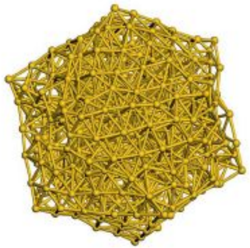
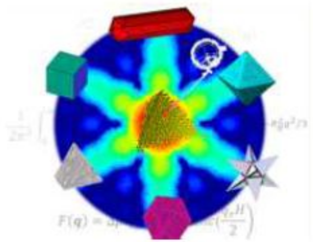
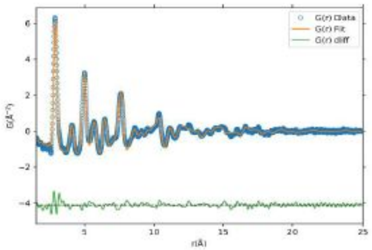
Machine learning-assisted structural characterization of nanoparticles using X Ray scattering







By:

Pierre Boissier

Maïmouna Gadji

OUTLINE

I.CONTEXT

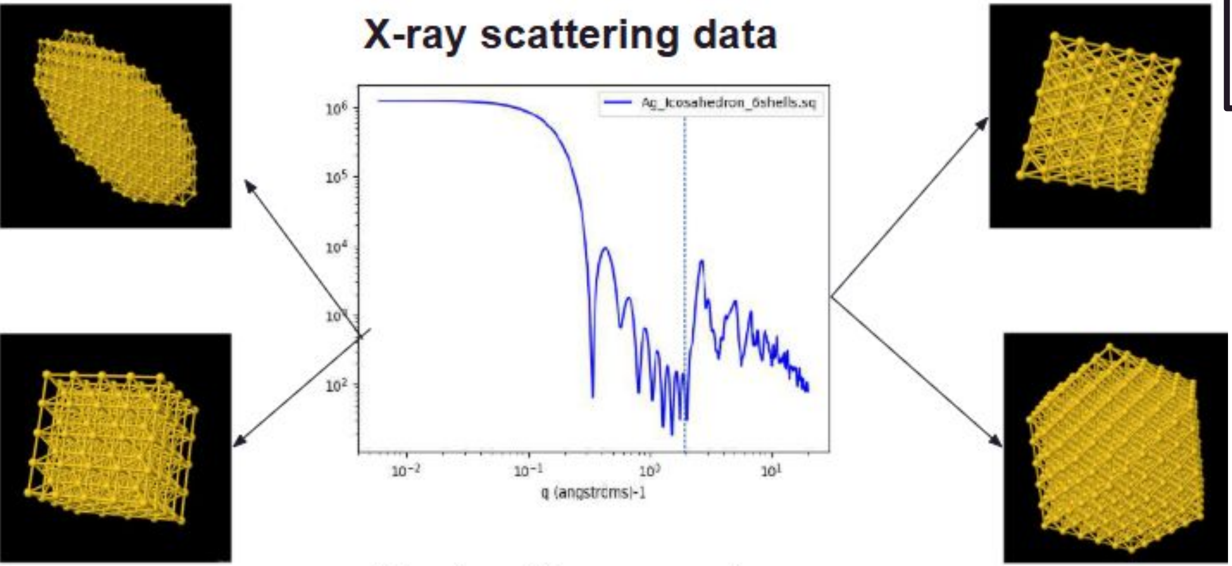
BiMAn Project:

- **Objective**: Develop efficient magnetic materials without rare-earth elements.

Various applications in **energy transition** like renewable energy system or data storage.

II. AIM OF THE PROJECT

Prediction of nanoparticle shape and size from X-ray scattering data



$$q = \frac{4\pi}{\lambda}\sin(\theta)$$

scattering angle

X-axis: q (Anstrome -1)
Y-axis: Intensities

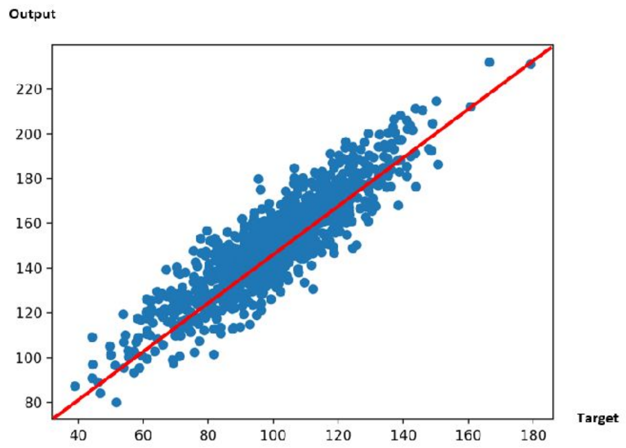
SWAXS METHOD

III.Size and Shape prediction

How?

- Size
  - n_atoms
  - Eq_radius
  - Size_parameter
- Shape
  - shape

III.1 Linear regression methods



Ridge Regression

$$J(\beta) = \|y - X\beta\|_2^2 + \alpha\|\beta\|_2^2$$

Logistic Regression

$$p_k = \frac{\exp(\beta_k^T x)}{\sum_{j=1}^{9} \exp(\beta_j^T x)}$$

$$\mathcal{L}(\beta) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{k=1}^{9} y_{i,k}\log(p_{i,k})$$

Idea of linear regression :

Find a linear relation between inputs and outputs

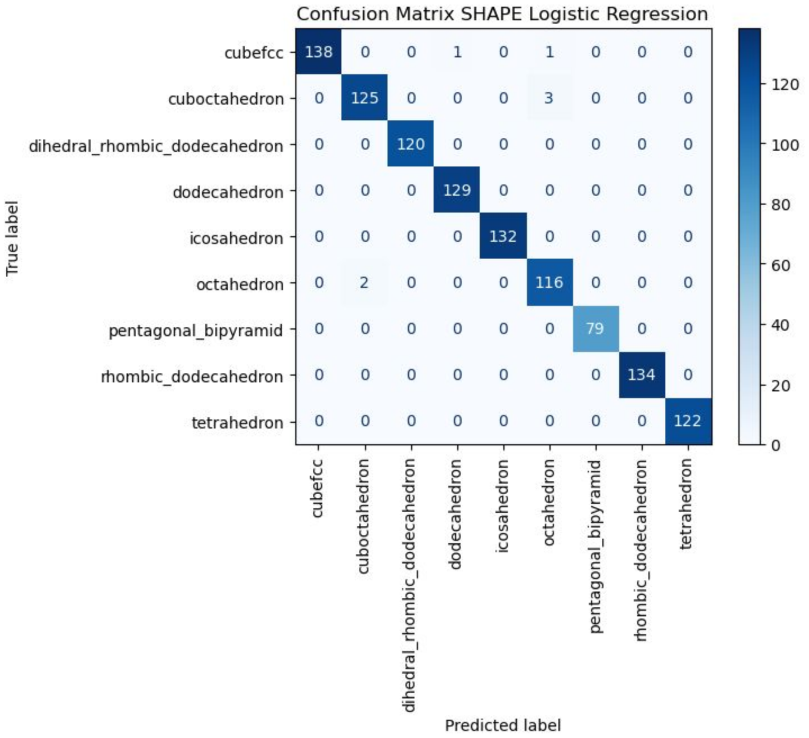
RESULTS: Linear reg

Size prediction = 3 quantitatives features to predict → Ridge Regression

Features	MSE	Variance of test data	Q2
log_n_Atoms	0.00015	3.196	0.999
Size_parameter_1	0.846	7.106	0.881
sqrt_log_eq_radius	0.310	0.695	0.554

RESULTS: Linear reg

Shape prediction = 1 qualitative features to predict → Logistic Regression



Accuracy = 99.4 %

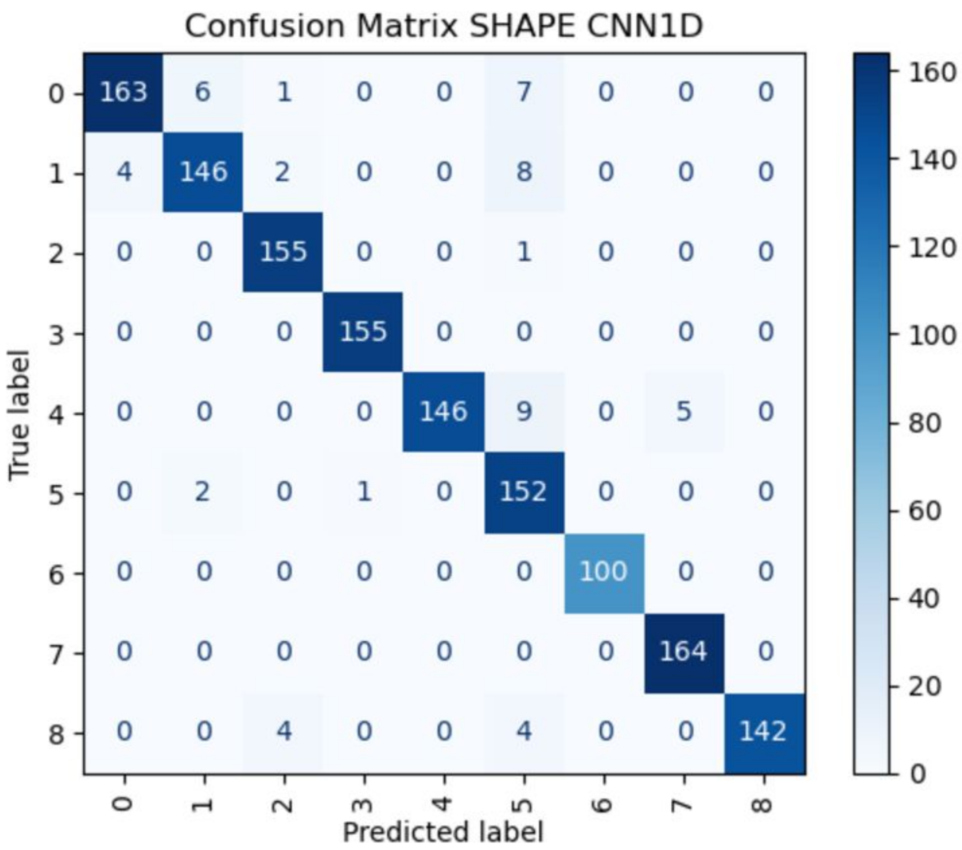
III.2 Convolutional neural network 1D (CNN 1D)

Layer (type)	Output Shape	Param #
conv1d_8 (Conv1D)	(None, 1997, 32)	128
max_pooling1d_8 (MaxPooling1D)	(None, 998, 32)	0
conv1d_9 (Conv1D)	(None, 996, 64)	6,208
max_pooling1d_9 (MaxPooling1D)	(None, 498, 64)	0
flatten_4 (Flatten)	(None, 31872)	0
dense_4 (Dense)	(None, 9)	286,857

Idea:

Searching for meaningful patterns in intensity curve and make the shape or size prédiction from them

RESULTS: CNN1D



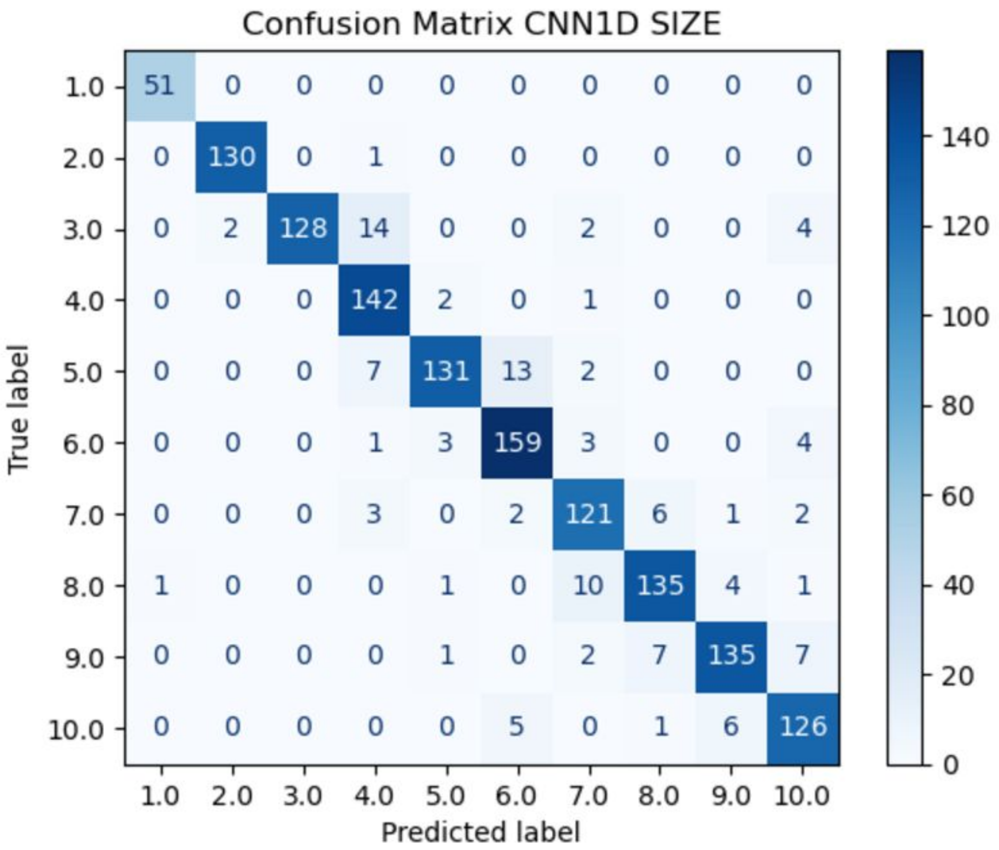
0	163	6	1	0	0	7	0	0	0
1	4	146	2	0	0	8	0	0	0
2	0	0	155	0	0	1	0	0	0
3	0	0	0	155	0	0	0	0	0
4	0	0	0	0	146	9	0	5	0
5	0	2	0	1	0	152	0	0	0
6	0	0	0	0	0	0	100	0	0
7	0	0	0	0	0	0	0	164	0
8	0	0	4	0	0	4	0	0	142
	0	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**

