

UNRAVELING UNCERTAINTY: QUANTIFICATION AND LOCALIZATION IN AN ERROR-RELATED POTENTIAL CLASSIFIER

Bachelor's Project Thesis

Martijn Wobbes, s4339312, m.s.wobbes@student.rug.nl, Supervisor: I.P. de Jong

Abstract: Accurate estimation of uncertainty plays a pivotal role in enhancing the reliability and interpretability of predictive models. This paper builds upon previous methods by proposing a novel approach that not only quantifies its uncertainty but also traces the sources of this uncertainty using a method from Explainable AI. In this study, a previously developed classification model for electroencephalogram signals is modified by incorporating an additional head predicting uncertainty. The contribution of features to the uncertainty prediction can be calculated, ultimately pointing towards the source of uncertainty. The proposed approach is evaluated on a dataset of Error-Related Potentials. To test this method's effectiveness, the signals have been modified by introducing artificial noise in specific regions to challenge the prediction and localization of the noise. The results show that the modified model is capable of predicting uncertainty with a high degree of accuracy. However, the tracing of sources of uncertainty proves to be challenging despite the accurate uncertainty estimation, and the exact sources of uncertainty remain elusive.

1 Introduction

Deep neural networks have emerged as the state-ofthe-art method for various machine learning tasks, exhibiting remarkable performance across domains such as computer vision, speech recognition, natural language processing, and even biomedical applications (Yoo, 2015; Zheng & Lu, 2015). However, because of their excellent performance, the outputs of these networks are often blindly trusted and presumed to be accurate, which is not always valid as the networks are generally overconfident. Generally, a network has no way of communicating how certain the model is with its predictions. Proper quantification of these uncertainties is becoming increasingly important in the practical field of machine learning. Uncertainty quantification gives the user a better insight into a model's prediction.

1.1 Uncertainty in machine learning

In machine learning, uncertainty refers to the lack of confidence or knowledge in the predictions or outcomes produced by a model. It can arise from various factors, such as limited or noisy data, model assumptions, or the complexity of the underlying problem. The uncertainty of a model can be divided into two types: epistemic and aleatoric uncertainty. Epistemic uncertainty arises from the lack of knowledge or understanding of the underlying data distribution or model parameters. This type of uncertainty can often be reduced by feeding the model more training data. Aleatoric uncertainty is the noise inherent in the data itself. It captures the inherent variability and randomness in the observed data and is typically caused by noise and measurement errors. This type of uncertainty cannot be reduced with more data or better model training.

Aleatoric uncertainty can be split up further into two types. Homoscedastic aleatoric uncertainty is uncertainty that is constant over all inputs. Heteroscedastic aleatoric uncertainty depends on the given input and differs between episodes. For example, homoscedastic aleatoric uncertainty can be sensor noise, constant across all episodes. In contrast, the heteroscedastic aleatoric uncertainty can

be a disconnected or faulty sensor, which only appears in a few episodes.

1.2 Uncertainty quantification

The quantification of uncertainty has been a subject of extensive research, with numerous previous studies proposing methods for measuring and quantifying these uncertainties.

One of the most studied approaches for modeling uncertainties is Bayesian Deep Learning Methods (Kendall & Gal, 2017; Chen et al., 2020). These models represent the weights as probability distributions rather than fixed values. The weights are treated as random values with prior distributions. After observing the data, the prior distributions are updated using Bayes' rule to obtain a posterior. The posterior can be used to make predictions, predicting a probability distribution rather than a fixed estimate. The spread of this final distribution indicates the uncertainty of the model.

Nix & Weigend (1994) suggested a different approach, initially designed for regression tasks. Their strategy was to use a non-bayesian network with two output heads. One predicts the target mean μ , and one predicts the variance σ with the variance capturing the heteroscedastic aleatoric uncertainty of the model. The model will learn to predict the variance indirectly with the loss function, with erroneous predictions getting punished less if the predicted variance is high. When using a sampling softmax method and a different loss function, this approach can also be used for classification (Kendall & Gal, 2017).

A different method of capturing predictive uncertainty involved deep ensembles (Lakshminarayanan et al., 2017). The core idea behind deep ensembles is to have multiple models, each trained independently on the same dataset. The variance between the different models can then be used to estimate the uncertainty. The variance reflects the level of disagreement between the models, which can be used to measure the overall uncertainty.

Monte Carlo Dropout is another method for predicting uncertainty (Gal & Ghahramani, 2016). This method sets random weights to zero, canceling out their contribution. Multiple passes will be done with random dropouts, resulting in an output distribution with which it is possible to calculate the uncertainty.

