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# Uncertainty quantification in Machine Learning

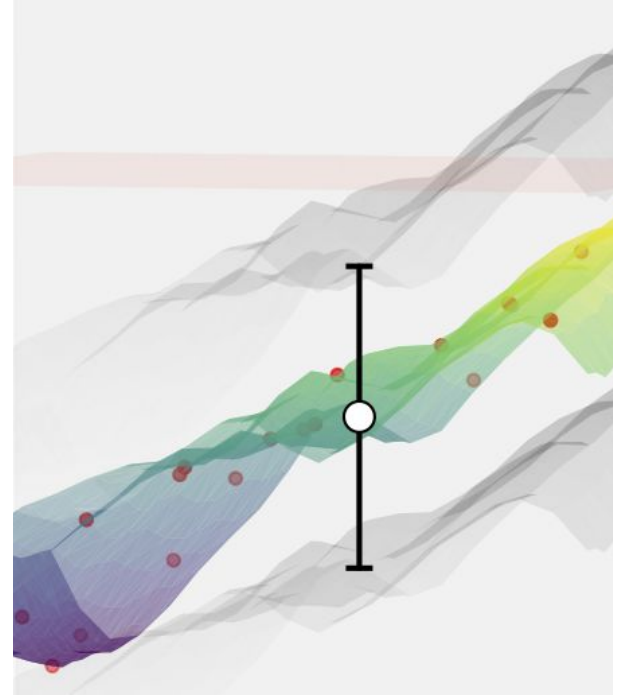
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# Summary

- I. Presentation of the project's interest
- II. The two types of uncertainties
- III. Tests on splitting uncertainties
- IV. Trying to estimate epistemic uncertainty
- V. Samples classification as functions of uncertainty



# I. Presentation of the project's interest

## Uncertainty quantification

- Informative purpose
- Many kinds of applications (including vision)

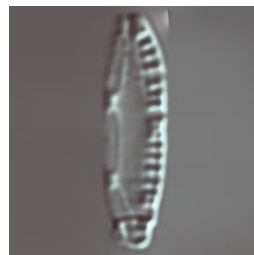
## The problem

Diatoms are hard to classify using AI and often require the eyes of an expert

## The proposed solution

Classify diatoms as functions of their classification uncertainty

- Identify uncertainties
- Measure uncertainties empirically
- Develop existing methods to predict potential outliers
- Use a framework to classify diatoms



# I. Presentation of the project's interest

## The pipeline

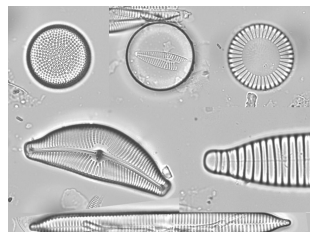


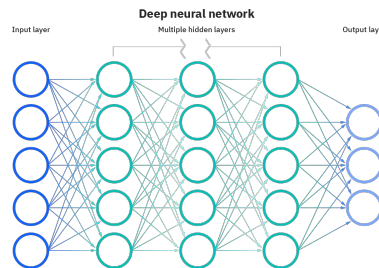
Image of diatoms

(1)



One instance

(2)



Neural Network

(3)

