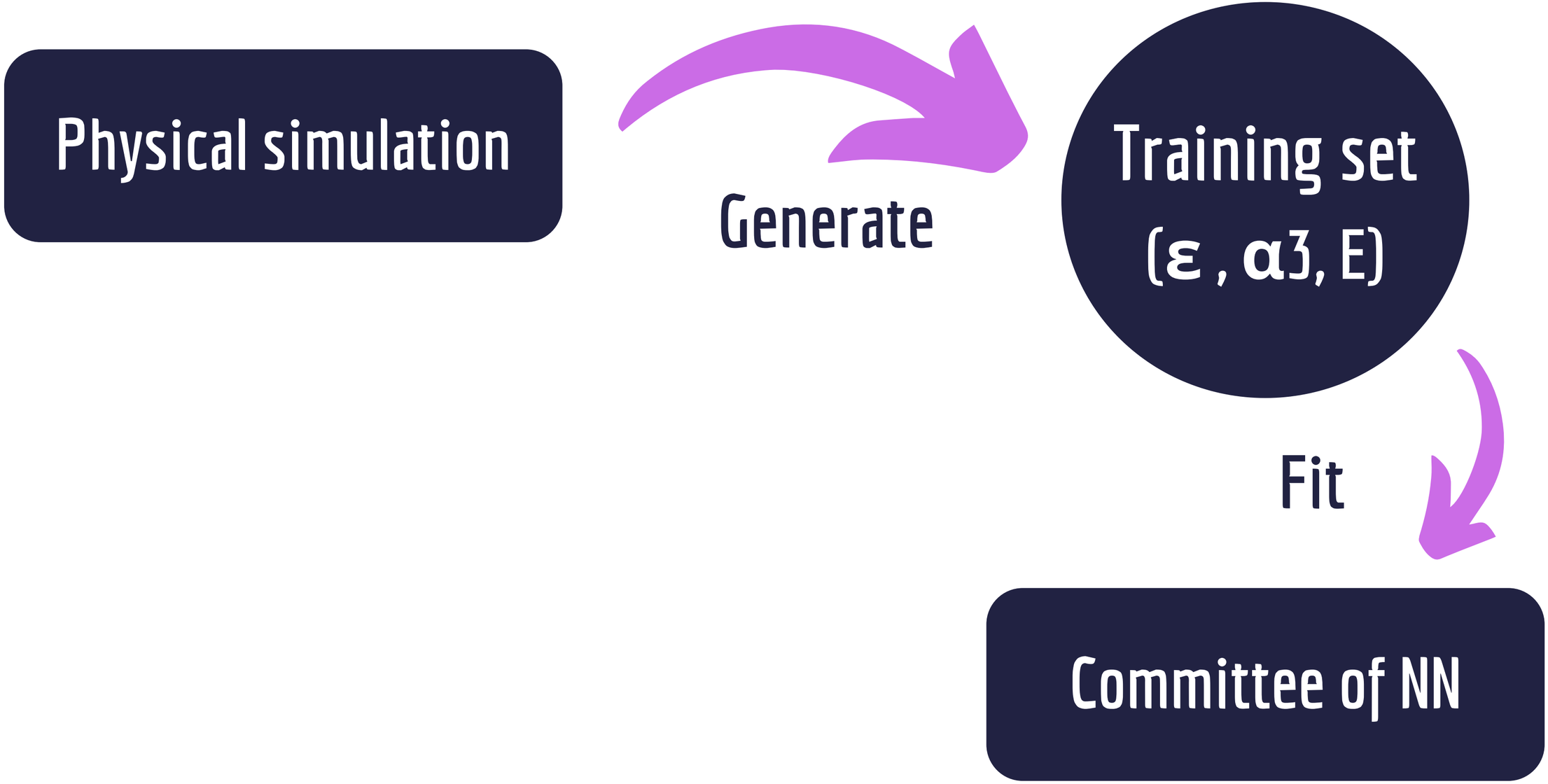
Physical simulation