Accuracy=96%

Labels

cubefcc 0
cuboctahedron 1
dihedral_rhombic_dodecahedron 2
icosahedron 3
octahedron 4
dodecahedron 5
pentagonal_bipyramid 6
rhombic_dodecahedron 7
tetrahedron 8

RESULTS: CNN1D



	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
1.0	51	0	0	0	0	0	0	0	0	0
2.0	0	130	0	1	0	0	0	0	0	0
3.0	0	2	128	14	0	0	2	0	0	4
4.0	0	0	0	142	2	0	1	0	0	0
5.0	0	0	0	7	131	13	2	0	0	0
6.0	0	0	0	1	3	159	3	0	0	4
7.0	0	0	0	3	0	2	121	6	1	2
8.0	1	0	0	0	1	0	10	135	4	1
9.0	0	0	0	0	1	0	2	7	135	7
10.0	0	0	0	0	0	5	0	1	6	126

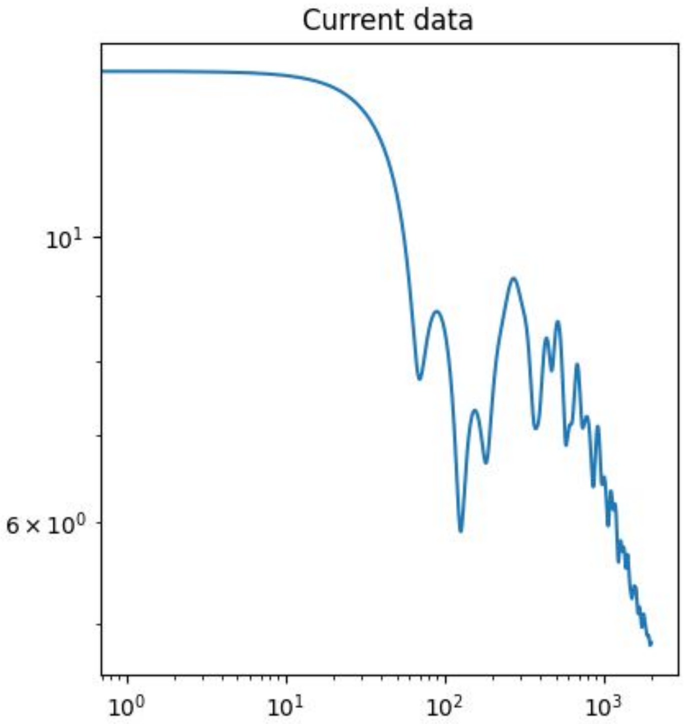
Accuracy=91%

IV. Testing the Robustness of Models

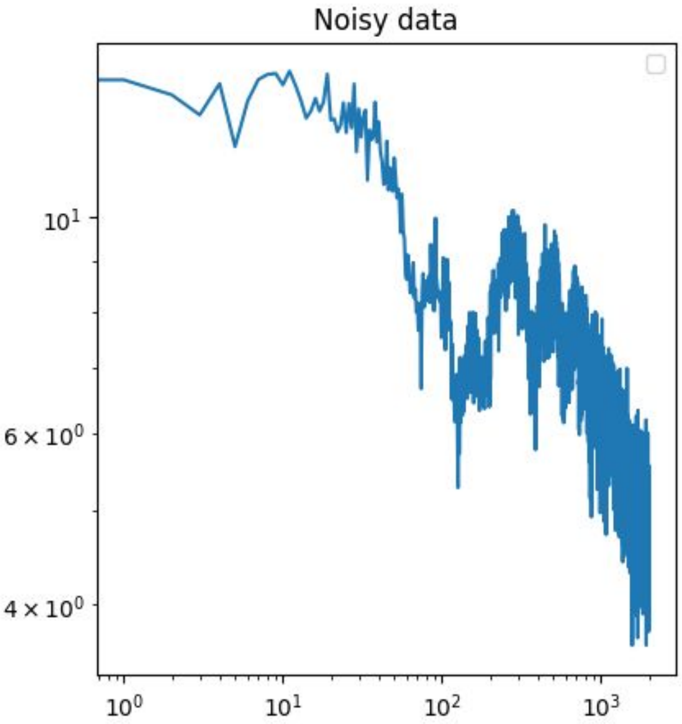
USING MORE REALISTIC DATA

Current data $\neq$ Realistic data.

I.V.1 Adding Noise

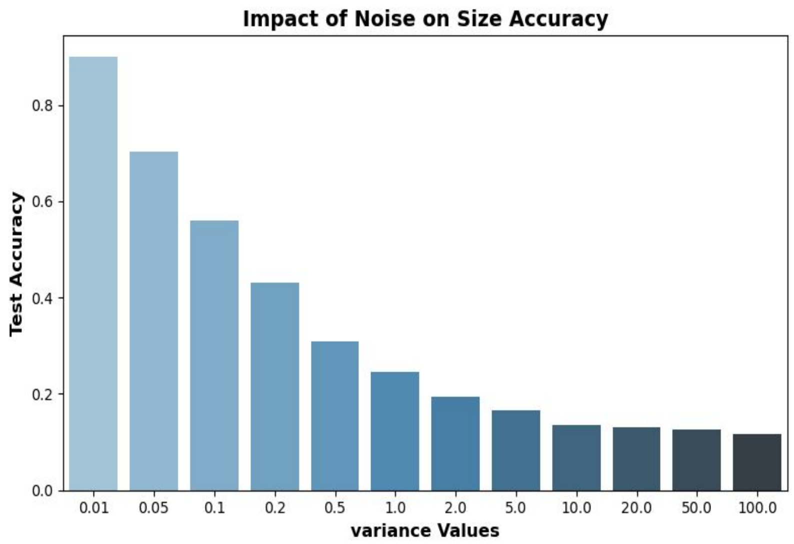


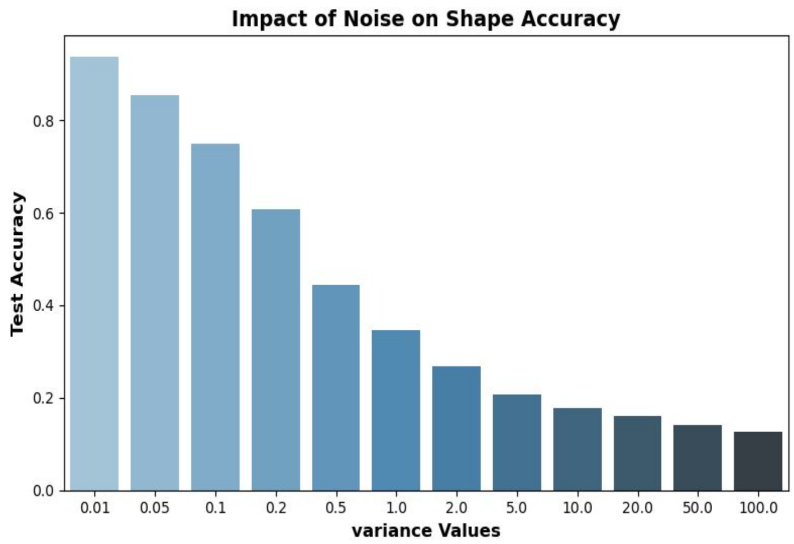
Gaussian noise



Impact of noise on prediction

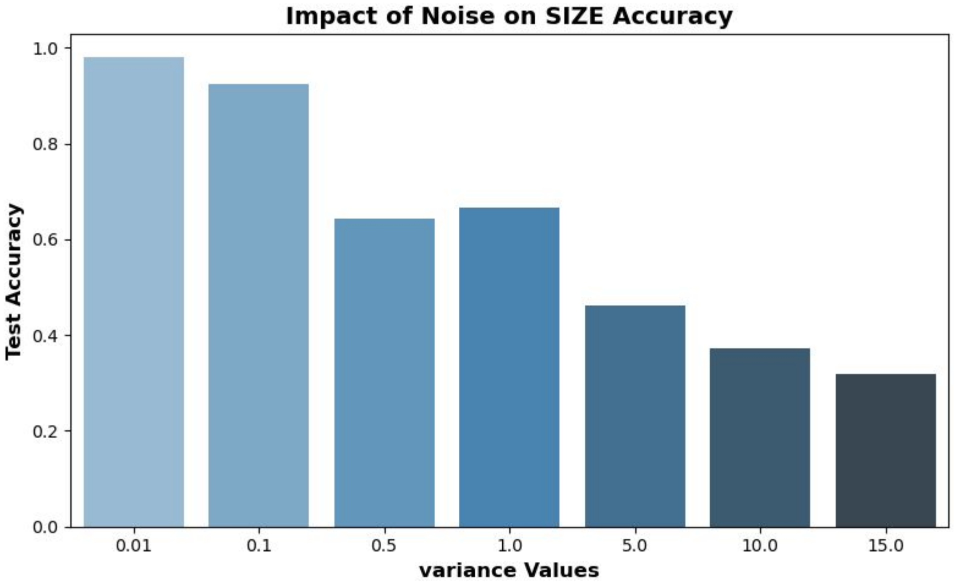
CNN1D model : Simple predictions on noisy data