C1 : Inliers of $c > 80\%$
C2 : Inliers of $c < 80\%$
C3 : Outliers

Classification given confidence

(1) Object detection

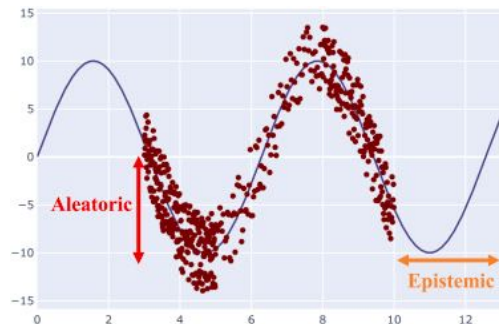
(2) Training given batch of instances

(3) Framework calculating uncertainty

## II. The two kinds of uncertainties

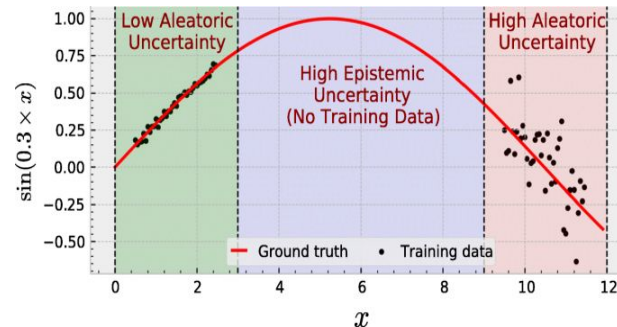
### Epistemic uncertainty

- Accounts for uncertainty in the model parameters
- Uncertainty on the model generated by the data
- Can be reduced with training



### Aleatoric uncertainty

- Captures noise inherent in the observations (sensor noise or motion noise for instance)
- Doesn't depend on the model
- Cannot be reduced



# III. Tests on splitting uncertainties

## Why ?

Could be useful to understand if uncertainty more comes from noised data or from model parameters.

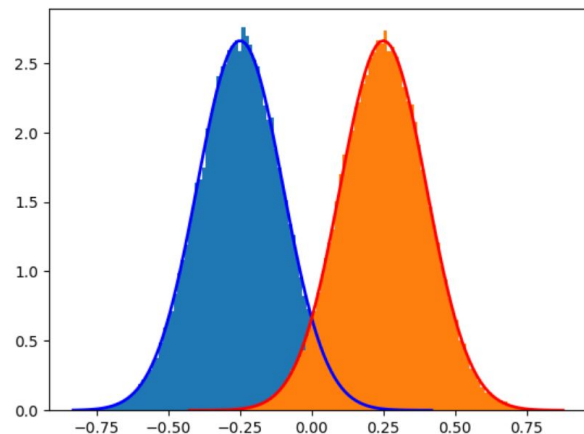
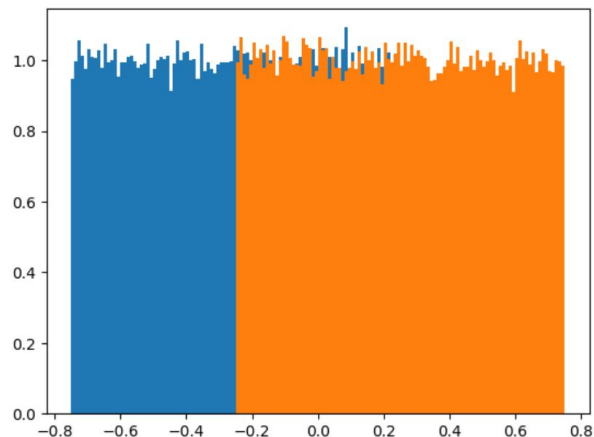
## A simple classifier : the 1D classifier

$$f(x, \lambda) = \begin{cases} -1, & x < \lambda \\ 1, & x \geq \lambda \end{cases} \quad \text{with } \lambda \sim N(0, \sigma^2)$$