These methods can all quantify uncertainty, each with its strengths and weaknesses. These methods can all answer the question of how uncertain a model is. However, they cannot answer why the model is uncertain and where this uncertainty comes from. Knowing the source of uncertainty can be very useful in real-time applications. For example, an unusually high source of uncertainty from one sensor can indicate that the sensor in question is faulty and must be replaced. Without this localization of uncertainty, this may have been overlooked, which could have affected the model's performance. An approach to localizing such sources of uncertainty is introducing methods of Explainable AI. By calculating the model's Shapley Values, the features' contribution to the uncertainty can be approximated (Merrick & Taly, 2020). Ultimately, a cluster of features with a high contribution to the uncertainty is a source of uncertainty.

1.3 Error-related potentials

The medical field stands to greatly benefit from the quantification of uncertainty, especially in tasks of great importance and significance, such as medical diagnoses. However, data collection methods in this field, such as an electroencephalogram (EEG), are highly susceptible to noise. EEGs involve placing electrodes on the scalp to detect the small electric signals originating from the brain's neurons. They provide a high temporal resolution, allowing researchers to study various aspects of the function of the brain, such as cognitive processes. However, due to the sensitive nature of this method, it introduces various sources of noise and interference. For example, small interferences, such as the frequencies originating from the AC powerlines and physiological artifacts like blinking and muscle movements, can contaminate the recorded signals, posing a challenge for accurate analysis.

A common use for the analysis of EEGs is the field of Brain-Computer Interfaces (BCIs). These systems use the brain's electrical activity to extract intention from a user and translate it into computer instructions. These systems are helpful in fields such as neuroprosthetics, where the user's intent can be translated into the movements of said prosthetic. Recently, Error-Related Potentials (ErrP) have become a topic of interest within this field. An ErrP signal is a response to error percep-

tion after feedback. These signals spark interest for BCIs since they indicate an erroneous extraction of intention, in which case the system can reconsider the translated action. Alternatively, the erroneous episode can be used as a training example to improve future performance.

Two crucial channels for studying Error-Related Potentials are FZc, located at the midline frontal scalp, and Cz, located at the midline central scalp. ErrPs exhibit a characteristic waveform as seen in figure 2.1, typically showing a negative peak at around 200ms after the erroneous event, followed by a positive peak at approximately 300ms.

Previous research has shown promising results in predicting ErrP signals (Correia et al., 2021). Specialized machine learning architectures designed explicitly for EEG signals have been designed and can be used for these tasks (Lawhern et al., 2018). This model, and most other models for classifying EEGs, are Convolutional Neural Networks (CNNs). A CNN uses convolutional layers designed to capture local patterns in the input data while pooling layers help reduce dimensionality and extract import features. In the context of EEGs, they can learn discriminateive representations directly from the raw EEG data, allowing them to classify and detect specific patterns. They have shown excellent accuracy in various EEG-based tasks such as braincomputer interfaces (Cecotti & Graser, 2010) and seizure detection (Zhou et al., 2018).

1.4 Proposed method

This paper proposes a multi-headed Convolutional Neural Network classifying EEG signals on Error-Related Potentials. The proposed model has two output nodes. One outputting the classification label and one outputting an estimate of the model's uncertainty associated with that classification. This model will be tested on the Monitoring Error-Related Potential dataset (Chavarriaga & Millán, 2010), to which artificial noise is added to challenge the model's ability to predict uncertainty. Furthermore, this model will be paired with a method from Explainable AI called Shapley values to approximate the contribution of features to the uncertainty prediction. Using this method, we test whether it is possible to use Explainable AI to locate the source of the artificial noise.

2 Methods

2.1 Dataset

The data used for this paper originates from the 'Monitoring error-related potentials' dataset, created by Chavarriaga & Millán (2010). This dataset is publically available on the BCNI Horizon 2020 project website. For this experiment, users were placed in front of a screen where they had to observe a moving cursor. The working area of the screen consisted of 20 locations along the horizontal plane. A coloured square would appear on the cursor's left or right side. This square indicates the target the cursor should move towards. At each trial, the cursor would move along the horizontal axis towards the target. Once the target has been reached, the cursor will stay in place, and a new target will appear along the horizontal plane, no more than three positions away from the cursor.

During the experiments, users were asked to solely monitor the agent's performance, knowing the goal of reaching the target. They had no control over the cursor. At each trial, there was a 20% chance for the cursor to move in the opposite direction relative to the target, which contradicts the agent's goal. These trials indicate a different outcome than the participant anticipated for, to induce an Error Related Potential signal.

Six users participated in this experiment, each performing two separate recording sessions. Each session consisted of 10 blocks, of 3 minutes each. Each block consisted of approximately 50 trials. The EEGs were recorded at a sampling rate of 512 Hz.

Since the participants have no control over the cursor, fewer signals originating from the motor complex are present in the EEG signals, reducing the number of artifacts. However, the lack of physical movements, and the need for constant attention, also makes it easier for participants to lose focus and start mind wandering. This would create the risk of participants not properly observing the screen and thus not properly inducing an ErrP, leading to invalid labels.