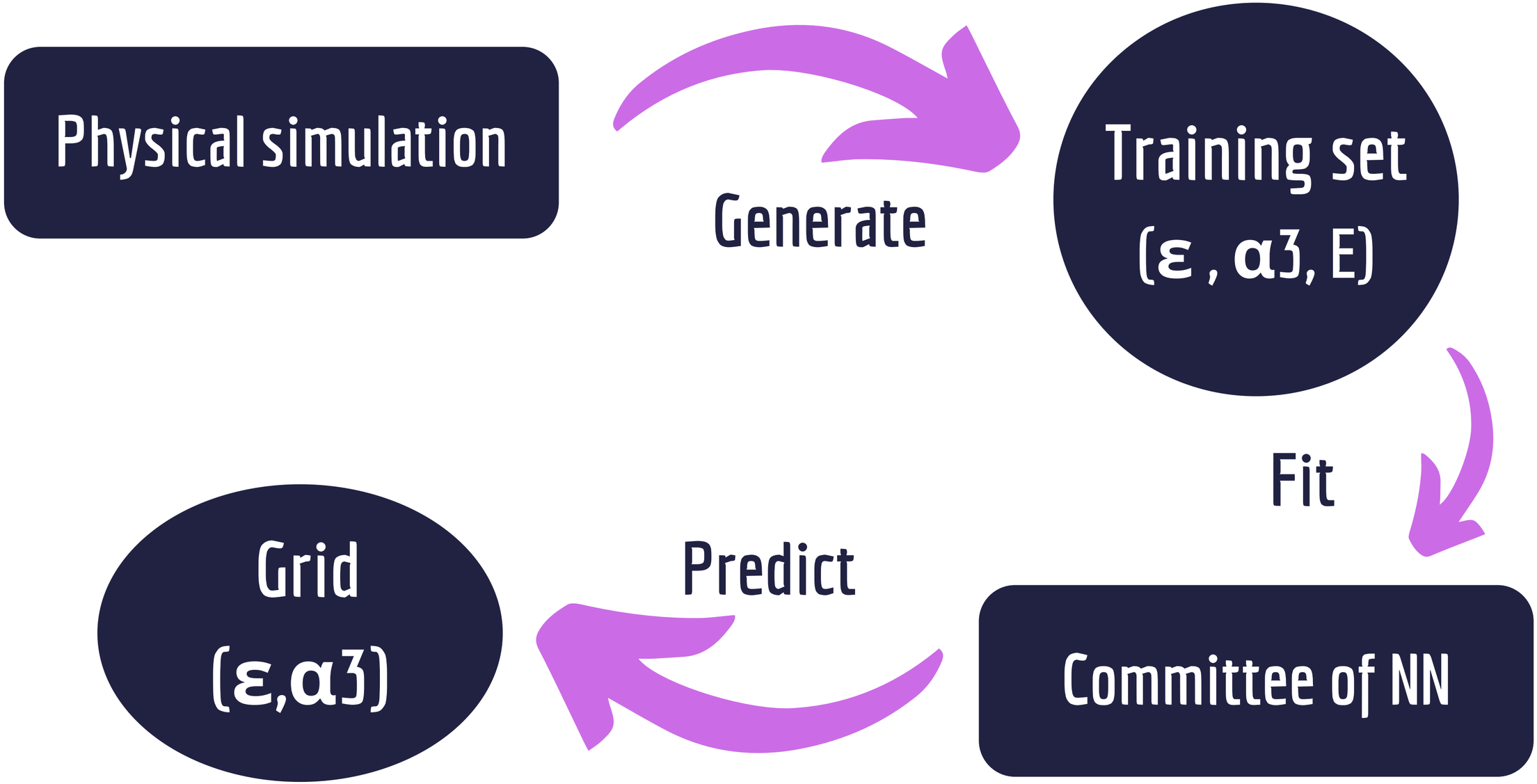
Generate

Training set
(ε , α3, E)