Homoscedastic case  $\rightarrow$  constant standard deviation

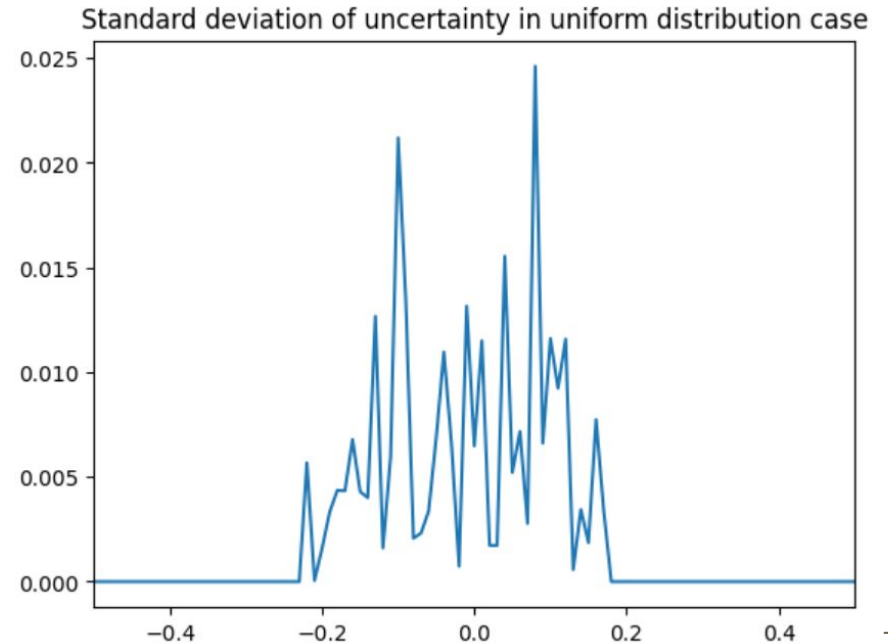
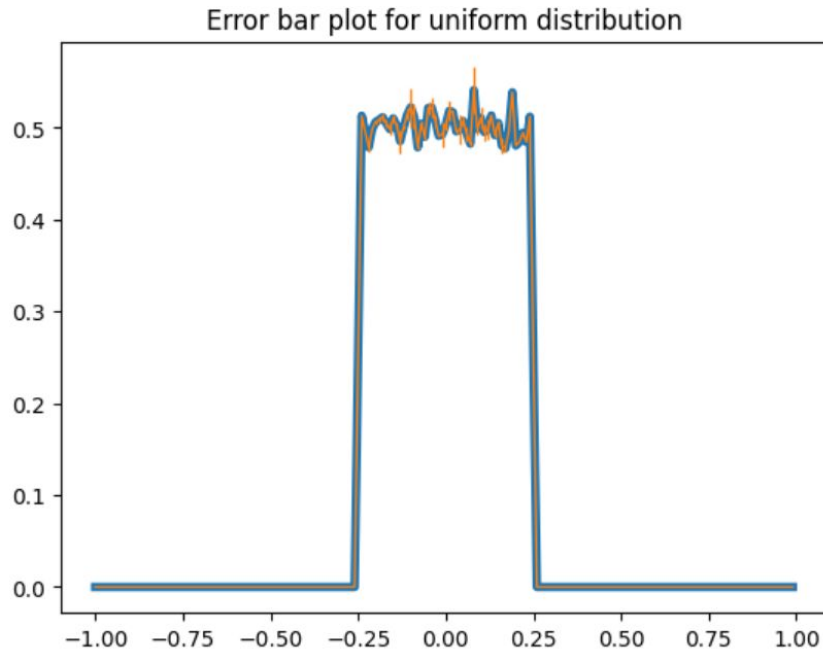
## 2 simple datasets