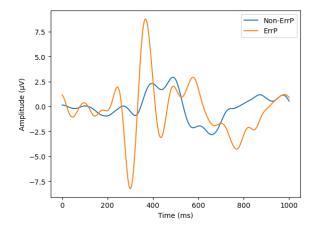


Figure 2.1: The average non-ErrP and ErrP signal on the FcZ channel. These signals originate from subject 1 during session 1.

2.2 Preprocessing

2.2.1 Filtering

EEG data is very prone to noise originating from its environment. One such example is the frequencies originating from the power line. To reduce this noise, the raw data is fed through a Butterworth filter with a bandpass for the range [1, 10] Hz.

2.2.2 Labeling

The used dataset contained six different labels for trials. Two labels indicate that the cursor moved towards the target, which will be labeled as a 'non error-related potential'. Two other labels indicate that the cursor moved in the opposite direction compared to the target. These are labeled as 'error-related potentials'. In the remainder of this paper, these two labels will be referred to as ErrP and non-ErrP signals. The two remaining raw labels are ignored.

2.2.3 Epoching

Figure 2.1, aswell as previous research on ErrP signals (Lopes-Dias et al., 2021; Omedes et al., 2015) shows that the most considerable difference between ErrP and non-ErrP signals occurs between 200 and 500 milliseconds after the feedback presentation. For this reason, the window size will be 600ms to capture these differences between signals.

Previous findings by Correia et al. (2021) also show that this size results in the best accuracy.

This window size results in the input EEG data being a matrix of size 64×308 . The number of rows is the 64 channels of the EEG, and the number of columns is the length of the windows, 600 ms of a 512 Hz sampling rate.

The decision to feed all 64 channels into the model was made for two reasons. First, previous experiments have shown that feeding all channels instead of pre-selecting electrodes consistently resulted in higher accuracy (Correia et al., 2021). Second, the main aim of this research is to study uncertainty. Using all channels could present more exciting results concerning the amount and origin of uncertainty instead of only using a select amount of channels.

2.2.4 Balancing

Due to the nature of the experiment of the used dataset, the data is inherently unbalanced with a 1/5 ratio. Only 20% of the trials are ErrP trials. Rebalancing is necessary to prevent the model from predicting all input episodes as non-ErrP. The under-represented class ErrP is over-sampled in the training set until the two classes are represented equally.

The dataset split for the model's training, validation and testing was carefully considered to stick as close as possible to the real-world application of these classifiers. One participant is put aside for the testing set, and the remaining five participants will be used for training. Furthermore, 20 trials are randomly sampled from the training set to be used as a validation set. This results in approximately 66.7% of the data being used for training, 16.7% for validation, and 16.7% for testing, with the latter being a participant the model has not yet seen in training and validation.

2.3 Model

The model used for this paper was created using PyTorch Lightning, a machine learning framework for the Python programming language (Falcon, 2019).

2.3.1 Model architecture

The main body of the model architecture consists of a model called EEGNet, a compact convolutional network tailored explicitly for BCI EEG classification (Lawhern et al., 2018). This model consists of two distinct sequential blocks.

The first block consists of two convolutional steps in sequence. The first layer applies F_1 convolutional filters of size (1, 64), which capture the EEG signal at different band-pass frequencies. Setting F_1 to half the sampling rate allows for capturing frequency information at 2Hz and above. Next, a Depthwise Convolution is applied to learn a spatial filter. After each convolutional layer, batch normalization is applied. Next, an exponential linear unit (ELU) is applied, followed by a Dropout layer to help regularize the model. Lastly, an average pooling layer is used to reduce the sampling rate to a quarter of the original sampling rate.

The second block consists of a Separable Convolution, which is a Depthwise Convolution followed by F_2 Pointwise Convolutions. These convolutions help reduce the number of parameters to fit and explicitly decouple the relationship across feature maps. This operation separates the learning of how to summarize individual feature maps in time from how to combine these feature maps optimally. An Average Pooling Layer follows this block to reduce the free parameters in the model.

In the original model, inputs are passed through the two blocks sequentially, followed by a flattened layer. These blocks are followed by a linear layer, which gives the logits of the model's prediction. This output layer is where our model differs from the original mode. Rather than having only one layer returning the classification logits, our model uses two output layers called heads. The first head is a linear layer returning the logits representing the mean of the prediction. The second head is a linear layer followed by a softplus layer. This head returns logits representing the variance of the model. The softplus layer is necessary to make the variance positive.

2.3.2 Sampling softmax

The goal is to capture heteroscedastic aleatoric uncertainty in the model. Currently, the model predicts two vectors. One contains the prediction of the mean of both classes. The other contains the prediction of the variance of both classes. Normally, the output logits would be passed through a softmax to calculate the probabilities of each class. However, our model outputs a Guassian logit, with a mean and variance. To convert these Gaussian logits to class probabilities, we use a method called Sampling Softmax. With this method, we interpret the output mean and variance as a Gaussian distribution:

$$\hat{x}|w \sim \mathcal{N}(f^w, (\sigma^w)^2) \tag{2.1}$$

$$\hat{p} = Softmax(\hat{x}) \tag{2.2}$$

Here, f^w is the output of the mean head with parameters w. σ^w is the output of the variance head with parameters w. The prediction consists of f^w , which is sampled from a Gaussian distribution with mean w^w and variance of σ^w . This vector is then squashed with the Softmax function to obtain a vector of probabilities.