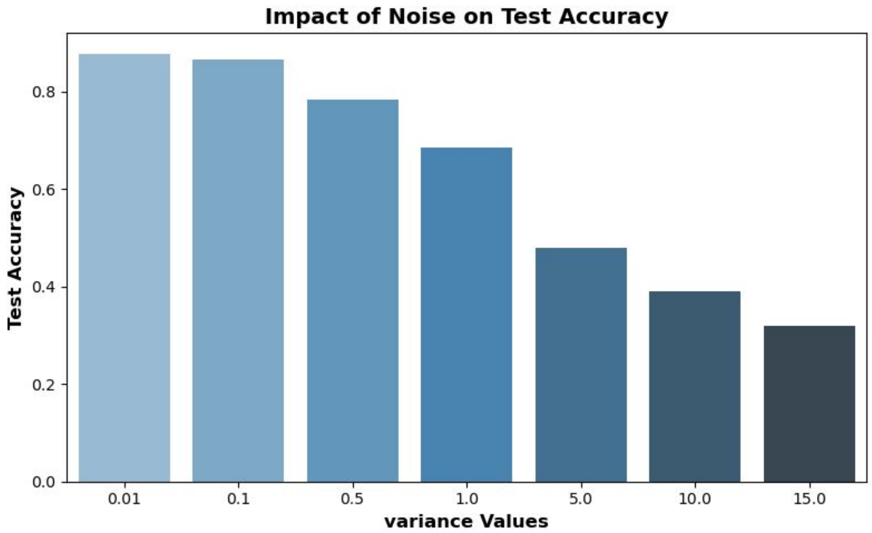


Impact of noise on prediction

CNN1D model : Training and prediction on noisy data



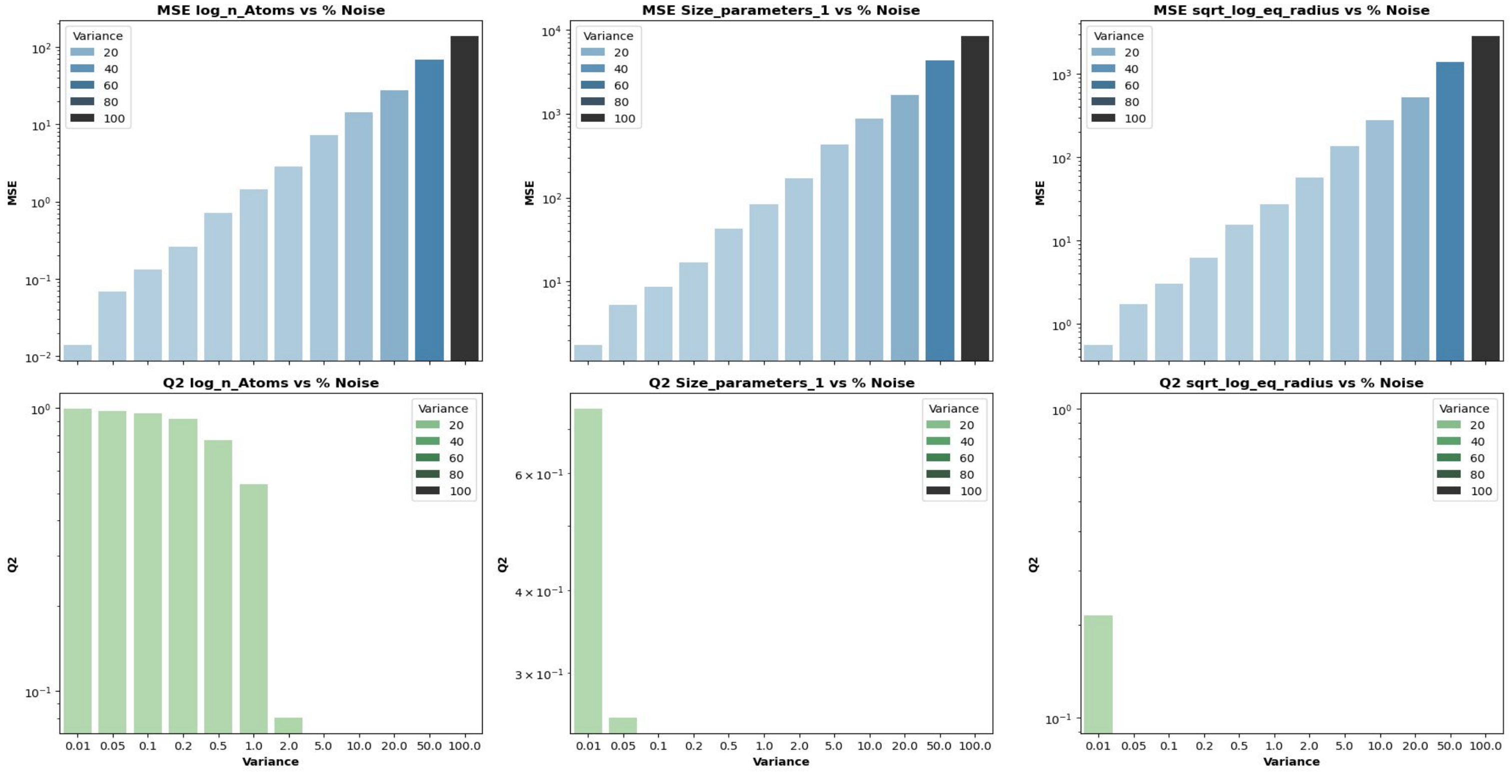
SIZE



SHAPE

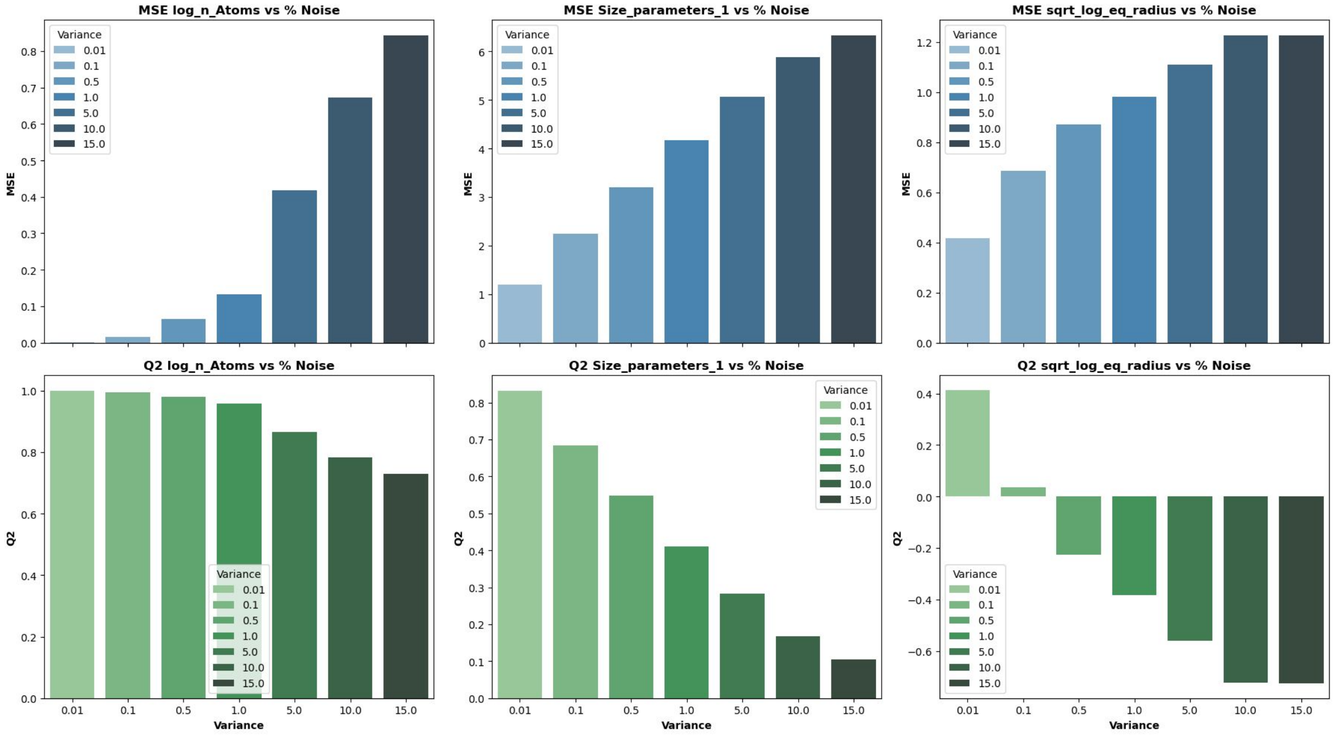
Impact of noise on prediction

Ridge Regression model: Simple predictions on noisy data



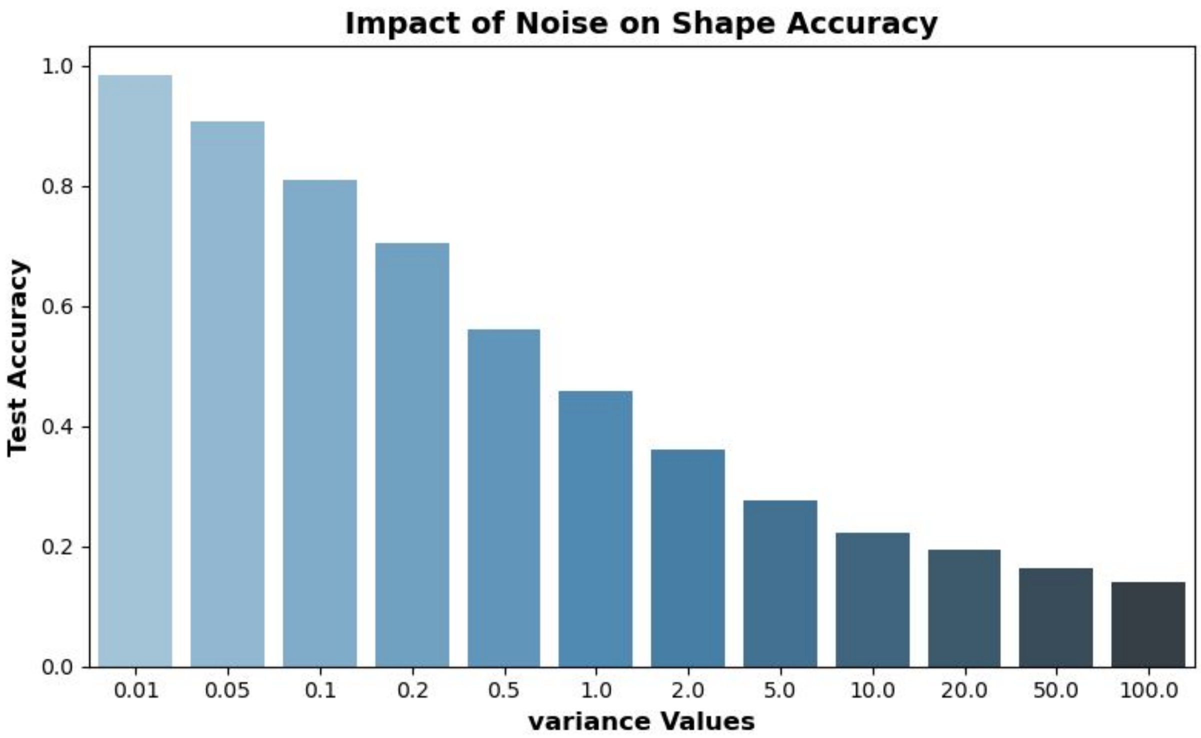
Impact of noise on prediction

Ridge Regression model: Training and predictions on noisy data



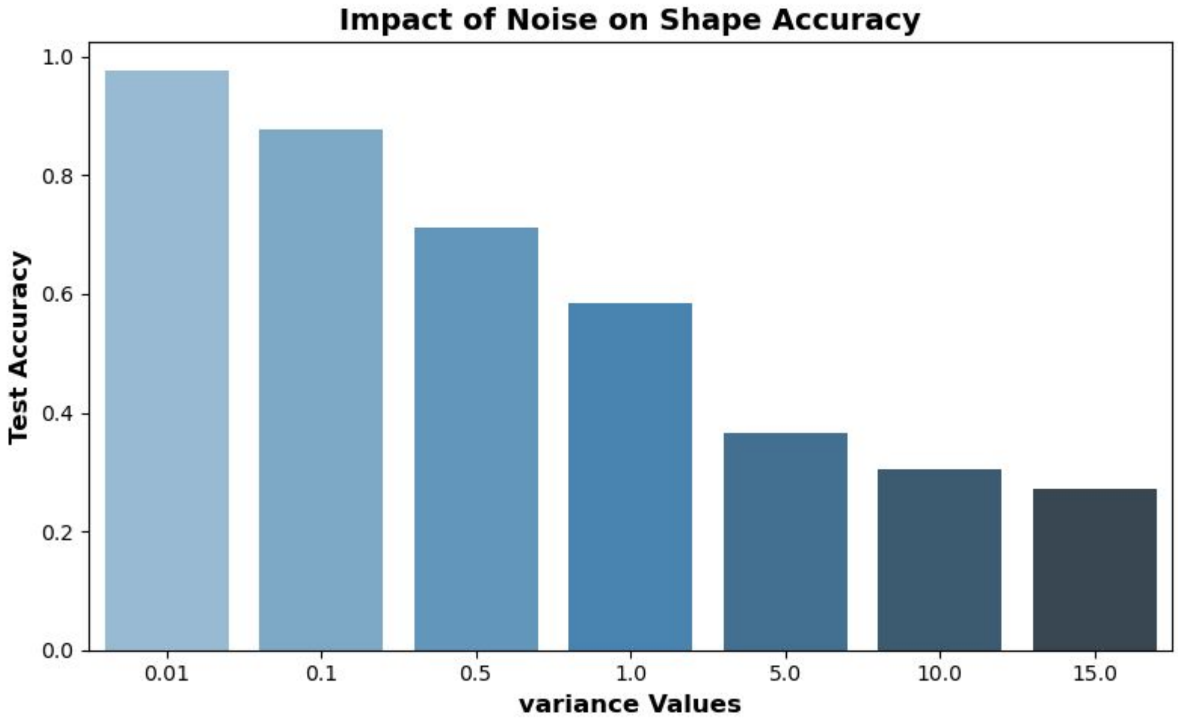