- Uniform distributions
- Gaussian distributions



# III. Tests on splitting uncertainties

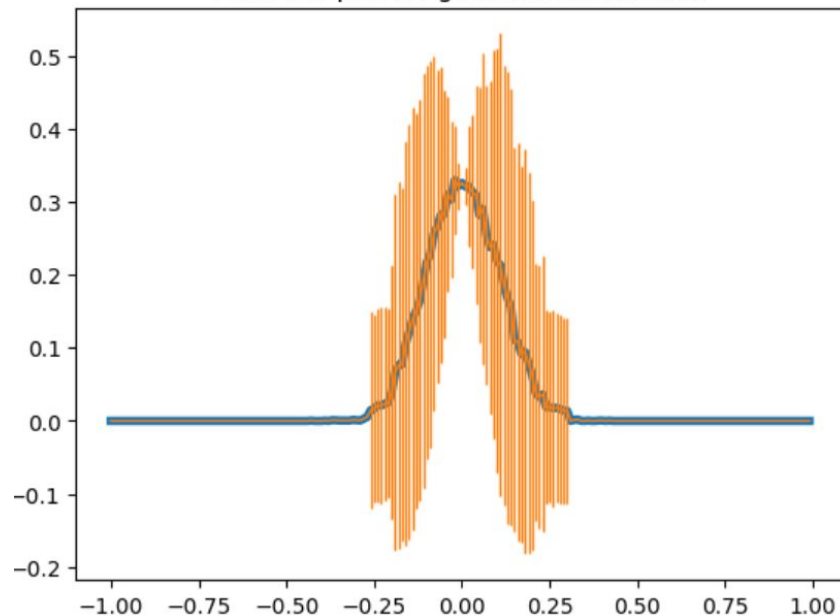
## Uniform case



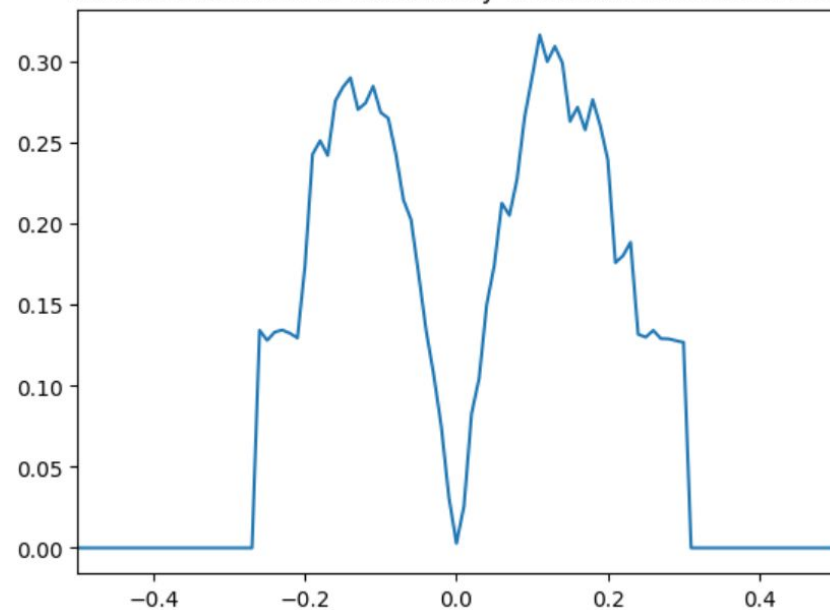
# III. Tests on splitting uncertainties

## Gaussian case

Error bar plot for gaussian distribution



Standard deviation of uncertainty in normal distribution case



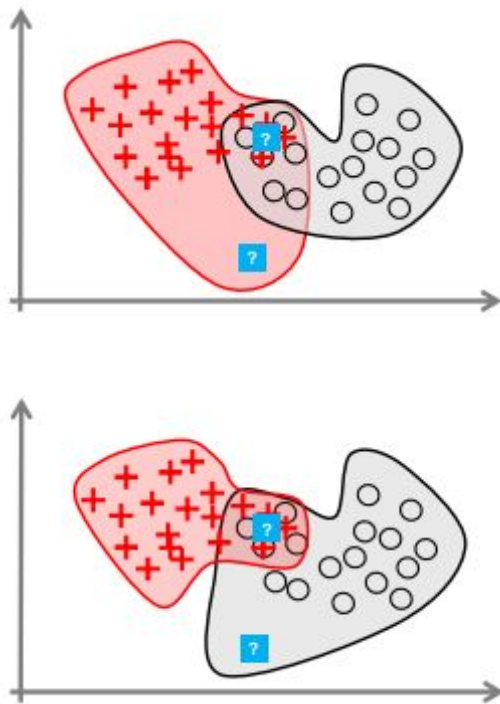


# IV. Trying to estimate epistemic uncertainty

## Fisher Information Matrix

$$I(\theta) = E \left[ \left( \frac{\partial}{\partial \theta} \log f(X; \theta) \right)^2 \middle| \theta \right]$$

- Used in Cramer Rao bound (lower bound of the variance of an estimator)
- The epistemic uncertainty is high in sparsely populated regions without training examples.
- The larger the region, the higher the epistemic uncertainty
- Therefore, it can be seen as a confidence region



# IV. Trying to estimate epistemic uncertainty

## Obtaining Fisher Information

$$\theta = \sigma^2$$

$$\lambda \sim N(0, \sigma^2) \xrightarrow{\text{yields}} f_{\lambda}(\lambda_i, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\lambda_i^2}{2\sigma^2}}$$

$$I(\sigma^2) = \frac{N^2(N-1)}{4\sigma^4} \approx \frac{N^4(N-1)}{4 \sum_{i=1}^N \sum_{j=1}^N \lambda_i^2 \lambda_j^2}$$

Regarding the results, it seems to have failed...

