Uncertainty quantification in Machine Learning

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Summary

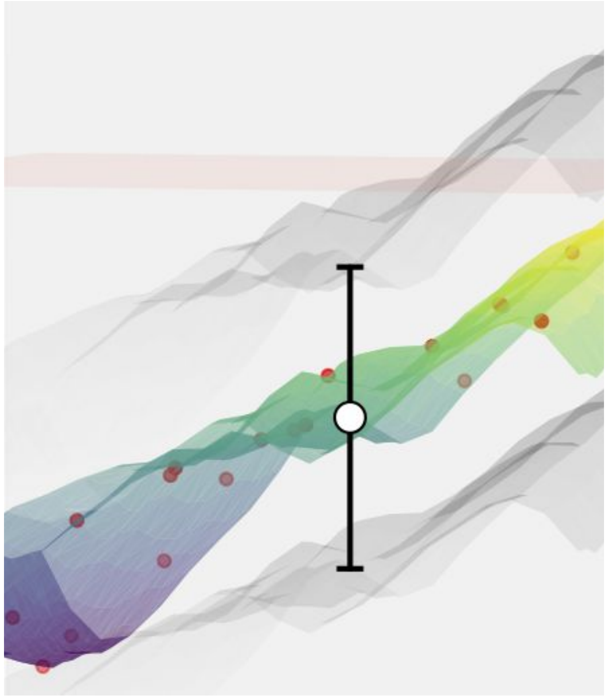
I. Presentation of the project's interest

II. The two types of uncertainties

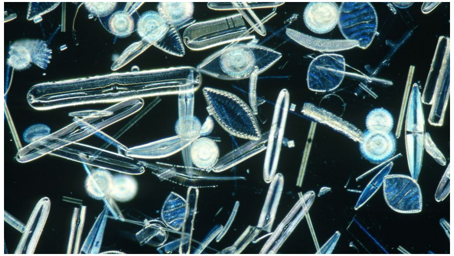
III. Tests on splitting uncertainties

IV. Trying to estimate epistemic uncertainty

V. Samples classification as functions of uncertainty



I. Presentation of the project's interest

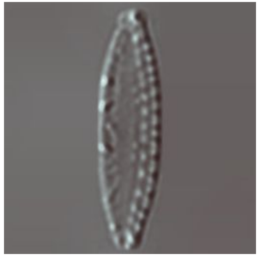


Uncertainty quantification

- 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

(1) Object detection

(2) Training given batch of instances

(3) Framework calculating uncertainty

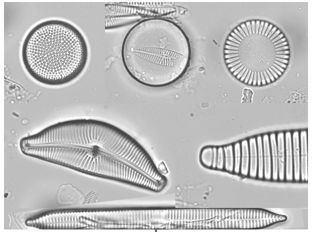
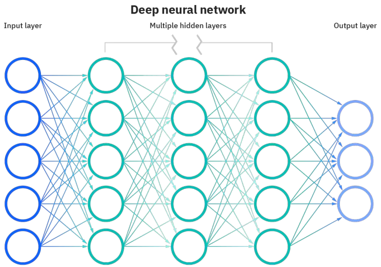


Image of diatoms

(1)

One instance

(2)



Neural Network

(3)

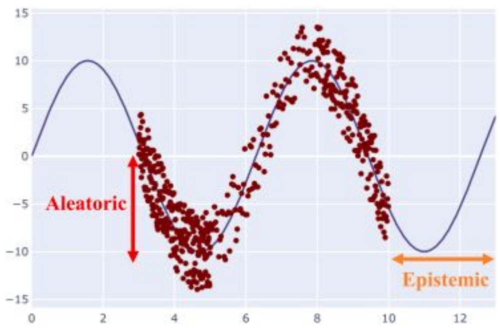
C1 : Inliers of c > 80%
C2 : Inliers of c < 80%
C3 : Outliers

Classification given confidence

II. The two kinds of uncertainties

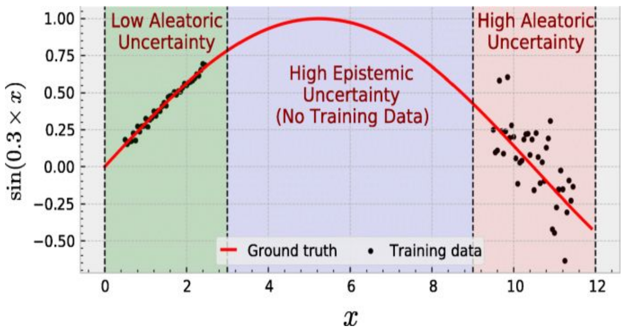
Epistemic uncertainty

- 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.