Ideally, an analytical integral should be taken from this Gaussian Distribution. However, no such solution exists to achieve this. Therefore, an approximation of the integral has to be made. This approximation is achieved through Monte Carlo integration. Here we sample from the aforementioned normal distribution and apply the softmax function to each sample. Using these samples, we can calculate the mean and variance.

2.3.3 Loss function

This used architecture raises a question. How can we find the optimal model parameters θ , which results in the most accurate predictions of the mean while simultaneously predicting a variance capturing the aleatoric uncertainty? The loss function should allow the model to reduce the received loss by predicting a high variance on incorrect predictions. However, it is undesirable if the model predicts high variance on all input sequences and thus needs to be punished for predicting high uncertainty on correct predictions. One may ask how this can be achieved. Previous research by Seitzer et al. (2022) found such a method to achieve this desired behavior. This method is called β -NLL:

$$\mathcal{L}_{\beta-NLL} := \underset{X,Y}{\mathbb{E}} \left[\lfloor \hat{\sigma}^{2\beta}(X) \rfloor NLL \right]$$
 (2.3)

Here, the $\lfloor . \rfloor$ indicates the stop gradient operator. This operator makes $\hat{\sigma}^{2\beta}(X)$ act as a learning rate, which is dependent on the variance prediction. If β is set to 0, the loss function behaves like a normal NLL loss. If the value is set to 0.5, interesting behaviour is observed. Now, all data points are weighted down by $\frac{1}{\sigma}$ (inverse standard deviation instead of inverse variance). Experiments by Seitzer et al. (2022) showed that $\beta=0.5$ achieved the best balance between accuracy and log-likelihood.

To find the optimal model parameters θ , the negative log-likelihood (NLL) is used:

$$NLL := \frac{1}{2} \log \hat{\sigma}^2(X) + \frac{\mathcal{L}_{\theta}}{\hat{\sigma}^2(X)}$$
 (2.4)

This loss measures the discrepancy between the predicted and target distributions, assuming a Gaussian distribution with mean μ and variance σ^2 . Here, the left term $\frac{1}{2}\log\hat{\sigma}^2(X)$ acts as a normalization factor for the NLL loss, which ensures the model learns to predict the best possible mean and variance parameters for the given data. In the right term, \mathcal{L}_{θ} is the loss function used nested in the NLL loss. This loss is divided by $\hat{\sigma}^2(X)$. By dividing this loss by the variance, we ensure that the NLL loss is sensitive to the accuracy of the predicted mean μ and the uncertainty estimation encoded in the predicted variance σ^2 , a higher uncertainty estimation, results in a higher dividing factor, and thus a lower loss. The first term ensures the model does not always predict a high σ^2 .

In the original paper, the task was a regression task, and the used loss function \mathcal{L}_{θ} was the mean squared error loss (MSE). In our case, the task at hand is a classification task. For this, we will use the Binary Cross Entropy loss (BCE):

$$\mathcal{L}_{\theta} := -(Y \log \hat{\mu}(X) + (1 - Y) \log(1 - \hat{\mu}(X)))$$
 (2.5)

The BCE loss measures the difference between the variable's predicted probability distribution and the variable's true probability distribution. The first term in this function, $Y \log \hat{\mu}(X)$, punishes the model when it predicts a low probability $\mu(X)$ for the positive class. Similarly, the second term punishes the model when it predicts a high probability for the negative class. These two terms ensure that BCE loss penalizes the model for incorrect predictions.

The combination of these three elements allows β -NLL to ensure that the model learns to predict an optimal mean μ and variance σ^2 , capturing the aleatoric uncertainty of the model.

2.4 Explainable AI

To understand what our model is doing and explain where the uncertainty originates from, we need to introduce a method of Explainable AI to our model. For this, a method based on Shapley values will be

Shapley values are a concept originating from the cooperative game theory field. They provide a way of allocating a value generated by a group of players to each player. This strategy has been widely adapted to the field of machine learning. They attribute each input feature's contribution to the model's final prediction. This resulting attribution method is called SHAP (SHapley Adaptive exPlanations)

The key idea behind SHAP values is to decompose the model's output into the contribution of each input feature while also considering their relations with the other features. Exact calculations are practically impossible to calculate for larger inputs. Instead, the SHAP values are calculated by approximation. This algorithm involves sampling a subset of the features and computing the SHAP values for each sample. The final values are then averaged over all samples to estimate the feature importance.