Impact of noise on prediction

Logistic Regression model: Simple predictions on noisy data

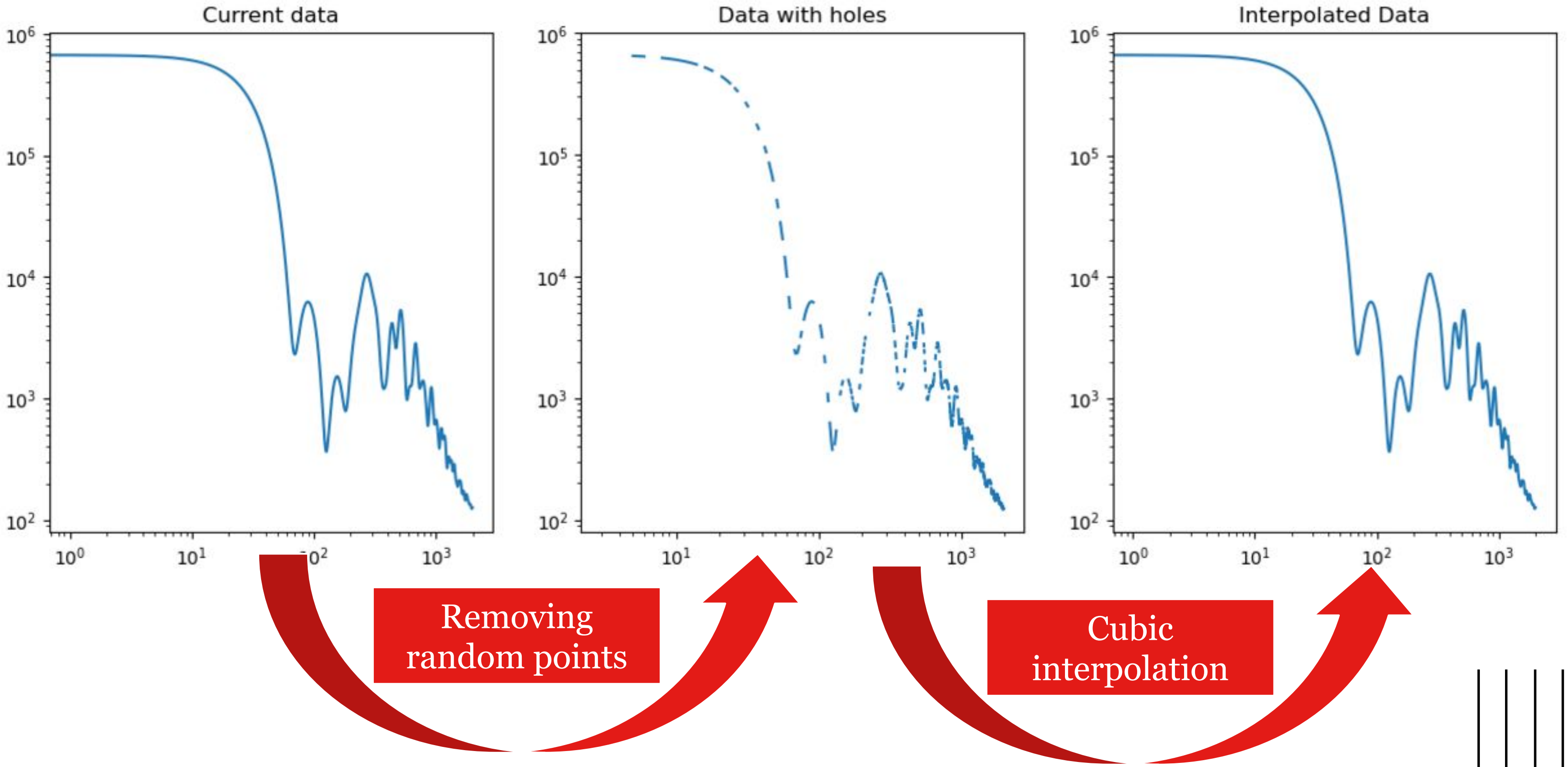


Impact of noise on prediction

Logistic Regression model: Training and predictions on noisy data

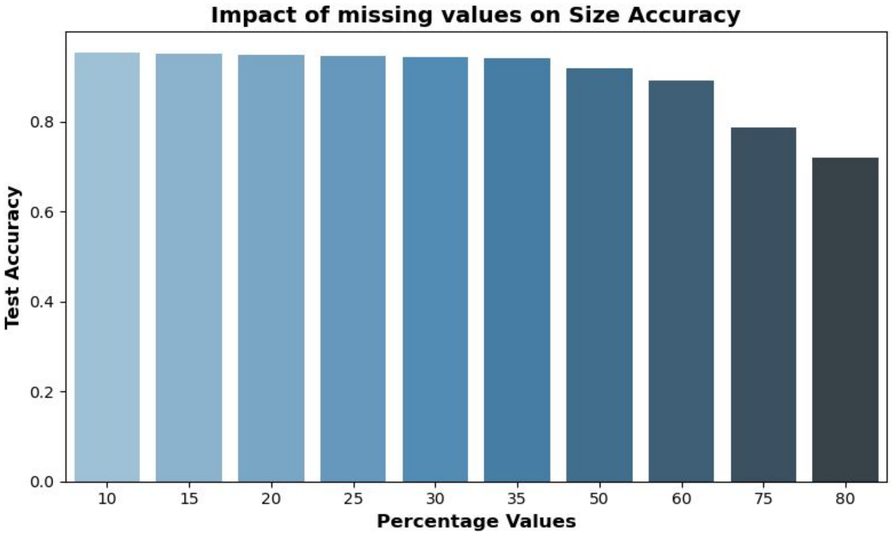


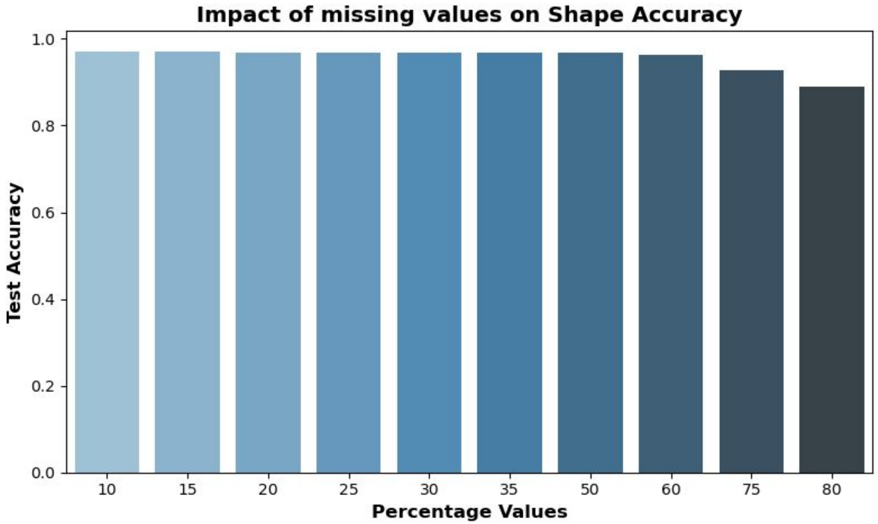
I.V.2 Adding Missing values



Impact of missing value + interpolation

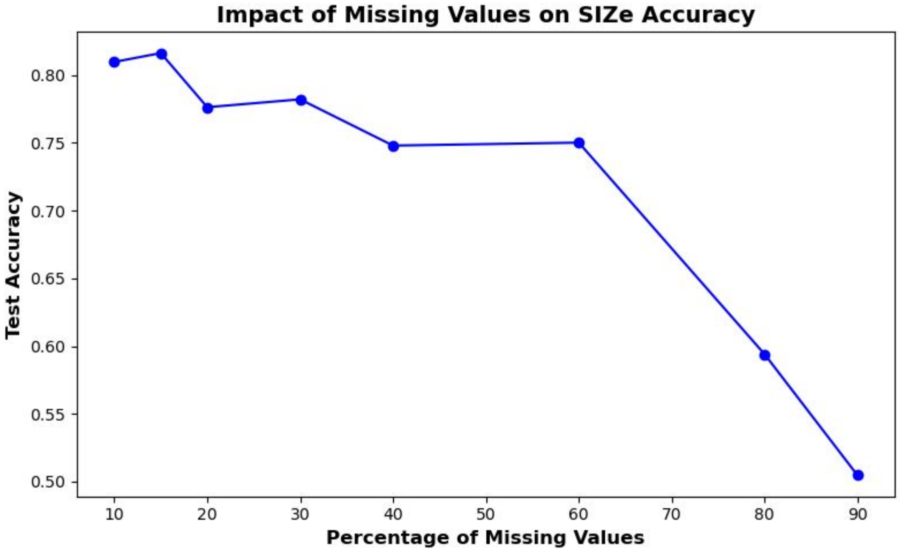
CNN model : Simple predictions on interpolated data