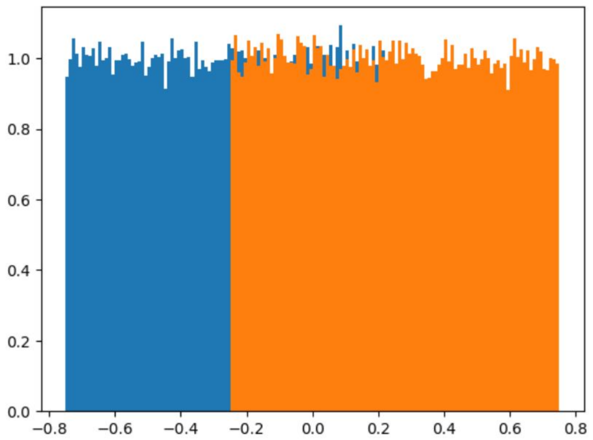
A simple classifier : the 1D classifier

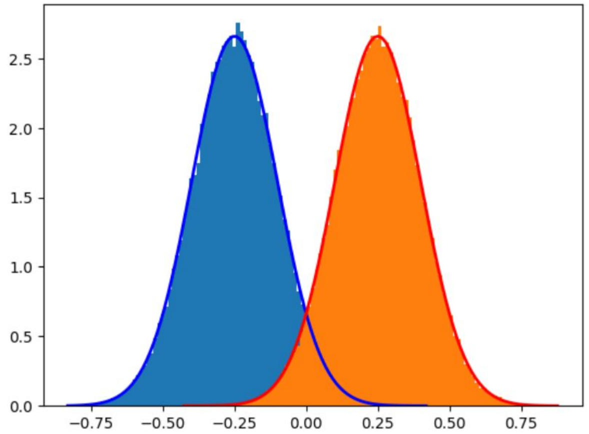
$$f(x,\lambda) = \begin{cases} -1, & x < \lambda \\ 1, & x \geq \lambda \end{cases} \qquad \text{with } \lambda \sim N(0,\sigma^2)$$

Homoscedastic case → constant standard deviation

2 simple datasets

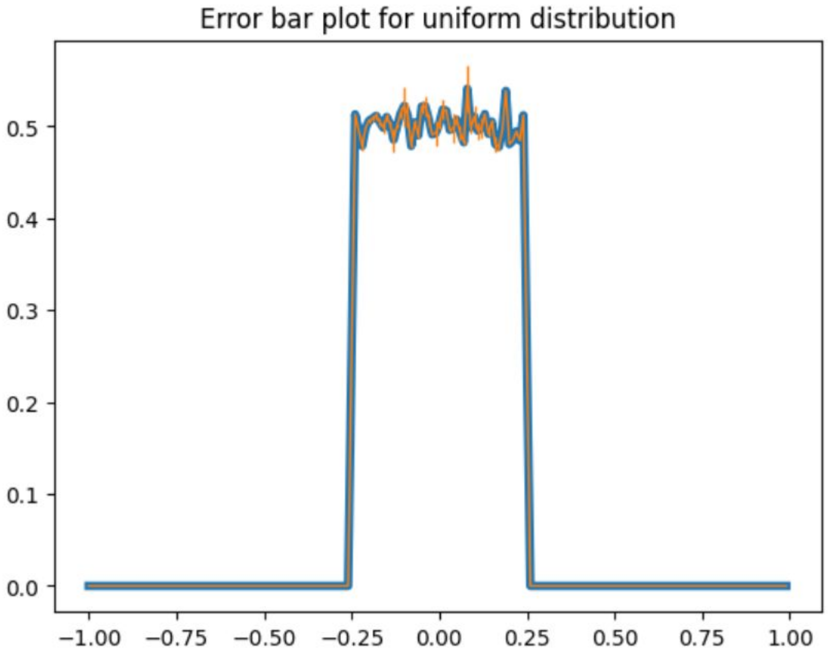
- Uniform distributions
- Gaussian distributions