The advantage of using the SHAP approach is its flexibility and generality. They can be applied to various models, including classification tasks. Moreover, they provide a rich and interpretable representation of the model's behaviour. Another advantage of SHAP values is that we can differentiate between the two heads. Using SHAP, we can build an understanding of how each feature contributed solely to the mean prediction and how they contributed solely to the variance prediction. The latter is of high interest in explaining the origins of the uncertainty.

2.5 Experiment design

To test the uncertainty quantification of the model three experiments were conducted. The first experiment aims at measuring the impact of overall noise

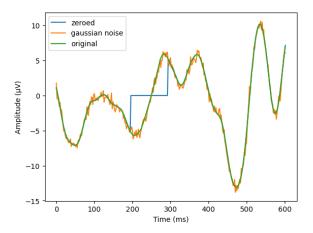


Figure 2.2: FcZ signal with artificially introduced Gaussian noise and localized zeroing.

on the predictive uncertainty. The second experiment expands upon this and tests whether the location of the noise effects the predictive uncertainty. Lastly, the final experiment attempts to use DeepLift to identify the location of the artificially added noise that induce uncertainty.

2.5.1 Artificial noise

To properly test whether our suggested approach captures aleatoric uncertainty, we need a method of artificially introducing noise to our data to invoke this uncertainty. Optimally, in the bane of BCIs, we would like to add noise to the data, which frequently occurs on EEG data. However, artificially adding physiological artefacts, such as muscle movements, is beyond our reach and could be an exciting topic for further research. For this paper, we keep the artificial noise simple. The first method of artificial noise generation is adding Gaussian noise to our data. Each data point, within the desired range, will receive noise sampled from a Gaussian distribution of varying intensity. The second method of applying artificial noise is designed to simulate faulty or improperly connected sensors. This method will set a random amount of data points to zero within a specific range.

Figure 2.2 shows an example of artificially generated noise. The green signal is the original FcZ signal, whereas the orange signal has artificially introduced Gaussian noise across the entire signal, with a standard deviation of 0.5. The blue signal

shows an artificial local zeroing between 200 and 250 ms.

2.5.2 Experimental setup

Each experiment uses the same hyperparameters optimal for EEGNet, suggested by Lawhern et al. (2018). Each training run will last for 50 epochs. This amount showed to be a good balance between performance and computational time. Each training session is averaged over a total of six runs. Each run uses a different participant as the test participant. The training was done using an NVIDIA GTX 1070 and took around 30 minutes per training session of six runs with 50 epochs each.

2.5.3 Effect of general noise

The first experiment adds noise to the entire input length, increasing the noise amount and intensity with every training session. It is expected that the addition of noise should result in a higher overall uncertainty compared to the clean data. The increase in the amount and intensity of the noise between training sessions is also expected to increase the predicted uncertainty between these sessions.

This experiment will accompany a test where labels are shuffled with increasing intensity. Here it is also expected that the uncertainty increases linearly with the number of shuffled labels.

2.5.4 Effect of localized noise

The second experiment will test whether the location of the added noise affects the predicted uncertainty. Two training sessions will be completed here, each with a different input data section corrupted. Both sections have an equal length and intensity of noise. One section will be located on the area with the most contribution to input data, which will be located using the SHAP approximation on the mean head. The second location will be an area with the most minor contribution to the output. Adding noise to the high-contribution areas is expected to result in a more substantial increase in uncertainty than adding noise to the low-contribution areas.

2.5.5 Tracable noise

For the final experiment, we test whether we can trace the uncertainty through the SHAP approximation. Here, we add localized noise to some regions of the input data. Afterwards, the SHAP approximation is taken and compared to the SHAP approximation of the original input data. We expect that a shift in the SHAP values is noticeable. Ultimately, the area where we added noise should have higher uncertainty than the other areas and can be located by plotting the SHAP values.

3 Results

3.1 Base variance predictions

Figure 3.1 shows a histogram with the variance distribution on correct and incorrect predictions. From this histogram, one can observe that the model's classification is almost always correct when it is paired with a low variance prediction. The higher the model's predicted variance becomes, the more often the classification is incorrect. Although the two histograms overlap, there is a clear skew towards higher variances for the incorrect predictions. On the highest variance predictions ranging from 0.24 to 0.25, the distribution between correct and incorrect classifications is nearly equal, indicating that the model is randomly guessing the classification.

3.2 General noise

Figure 3.2 shows the effect of shuffling the labels of training and testing data on the model's predicted variance. Here, it is clear that there is an increase in variance as more labels in the training and testing set are shuffled. However, this difference is not very large, as there is only an increase of approximately 0.027, with relatively high variance between runs. However, the overall increasing behavior of the variance's head output is as expected. It indicates that the model is working as intended and is predicting the variance based on the quality of the input.