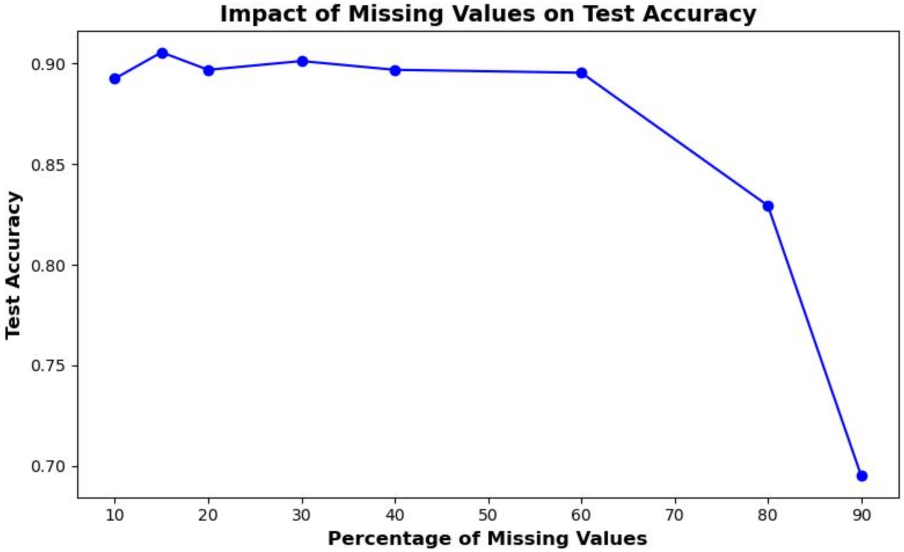


Impact of missing value + interpolation

CNN model : Training and prediction on interpolated data



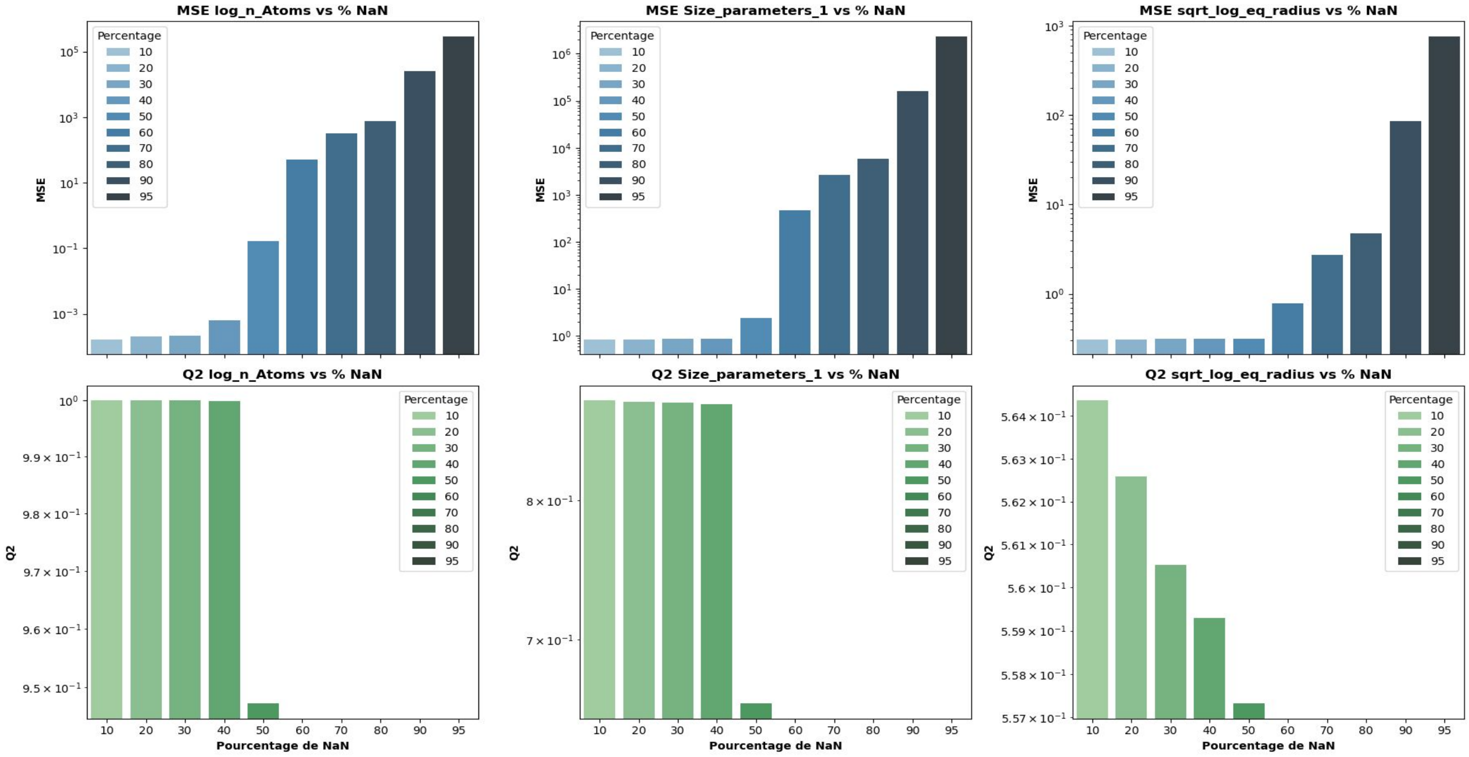
SIZE



SHAPE

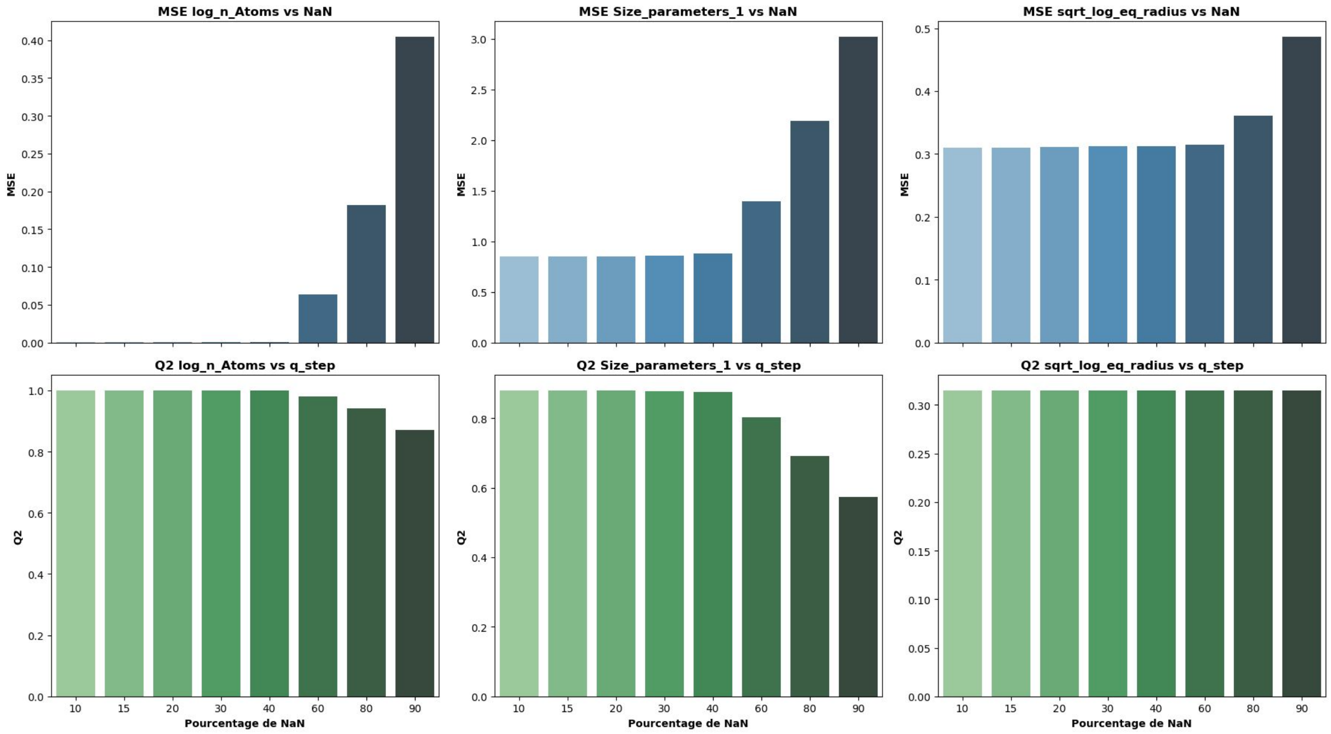
Impact of missing value + interpolation

Ridge Regression model: Simple predictions on interpolated data



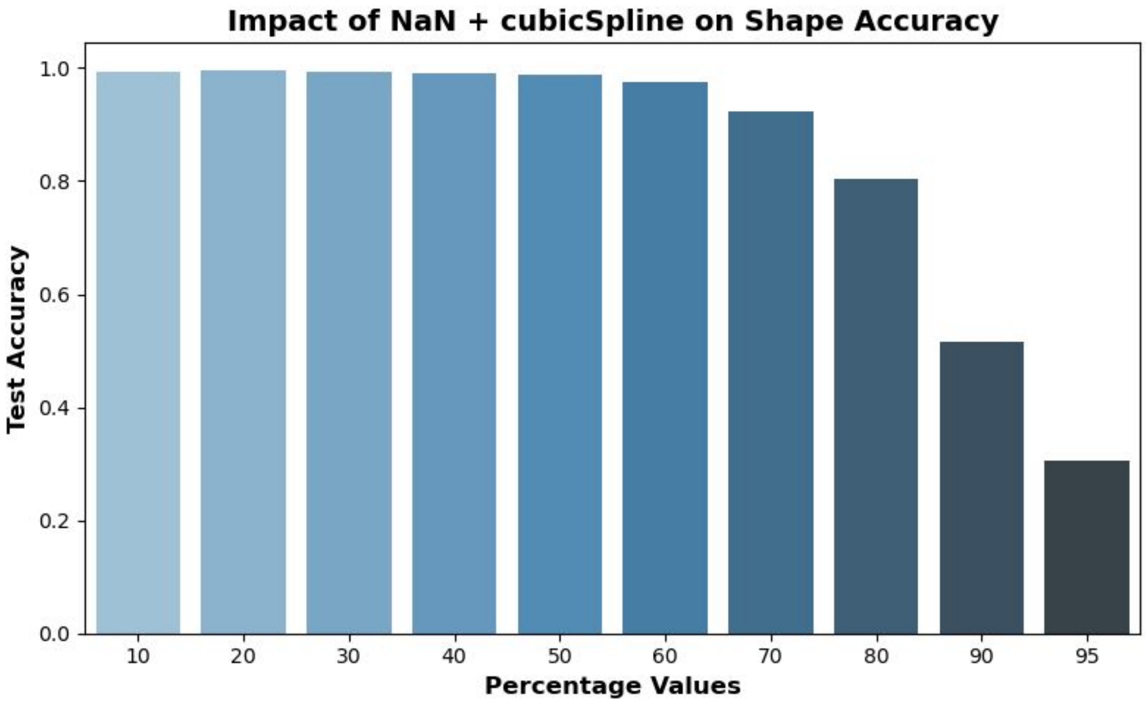
Impact of missing value + interpolation

Ridge Regression model: Training and predictions on interpolated data



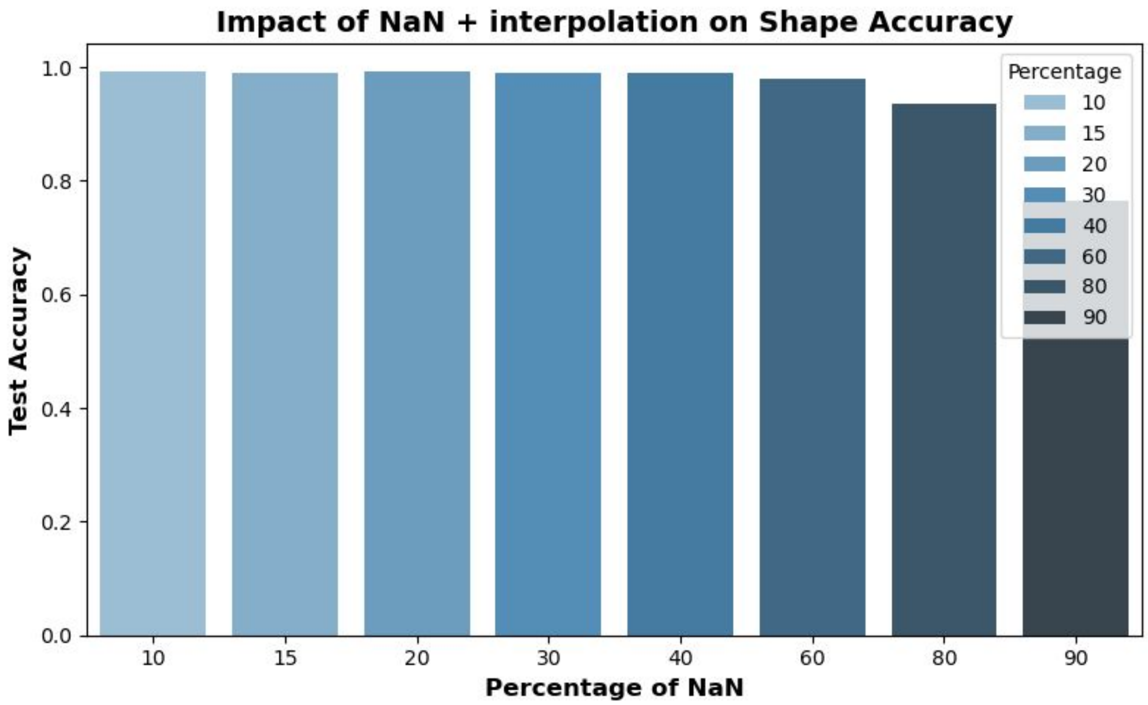
Impact of missing value + interpolation

Logistic regression model : Simple predictions on interpolated data

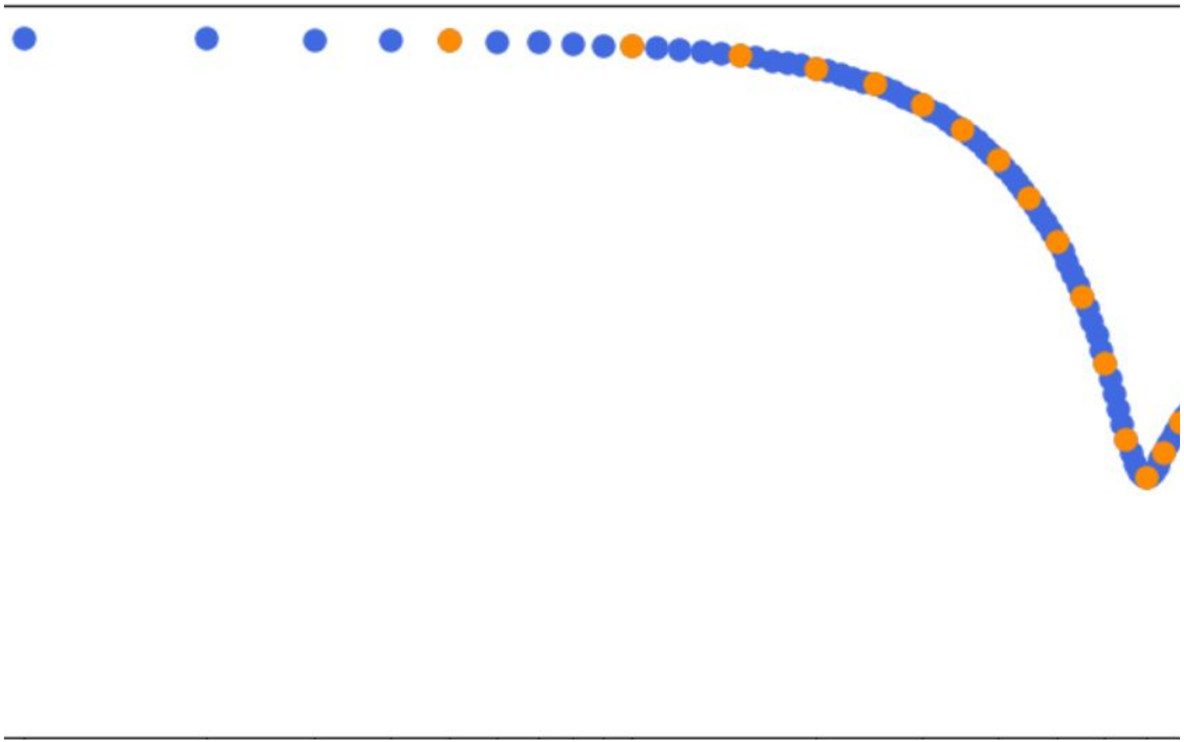


Impact of missing value + interpolation

Logistic regression model : Training and predictions on interpolated data



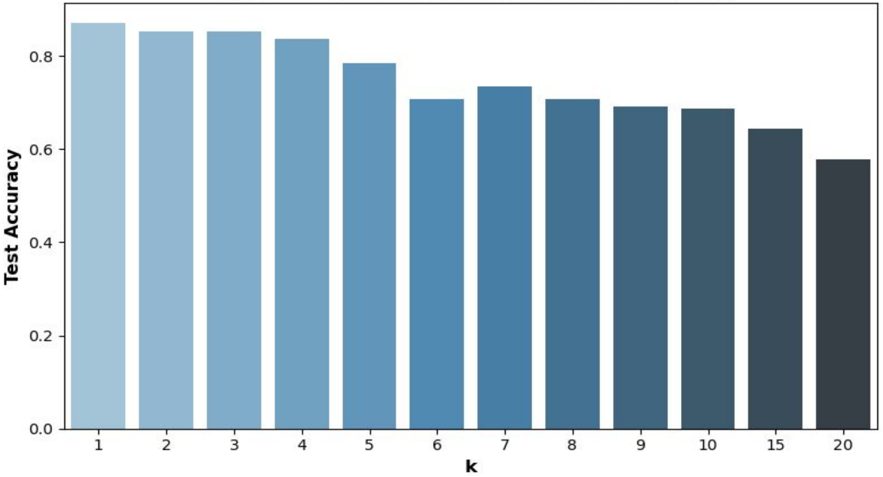