Therefore, it may be aimless trying to split uncertainties.

## The results

```
1 fisher_uni = fisher(lambda_uni, n_test)
2 1/fisher_uni
```

✓ 0.4s

3.980242134859097e-10

```
1 fisher_gauss = fisher(lambda_gauss, n_test)
2 1/fisher_gauss
```

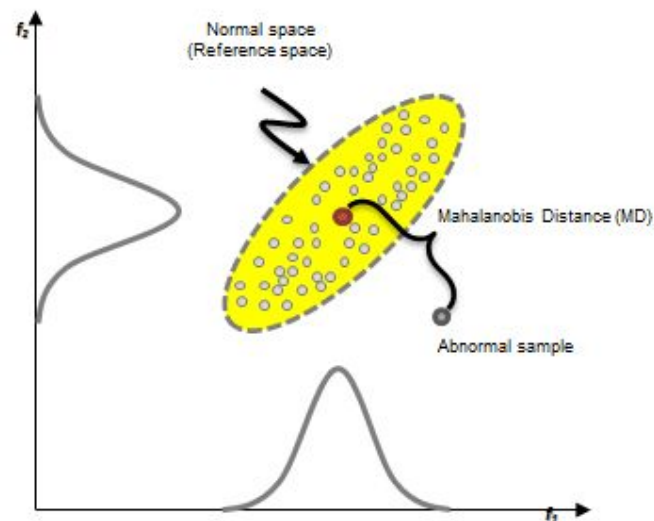
✓ 0.5s

2.3169135765420645e-10

# V. Samples classification as functions of uncertainty

## Process

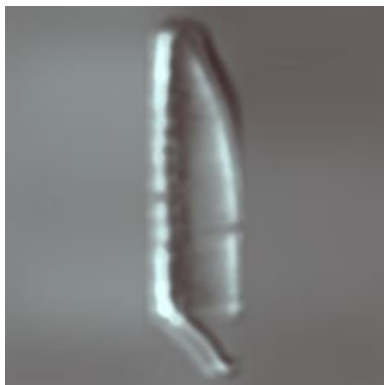
1. Extract instances from images (each instance is a diatom and there can be several in one image)
2. Train a network with the extracted instances
3. Calculate Mahalanobis distances of samples from centroids
4. Identify and rank the diatoms given the confidence returned for each instance



# V. Samples classification as functions of uncertainty

## Let's look at the results

Test on individuals belonging to the NPAE class give **bad results**...



Very high confidence  
(to belong to UULN)



Low confidence  
(to belong to NPAE)

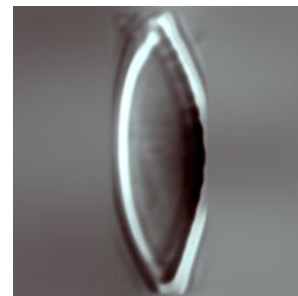
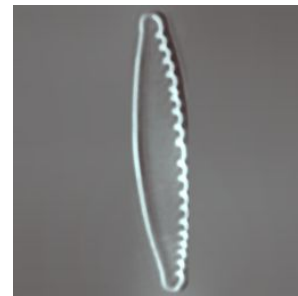


Predicted outlier  
(while it belongs to NPAE)

# Conclusion

- Uncertainty can be split **empirically** but it seems hard to do it theoretically as shown with Fisher Information Matrix
- Mahalanobis distance is a good way to take into account data covariance but is not always efficient
- Disappointing results with the neural network and the framework: **the network is overconfident on predicting a wrong class**
- **Hard problem** since :
  - diatoms of different classes can look very similar
  - diatoms of the same class can look very different

Individuals from  
class NPAE



**Thank you for your attention.  
Don't hesitate if you have any questions!**

**And thanks, once again, to Cédric Pradalier and  
Aishwarya Venkataramanan for their help during the  
whole project**