Figure 3.3 shows two measurements of the model. The two leftmost plots show the predicted variance of the model, whereas the two rightmost plots show the model's accuracy. The top plots show the behavior when Gaussian noise is added to the entire

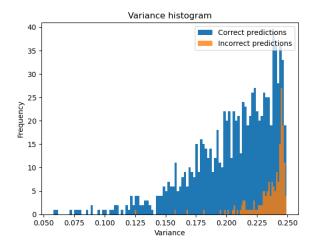


Figure 3.1: Histogram with the frequencies of variance predictions for correct and incorrect predictions.

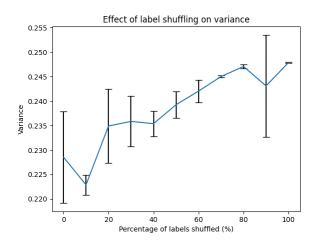


Figure 3.2: The effect of label shuffling on the output of the variance head.

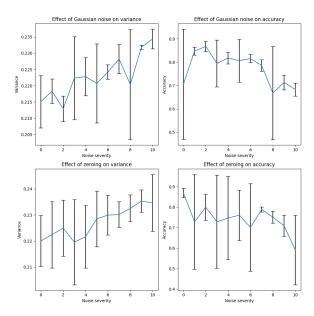


Figure 3.3: The effect of different intensities of artificial noise added to the entire signal length on the model's accuracy and variance.

length of the signal, whereas the bottom plots show the behavior when channels are entirely zeroed. The x-axis here represents the **severity**, which indicates the strength of the noise. Higher values indicate that the added noise is of higher magnitude (in the case of Gaussian noise), occurring in more channels per episode and affecting more episodes in general.

As can be seen from these plots, there is a clear increase in the predicted variance as the severity of the noise increases. This increase is present for the Gaussian noise and zeroing methods. Secondly, there is a clear decrease in accuracy as the severity of the noise increases. This behavior is also present for both types of noise. However, like the previous experiment, it is paired with a high variance between runs.

3.3 Localized noise

Figure 3.4 shows the influence of the location to which the noise has been added on both the variance and accuracy of the model. The leftmost plots show the predicted variance of the model, whereas the rightmost plots show the model's accuracy. The top plots show the behavior when Gaussian noise is

added to the data, whereas the bottom plots show the behavior when channels are zeroed. The left-most column shows the effect of the noise being added on the 0-250ms region, whereas the right-most column shows the effect of the noise being added on the 250-500ms region.

As can be observed from these plots, the general trend for both models is that the variance is higher when noise is added to the 250-500 ms region than the 0-250 ms region. The accuracy is slightly lower when the noise is added to the 250-500 ms region than the 0-250 ms region. It also observed that zeroing has a stronger effect on the variance and accuracy than Gaussian noise. This behavior is according to expectation since a Gaussian noise corrupted signal still resembles the original signal to some extent, regardless of the degree of Gaussian noise. Moreover, when averaging many signals corrupted with Gaussian noise, the noise will balance each other out. In contrast, the zeroing of signals does not resemble the original signal. The observation that noise on the 250-500 ms region substantially influences the accuracy and variance compared to the 0-250 ms region is as expected, as previous research showed that the most prominent part of the ErrP signal occurs within this window.

However, the differences between these two regions in accuracy and variance are minimal and are similar to the previous experiments, paired with high variance between runs.

3.4 Tracable noise

Figure 3.5 shows the single-dimensional heatmaps of the Shapley values of the predictions of the variance head. Here, the Shapley values are depicted as a continuous color palate referring to the contribution of the data points. Lighter colors (yellow) indicate a strong positive contribution to the prediction, and darker colors (blue) indicate a strong negative contribution to the variance prediction. Here, the Shapley values are averaged over all channels.

Comparing these single-dimensional heatmaps yields various observations. Firstly, there is a noticeable difference between the Shapley values of the original signals and the signals with artificial noise added to them. In the case of the Gaussian Noise variant, it is clear to which area the noise has been added due to the oscillating behavior of the Shapley values. This oscillating behavior originates

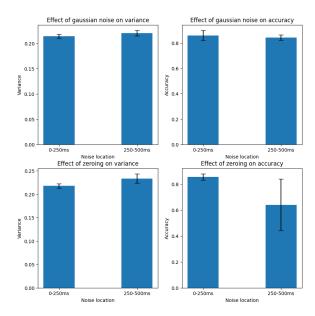


Figure 3.4: The effect of strong noise added to two different regions of the signal on the accuracy and variance of the model. The two regions tested are the ranges of 0ms to 250ms and 250ms to 500ms.

from the Gaussian noise adding large differences between adjacent data points. This oscillating behavior will most likely disappear when computing and averaging the Shapley values over more episodes since the noisy signal will average to the original signal. However, the computational cost of approximating these Shapley values is very high. Thus this plot only shows an average of 10 test episodes. When ignoring this oscillating behavior and judging only from the contribution distribution, one cannot find the location of the noise present in the signal. The contribution distribution between the data with noise on the 0-250ms and 250-500ms regions is nearly indistinguishable.