I.V.3 Step increase

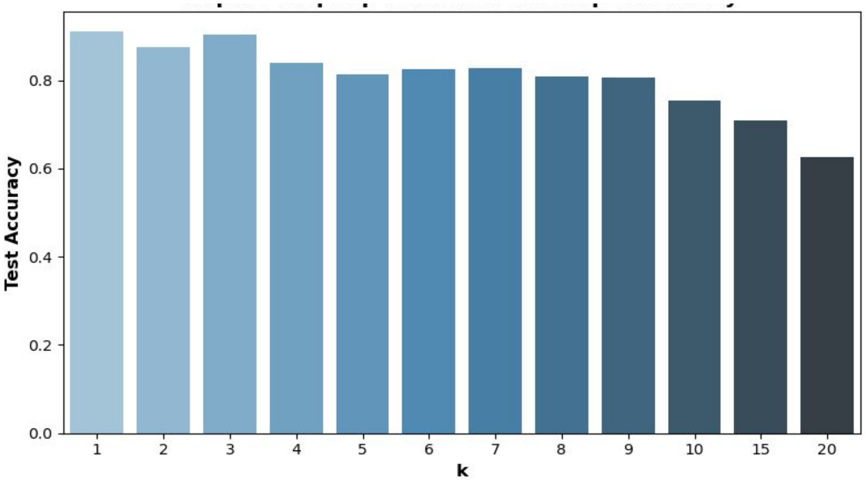


- original values
- Selected values

I.V.3 Step increase: Results

CNN1D model : Training and prediction on edited data





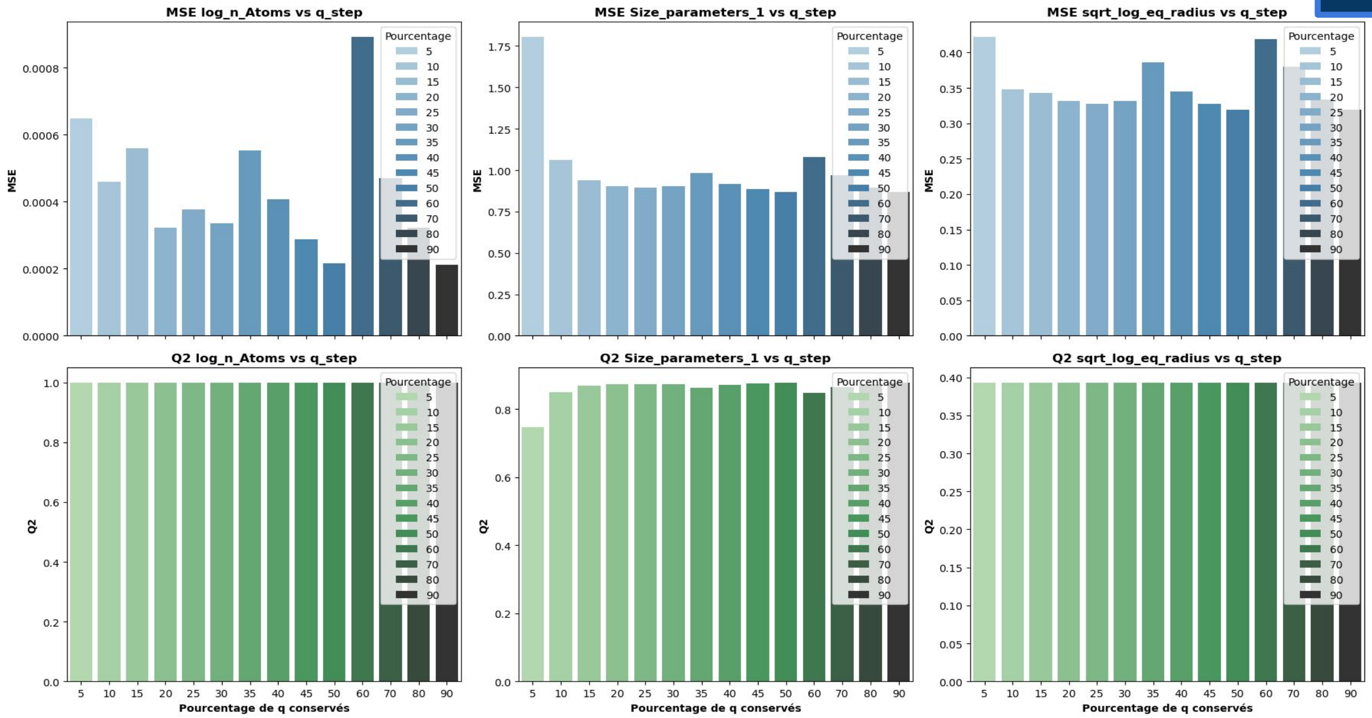
Impact of step increase on Size prediction

Impact of step increase on Shape prediction

I.V.3 Step increase: Results

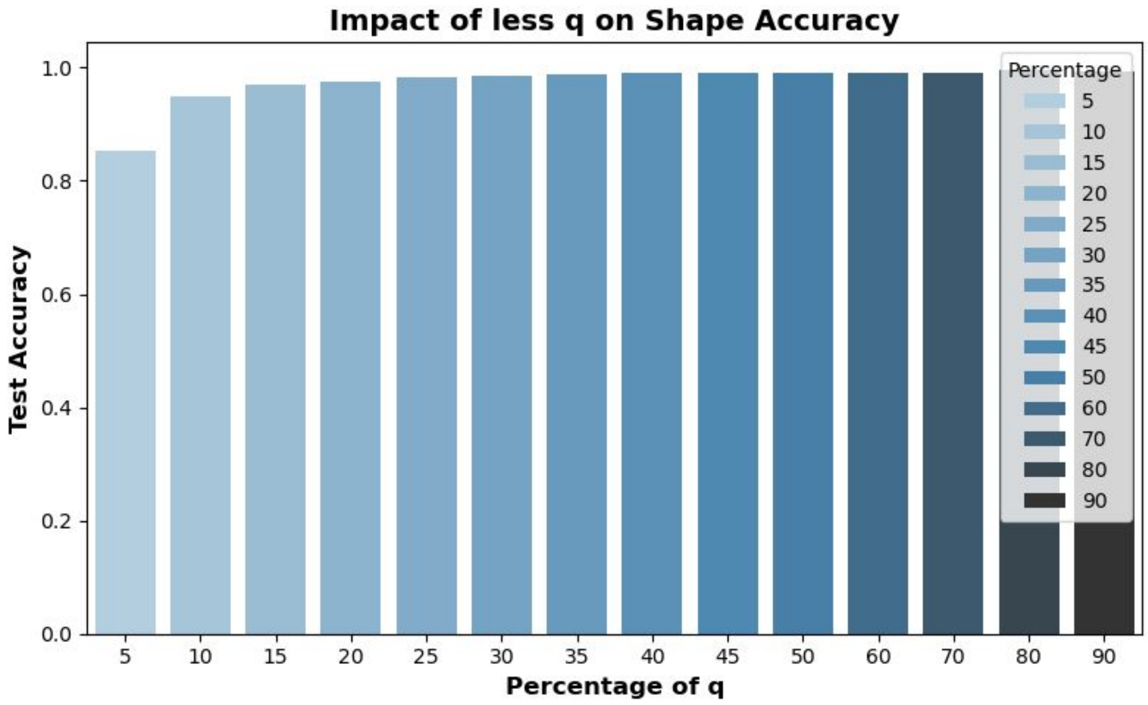
Ridge model: Training and prediction on edited data

Impact of step increase on size prediction



I.V.3 Step increase: Results

Logistic model: Training and prediction on edited data



Impact of step increase on shape prediction

V. USING Only SAXS or WAXS

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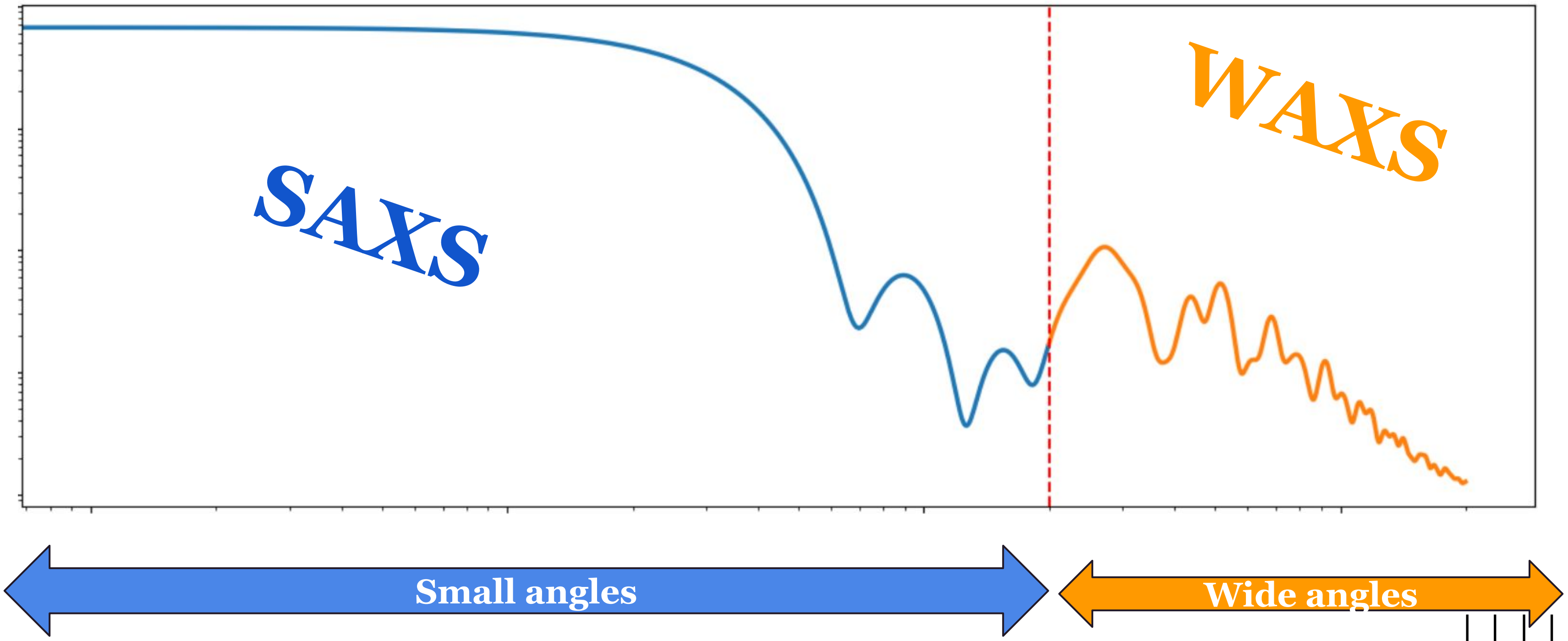
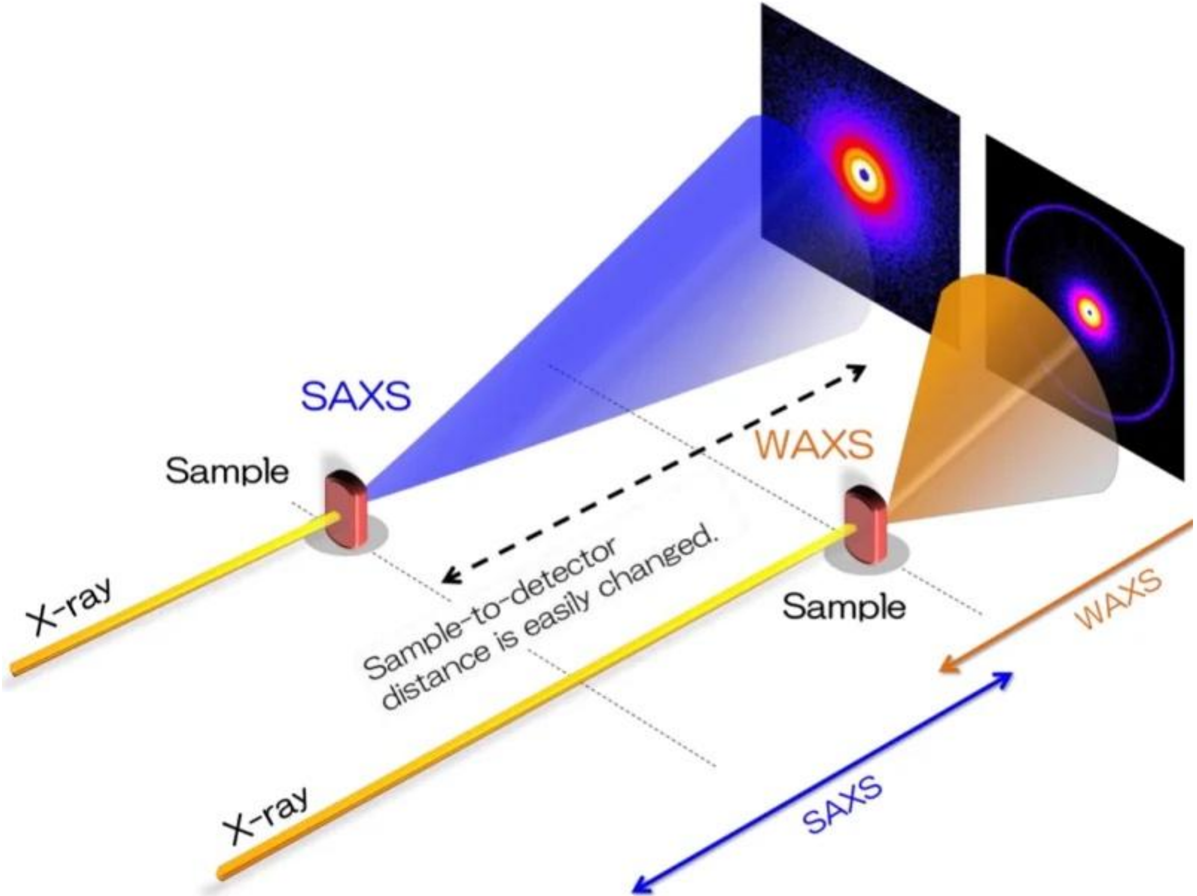
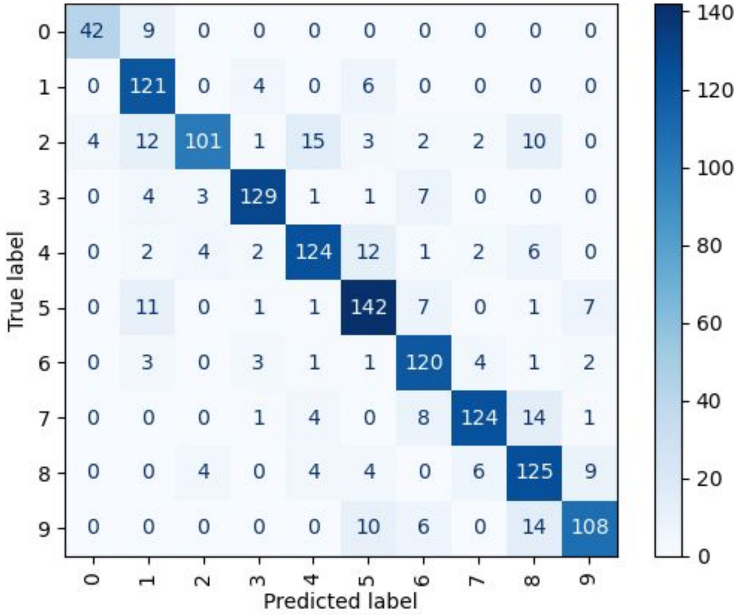