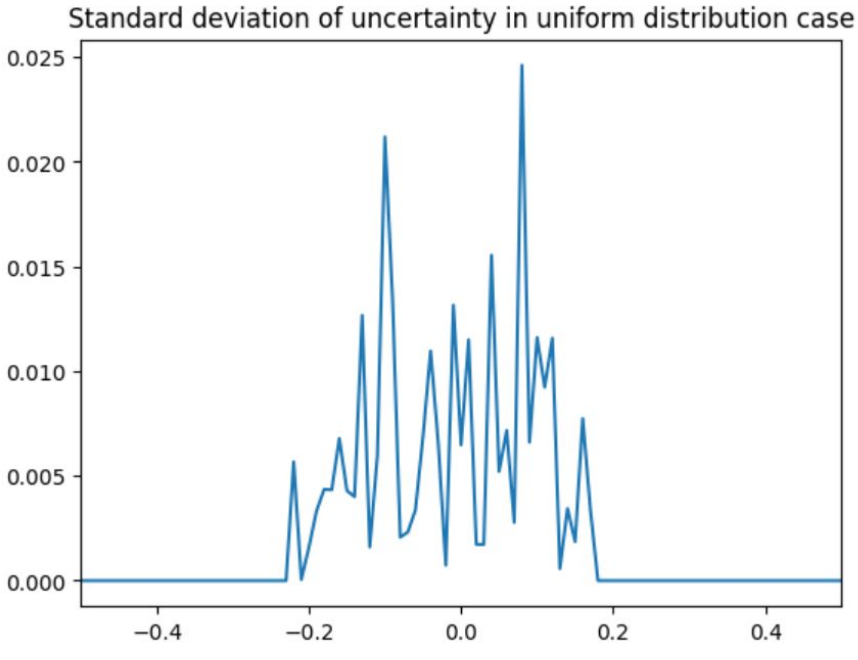




III. Tests on splitting uncertainties

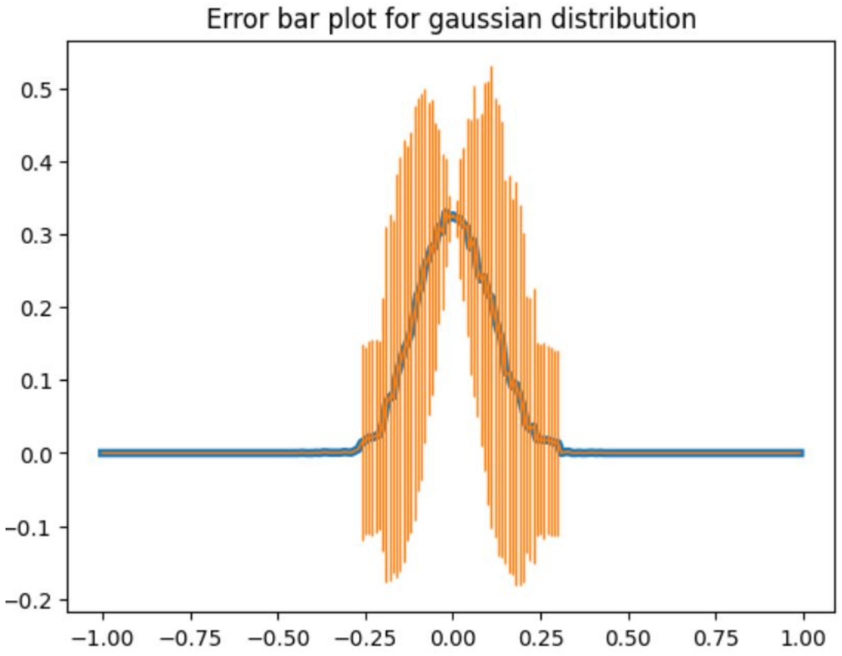
Uniform case

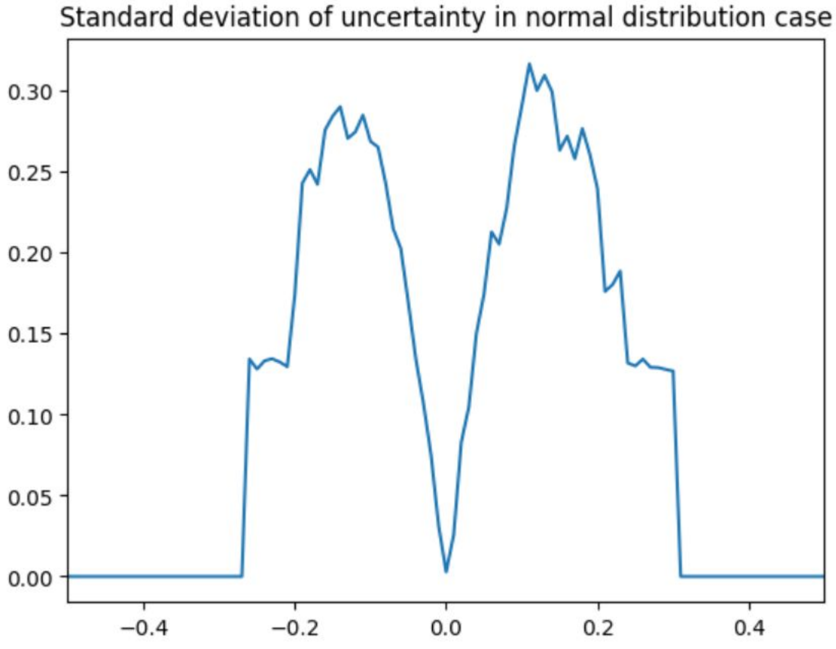




III. Tests on splitting uncertainties

Gaussian case



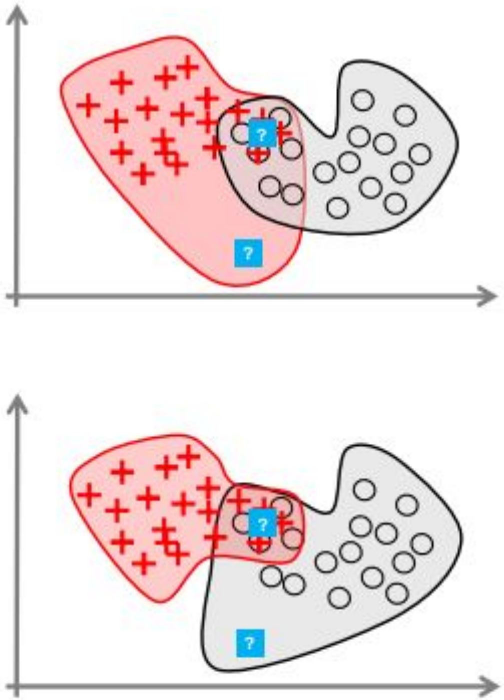


IV. Trying to estimate epistemic uncertainty

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

$$\theta = \sigma^2$$

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

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

Regarding the results, it seems to have failed…

Therefore, it may be aimless trying to split uncertainties.

The results