As for the signal with the artificially zeroed channels, much of the same behavior is present. There is a clear distinction between the Shapley values of the original and modified signals. In this case, there is a noticeable difference between the two noisy signals, and in the case of the zeroing being added to the 0-250ms region, a higher contribution to the variance is present in this region. However, this behavior is unclear on the signal zeroed on the 250-500ms region.

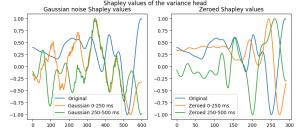


Figure 3.5: Plot with the Shapley values of the various signals. The left plot holds the Guassian noise signals, and the right plot holds the zeroed signals. All values have been normalized to the range of -1 to 1

4 Discussion

In this section, the results of the experiments, as mentioned earlier, will be discussed, and problems with the current experimental setup and points for improvement, as well as opportunities for further research, will be addressed.

4.1 Uncertainty quantification

The results from the first experiment, as seen in figure 3.1, showed that the model predicts high variance on incorrect classifications, with the highest variances pointing towards random guessing of the model. This observation allows for an interesting implementation of a sanity check for the model. This applies not only to these specific EEG classification models but to classification models in general. Moreover, it can even be extended beyond classification tasks when using a different noisecapturing method. One could put a threshold on the maximum variance, which is allowed in a prediction. All classifications with a predicted variance below this threshold are accepted, whereas all classifications with a variance exceeding this threshold are rejected. This method can drastically improve the accuracy of the model. However, this does come at the cost of rejecting some classifications, which would have to be resolved manually. This can be a worthwhile trade-off for classification tasks in which false positives and negatives must be avoided at all costs, such as medical classifications and diagnoses.

The experiment in which the labels were shuffled (Figure 3.2) showed an increase in the predicted variance as the percentage of labels shuffled increased. In the general noise experiment (Figure 3.3), it was observed that the addition of noise, in the form of Gaussian noise and the zeroing of channels, on the entire length of the signal results in an increase in variance. These two experiments indicate that the model behaves as expected, actively basing its variance prediction on the data quality and captures the artificially added noise as uncertainty in the variance output head.

The results from the localized noise experiment, seen in figure 3.4, show that the noise location affects the predicted variance, with noise on the 250-500ms region resulting in higher variance and lower accuracy than noise on the 0-250ms region. However, this difference is small. Smaller than one might expect, with the majority of prominent features of the ErrP signal being located in this region. However, previous research shows that this small difference was to be expected. Experiments with varying lengths of the input windows showed that there was only a 6% increase in accuracy when increasing the window from 300ms to 600ms after the event's presentation (Correia et al., 2021). Thus, the model was already capable of predicting the label reasonably accurately. However, the slight difference in accuracy and variance between noise in the two regions does suggest that the model shifts its attention to the 250-500 ms region when it has access to it since noise in this range has a stronger effect. This behaviour aligns with the expectations of this region's prominent features of the Error-related potential.

From the localized and global noise experiment, one can observe that the type of noise added to the signal matters in the variance and accuracy of the model. This behaviour is to be expected. Zeroing has a larger effect since the zeroed signal does not resemble the original signal, and thus the original signal cannot still affect the model. In Gaussian noise, the signal still resembles the original signal, regardless of the intensity of the noise. The original signal will still affect the model.

4.2 Uncertainty traceability

The results of the fourth and final experiment on the traceability of the noise using Shapley values shows, as seen in figure 3.5, that there is a clear difference between the original signals and the signals with artificially added noise. There is also a clear indication that the type of noise affects the resulting Shapley values. The point of highest variance is located in a different spot on the signals with Gaussian noise, compared to signals with zeroing. We can notice one very interesting behaviour from this, especially on the Gaussian noise signals. Interestingly, the peaks of the contribution of variance for the two noisy signals are both at the same location, which is noticeably different from the original signal. This similarity is unexpected. If the noise were to affect the contribution of the variance, one would expect the peaks to be different for the signals with noise in the 0-250ms region and for signals in the 250-500ms region. This is not the case. Moreover, if the noise did not affect the variance, the peaks would be the same as the original signal, which is also not the case. This same behaviour is also noticed on the zeroed signal but less extreme. This behaviour suggests that noise affects the feature contribution to the variance, but not in the way initially expected.

Regardless of this unexpected behaviour, the main goal of this paper is to see whether the location of the noise can be found from the Shapley values. For both signals, the variance on the 0-250ms region is higher when there is noise added to this region. However, this variance is still lower than observed in the original signals. On the 250-500 ms region, there is no increase in variance, with even a decrease in variance for the zeroed signal. Adding noise in different regions has a very inconclusive effect on the Shapley values.

Thus, one may notice from the Shapley values that a signal has been modified with artificial noise but cannot pinpoint the exact location of the source of uncertainty.