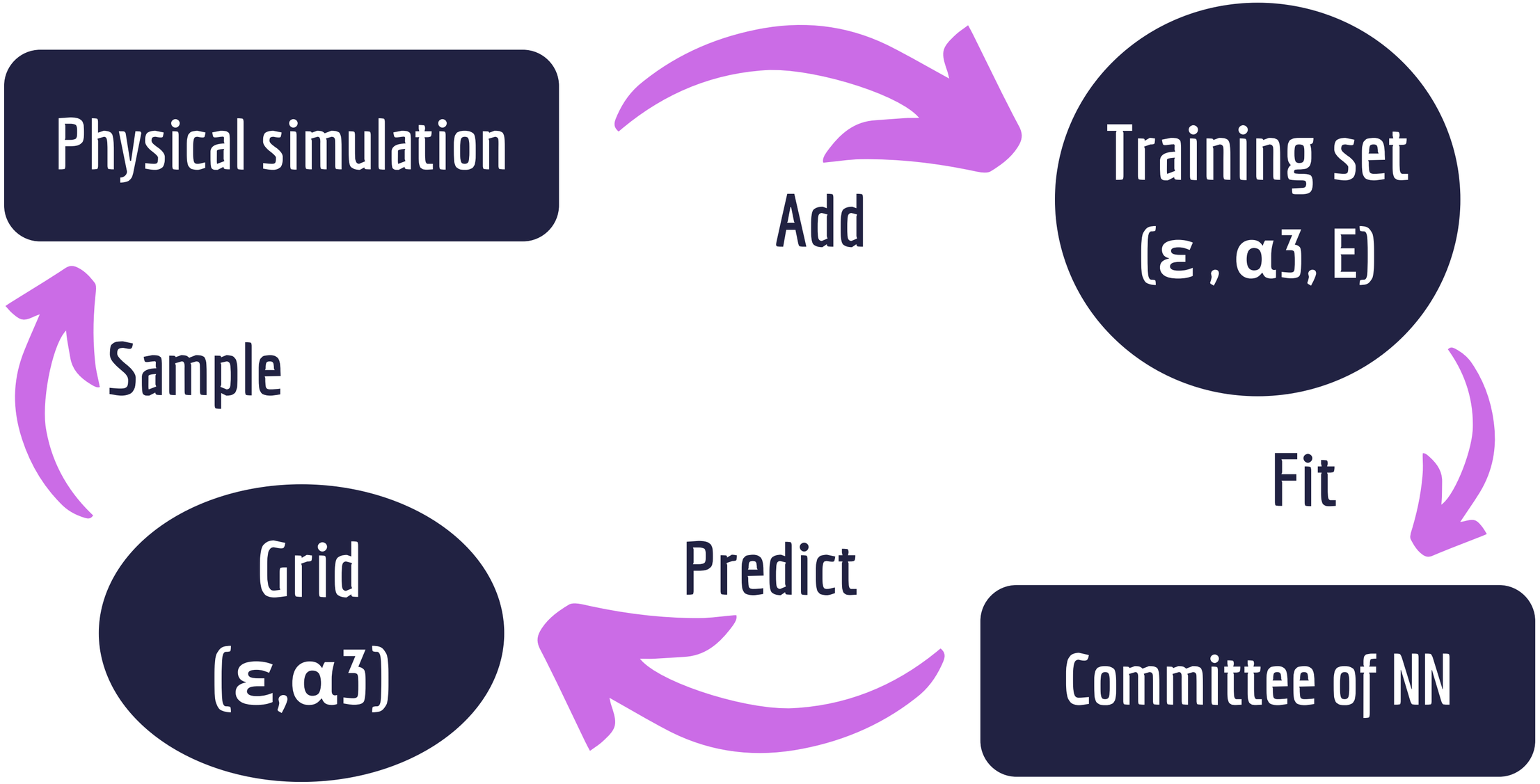
ACTIVE LEARNING - ALGORITHM



ACTIVE LEARNING - ALGORITHM



ACTIVE LEARNING - ALGORITHM



ACTIVE LEARNING - RESULTS

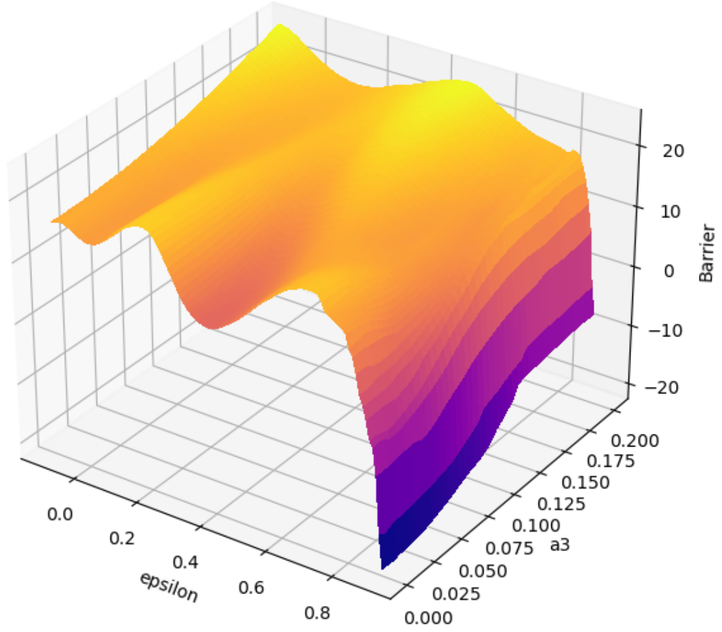
Starting with 3% of the dataset

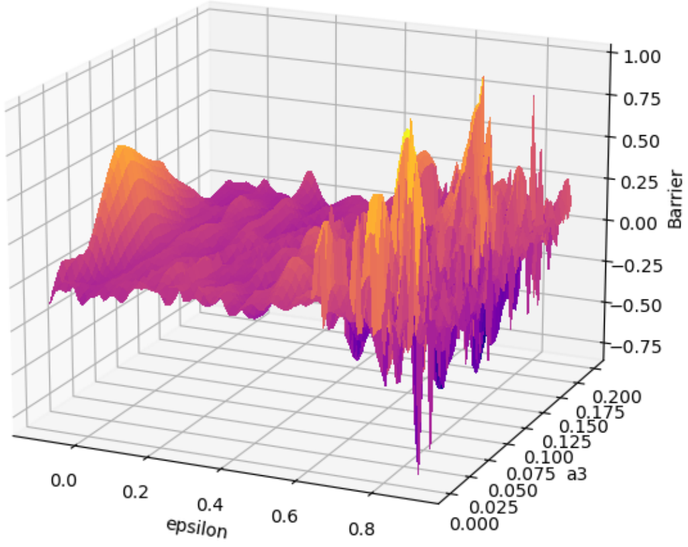
RUN 1: **final rmse = 302 keV**
10% of the dataset

RUN 2: **final rmse = 442 keV**
9.9% of the dataset

RUN 3: **final rmse = 154 keV**
25% of the dataset

Predicted PES
(Barrier in MeV)





Difference
between
predicted and
simulated PES
(Barrier in MeV)

ACTIVE LEARNING - FINAL THOUGHTS

No optimal hyperparameters for the active learning yet :

- Number of epochs per loop

- Number of models

- Sample size of the train dataset for each model

- Size of the initial train dataset

And most likely many other optimizations could be made

THANK
YOU