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

✓ 0.4s

```
3.980242134859097e-10
```

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

✓ 0.5s

```
2.3169135765420645e-10
```

V. Samples classification as functions of uncertainty

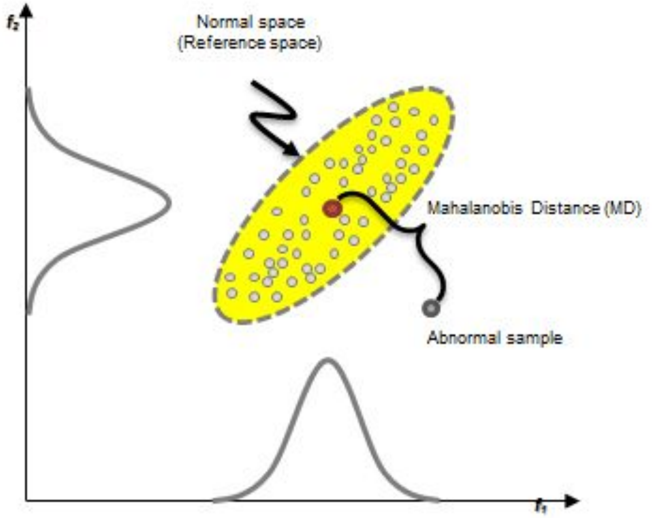
Process

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

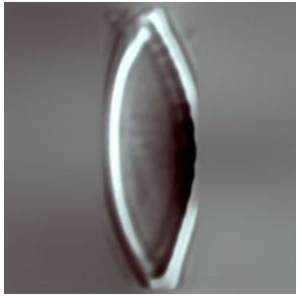
- Uncertainty can be split **empirically** but it seems hard to do it theoretically as shown with Fisher Information Matrix

- Mahalanobis distance is a good way to take into account data covariance but is not always efficient in a latent space

- 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