4.3 Experimental setup issues

As one may have noticed in this paper, the dataset consists of data from six participants. One may have also noticed that thus far, I have been training on the same participants (2-6) and testing on the same participant (1). This was done deliberately. EEG signals are prone to very high interparticipant variability. Due to this high variability and only having six participants, testing on all participants was not a viable choice due to the low consistency in results between participants. Due to this

high variance, it was impossible to gather concise results, and the difference between training sessions is much larger than the already quite large difference experienced with only one test participant.

The two methods of generating artificial noise, Gaussian noise and the zeroing of channels, used for the experiments are only rough simulations of noise and could be more realistic. The noise used in these experiments, which showed results are magnitudes higher than in real-life applications. A more realistic approach would be adding noise variants that are more common in EEG signals. One such approach would be the recreation of physiological artefacts, such as the signals originating from the motor complex for actions like blinking. This method drastically increases the experiment's complexity and is way beyond the scope of this research paper, but it could be interesting to research in the future.

For this experiment, I focused on a single model: EEGNet, developed by Lawhern et al. (2018). This model is a compact Convolutional Neural Network (CNN). However, this is one of many model architectures commonly used for EEG classification. One of these architectures which is commonly used is the Recurrent Neural Network (RNN). It might be possible that the localization of the noise can be achieved when using the other architectures since they observe and train from the data in different ways, and thus can be interesting research for the future.

References

- Cecotti, H., & Graser, A. (2010). Convolutional neural networks for p300 detection with application to brain-computer interfaces. *IEEE transactions on pattern analysis and machine intelligence*, 33(3), 433–445.
- Chavarriaga, R., & Millán, J. d. R. (2010). Learning from eeg error-related potentials in noninvasive brain-computer interfaces. *IEEE transactions on neural systems and rehabilitation engineering*, 18(4), 381–388.
- Chen, W., Zhang, B., & Lu, M. (2020). Uncertainty quantification for multilabel text classification. Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery, 10(6), e1384.

- Correia, J. R., Sanches, J. M., & Mainardi, L. (2021). Error perception classification in brain-computer interfaces using cnn. In 2021 43rd annual international conference of the ieee engineering in medicine & biology society (embc) (pp. 204–207).
- Falcon, W. A. (2019). Pytorch lightning. GitHub, 3.
- Gal, Y., & Ghahramani, Z. (2016). Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In *international conference on machine learning* (pp. 1050–1059).
- Kendall, A., & Gal, Y. (2017). What uncertainties do we need in bayesian deep learning for computer vision? Advances in neural information processing systems, 30.
- Lakshminarayanan, B., Pritzel, A., & Blundell, C. (2017). Simple and scalable predictive uncertainty estimation using deep ensembles. Advances in neural information processing systems, 30.
- Lawhern, V. J., Solon, A. J., Waytowich, N. R.,
 Gordon, S. M., Hung, C. P., & Lance, B. J.
 (2018). Eegnet: a compact convolutional neural network for eeg-based brain-computer interfaces.
 Journal of neural engineering, 15(5), 056013.
- Lopes-Dias, C., Sburlea, A. I., Breitegger, K., Wyss, D., Drescher, H., Wildburger, R., & Müller-Putz, G. R. (2021). Online asynchronous detection of error-related potentials in participants with a spinal cord injury using a generic classifier. *Journal of Neural Engineering*, 18(4), 046022.
- Merrick, L., & Taly, A. (2020). The explanation game: Explaining machine learning models using shapley values. In *Machine learning and knowledge extraction:* 4th ifip to 5, to 12, wg 8.4, wg 8.9, wg 12.9 international cross-domain conference, cd-make 2020, dublin, ireland, august 25–28, 2020, proceedings 4 (pp. 17–38).
- Nix, D. A., & Weigend, A. S. (1994). Estimating the mean and variance of the target probability distribution. In *Proceedings of 1994 ieee international conference on neural networks (icnn'94)* (Vol. 1, pp. 55–60).

- Omedes, J., Iturrate, I., Minguez, J., & Montesano, L. (2015). Analysis and asynchronous detection of gradually unfolding errors during monitoring tasks. *Journal of neural engineering*, 12(5), 056001.
- Seitzer, M., Tavakoli, A., Antic, D., & Martius, G. (2022). On the pitfalls of heteroscedastic uncertainty estimation with probabilistic neural networks. arXiv preprint arXiv:2203.09168.
- Yoo, H.-J. (2015). Deep convolution neural networks in computer vision: a review. *IEIE Transactions on Smart Processing & Computing*, 4(1), 35–43.
- Zheng, W.-L., & Lu, B.-L. (2015). Investigating critical frequency bands and channels for eegbased emotion recognition with deep neural networks. *IEEE Transactions on autonomous mental development*, 7(3), 162–175.
- Zhou, M., Tian, C., Cao, R., Wang, B., Niu, Y., Hu, T., ... Xiang, J. (2018). Epileptic seizure detection based on eeg signals and cnn. Frontiers in neuroinformatics, 12, 95.