V. USING Only SAXS or WAXS



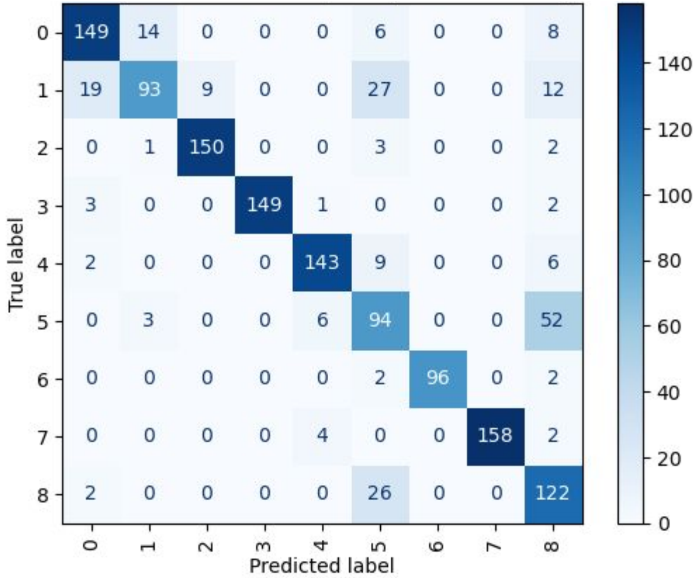
V.1 Prediction with WAXS

CNN1D : Size prediction



Accuracy=82%

CNN1D : Shape prediction



Accuracy=84%

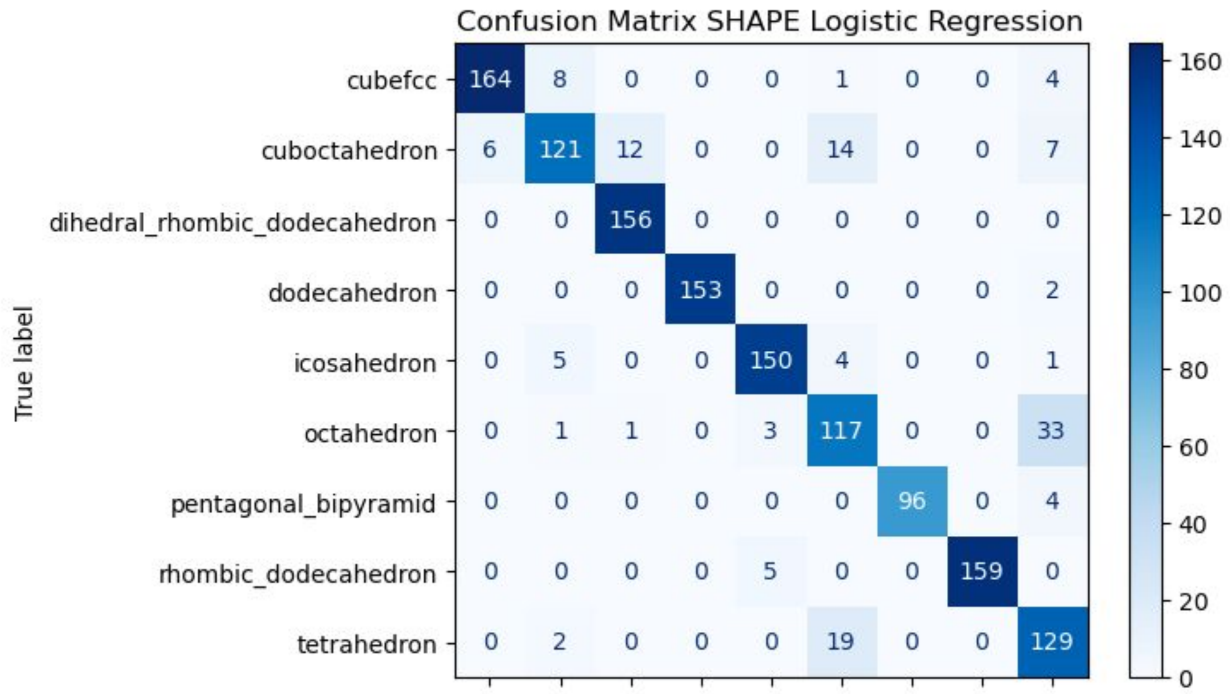
V.1 Prediction with WAXS

Ridge model : Size prediction

Features	MSE	Q2
log_n_Atoms	0.1152	0.9629
Size_parameter_1	2.0095	0.7158
sqrt_log_eq_radius	0.3200	0.5496

V.1 Prediction with WAXS

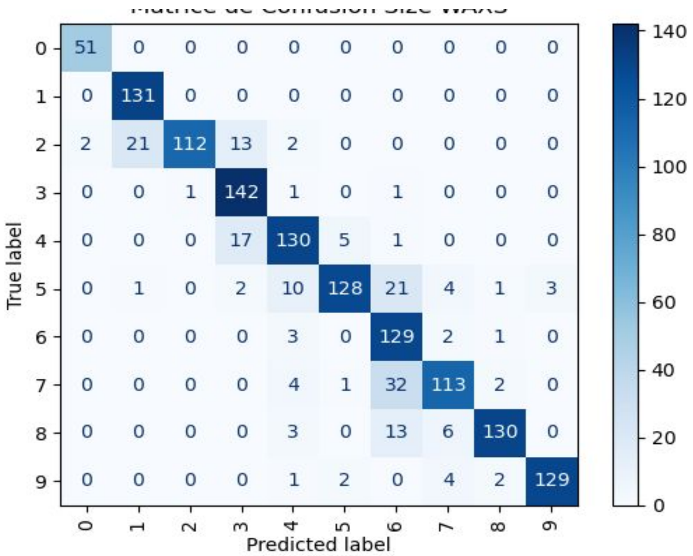
Logistic model : Shape prediction



Accuracy = 90%

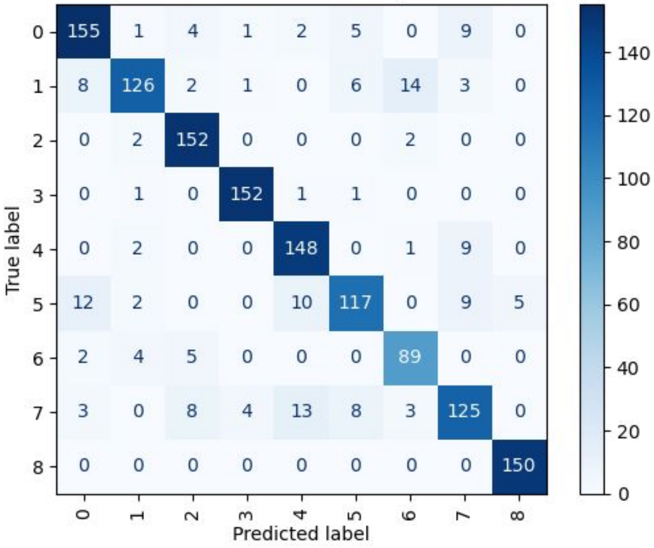
V.2 Prediction with SAXS

CNN1D : Size prediction



Accuracy=86%

CNN1D : Shape prediction



Accuracy=88%

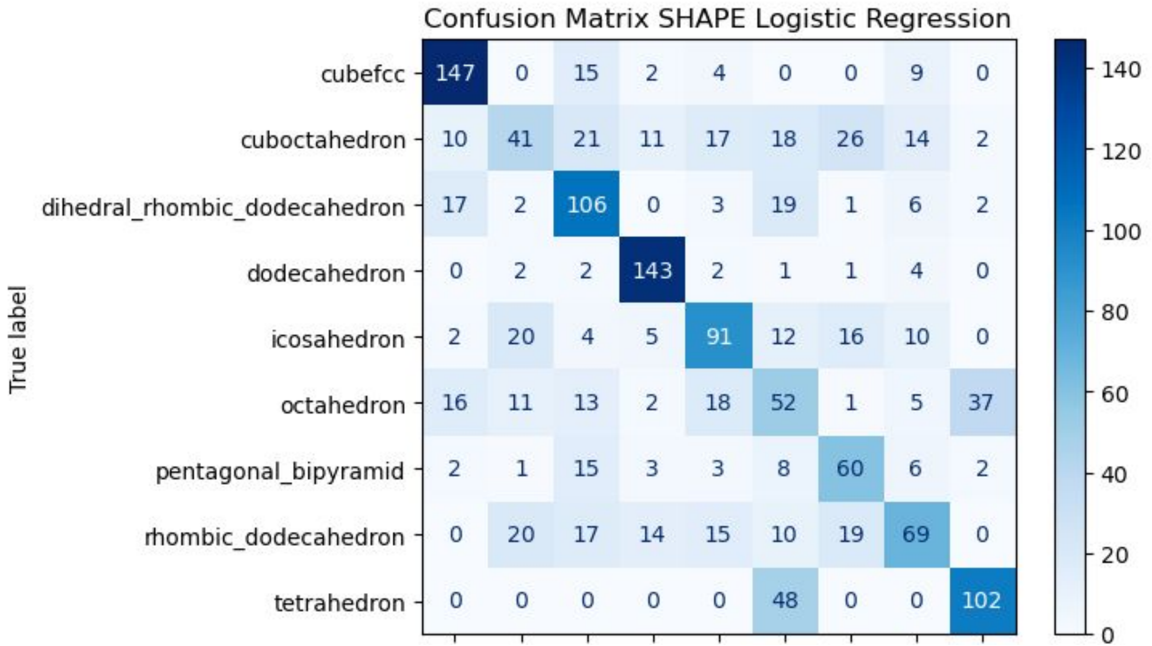
V.2 Prediction with SAXS

Ridge model : Size prediction

Features	MSE	Q2
log_n_Atoms	0.0300	0.9904
Size_parameter_1	2.1451	0.6966
sqrt_log_eq_radius	0.6271	0.1170

V.2 Prediction with SAXS

Logistic model : Shape prediction

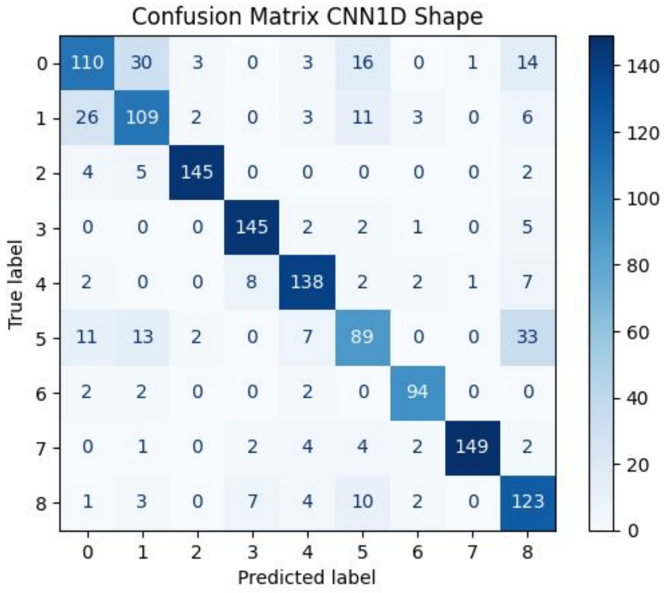


Accuracy = 59%

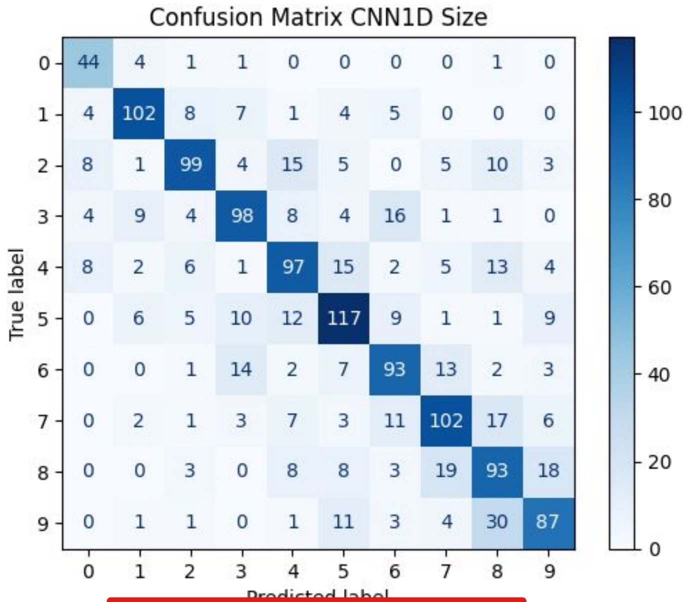
VI.Impact of Modifying Signal Bounds

CNN model

Training and prediction



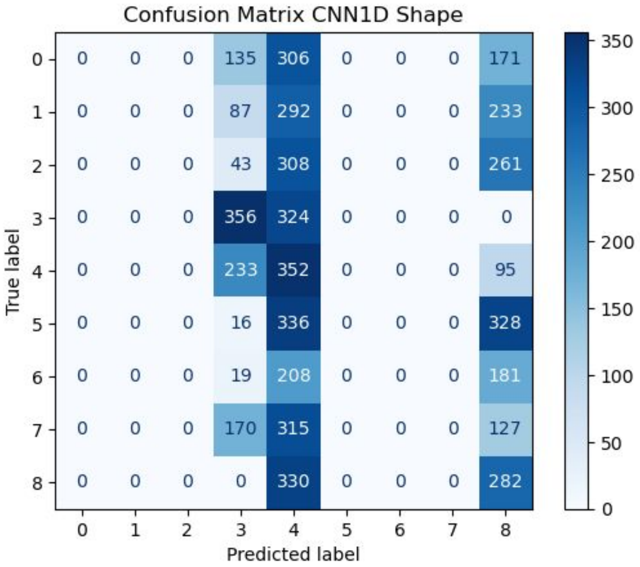
Shape Accuracy = 80%

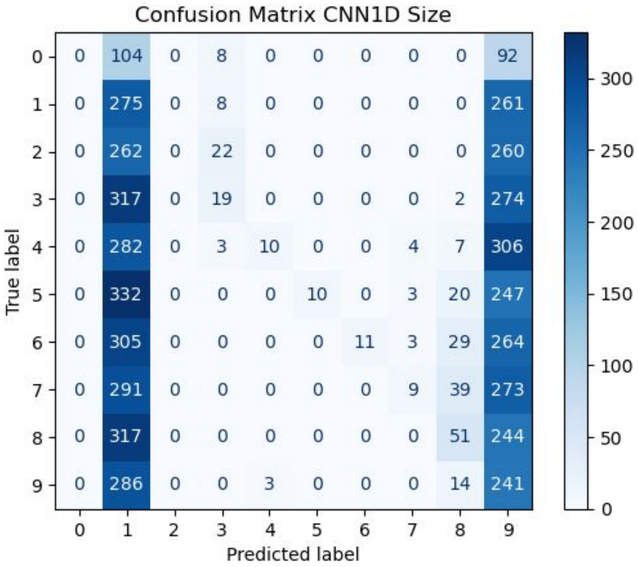


Size Accuracy = 66%

CNN model

Simple predictions

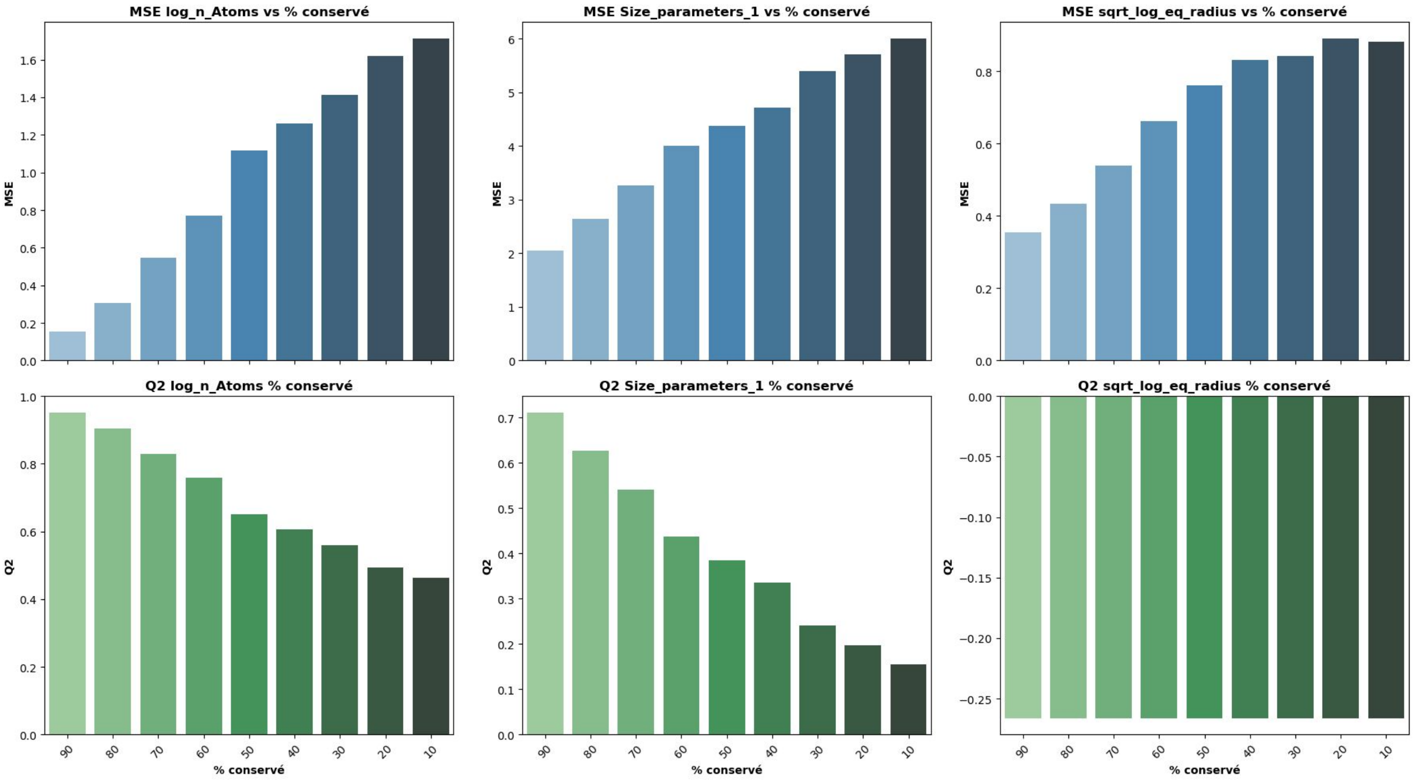




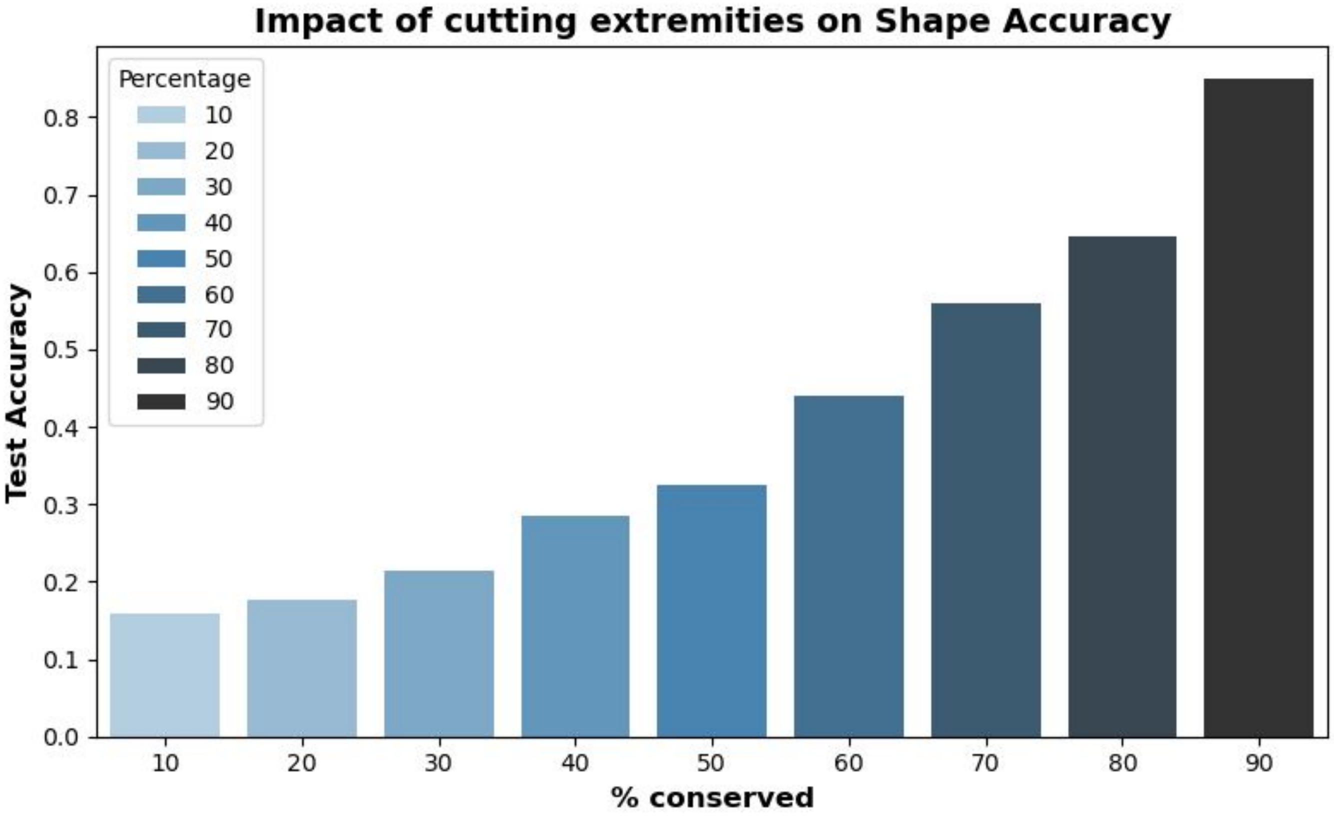
Shape Accuracy = 17%

Size Accuracy = 11%

Ridge model


MSE log_n_Atoms vs % conservé
MSE Size_parameters_1 vs % conservé
MSE sqrt_log_eq_radius vs % conservé
Q2 log_n_Atoms % conservé
Q2 Size_parameters_1 % conservé
Q2 sqrt_log_eq_radius % conservé
MSE
Q2
% conservé
90
80
70
60
50
40
30
20
10

Logistic model



CONCLUSION

- ★ **Work completed: Developing high-performance models using our simulated data**

  - ★ **Outlook:**
    - **working with more realistic data**
    - **Explainable Artificial Intelligence (XAI) methods to identify the specific q-range regions contributing to size and shape predictions**