Uncertainty Detection in EEG Neural Decoding Models

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Abstract

EEG decoding systems based on deep neural networks have been widely used in decision making of brain computer interfaces (BCI). Their predictions, however, can be unreliable given the significant variance and noise in EEG signals. Previous works on EEG analysis mainly focus on the exploration of noise pattern in the source signal, while the uncertainty during the decoding process is largely unexplored. Automatically detecting and quantifying such decoding uncertainty is important for BCI motor imagery applications such as robotic arm control etc. In this work, we proposed an uncertainty estimation model (UE-EEG) to explore the uncertainty during the EEG decoding process, which considers both the uncertainty in the input signal and the uncertainty in the model. The model utilized dropout oriented method for model uncertainty estimation, and Bayesian neural network is adopted for modeling the uncertainty of input data. The model can be integrated into current widely used deep learning classifiers without change of architecture. We performed extensive experiments for uncertainty estimation in both intra-subject EEG decoding and cross-subject EEG decoding on two public motor imagery datasets, where the proposed model achieves significant improvement on the quality of estimated uncertainty and demonstrates the proposed UE-EEG is a useful tool for BCI applications.

Our code repository is publicly available on https://github.com/tiehangd/UE-EEG

Index terms— Uncertainty Estimation, Model Calibration, Motor Imagery EEG Decoding, Brain Computer Interface

1 Introduction

Brain computer interfaces (BCI) aim to control computers and robots by directly monitoring human brain activities [1]. A common way to record such signals is to use the Electroencephalography (EEG) equipments, which have the advantage of being non-invasive, high temporal resolution and relatively low acquisition cost. Motor imagery EEG signal, which records the activity of human brain during user imagined movements, is currently being actively explored given their wide applicability for motion restoration of disabled people [2], neurorehabilitation [3] and gaming control [4].

Decisions made by BCI systems are based on EEG signal. However the EEG signal is volatile and has significant variance across different subjects and even across different sessions for the same subject. Such variance are from two sources: 1) the noise oriented from the electrodes and the recording equipment, 2) the erratic nature of brain activity. The first source mainly contribute to the homoscedastic data noise, and the heteroscedastic data noise is mostly generated from the second source. For application of BCI systems, an additional challenge is the efforts involved in labeling data for a new user, resulting in limited number of data points and brings in undesired uncertainty when applying previously trained model classifier to a new user.

Quantifying the uncertainties of EEG decoding caused by such variance in source signal is important for motor imagery BCI applications. Gaining knowledge on when and to what extent the model is unsure about its decision helps mitigate hazard movements in BCI controlled robotic systems. Please note the estimated uncertainty can be very different from the predicted probability of an EEG decoder. Significant uncertainty can incur even when predicted probability of target class is much higher than the other classes, which is the case for out of domain input data such as EEG signal from a new user.

The prediction uncertainty come from two sources:
1) uncertainty in the input signal, which is known as data uncertainty or aleatoric uncertainty, indicates the noise in EEG electrodes and recording equipments, 2) model uncertainty or epistemic uncertainty, which originates from the uncertainty lying in model parameters [5]. Model uncertainty is significant when there is a distribution shift between the training data and testing data, this is often the case for EEG classification due to the pattern difference across subjects, or when the amount of training EEG data is limited due to the significant manual effort involved in data annotation.

In this work, we proposed an uncertainty estimation method for EEG neural decoding models (UE-EEG), with a focus on motor imagery BCI applications. The model quantify data uncertainty through light weight probabilistic neural networks, which encode the variance in input data into probabilistic distribution, and forward propagates the moments all the way to output through Assumed Density Filtering (ADF). ADF derived a probabilistic formulation of propagation for most of the operations in neural network such as convolution, pooling, relu etc. and is computationally effective in practice. For model uncertainty, UE-EEG performs estimation with drop-out similar to [6]. Unlike direct modeling of model parameters with probability distributions, dropout based approaches don’t need to change model architecture and also computation ally efficient in nature.

In summary, our contributions are mainly three-fold:

1) We formed an end to end framework to perform uncertainty estimation in EEG neural decoding systems with a computationally efficient and versatile method. The estimation method can be integrated into current widely used EEG neural decoders and don’t need changes in the model architecture.

2) We conducted detailed experiment on two public datasets. The proposed method shows significant improvement on the quality of estimated uncertainty, at the same time predictive accuracy is on par with the other models.

3) We perform interpretation analysis on the estimated uncertainty, and visualizes the influence of different factors towards the result.

2 Related Work

2.1 Uncertainty in EEG Source Signal

EEG signals are generated with electrodes monitoring brain activities such as rehearsal of a motor act for motor imagery tasks [7]. Proper decoding of its pattern allows it to be interpreted as control commands to devices such as wheelchair [8][9], robotic arms [10] and gaming gadgets [11]. The EEG signal has high noise level with sources of noise including environment, recording equipment, experimental error etc., and its pattern is also highly subject specific [12]. Previous works have conducted research on noise estimation and variation analysis in the source signal [13][14][15], with widely adopted noise estimation approaches include recursive least square filtering, discrete wavelet transform [16], and combination of adaptive filtering with discrete wavelet transformation etc. The corresponding noise mitigation approaches are also proposed including . The noise estimation are performed in the pre-processing stage of EEG signal, and to our knowledge the uncertainty involved in the decoding process is largely unexplored.

2.2 EEG Neural Decoding Models

EEG neural decoding models utilize different types of deep neural networks for EEG decoding and classification, e.g. [17] proposed a computationally efficient convolutional neural network (CNN) that is effective across different BCI platforms. [18] adopted a novel cropped training strategy for the CNN model and achieved state of the art performance. [19] come up with a cascade and parallel CNN architecture for improved performance. [20] utilized attentional mechanism on top of LSTM to effectively extract temporal features and achieved promising result. Compared to classic signal processing and machine learning approaches such as filter bank (FB) and common spatial pattern (CSP) [21], power spectral density decomposition (PSD) [22] etc., most deep neural network oriented approaches are over-parameterized and only produces deterministic results without uncertainty control in the process, which can leads to over-confident incorrect predictions and pose challenge for its deployment in real world EEG systems, with its unknown behavior towards factors such as generalization across different subjects, the fitting of confounders, and interpretability.
2.3 Uncertainty Estimation for EEG Neural Decoding Models

Uncertainty estimation is being actively explored in machine learning with important applications in fields such as auto driving and robotics [23][24][25]. The estimation is done either through Bayesian probabilistic approaches [26] or Monte-Carlo sampling based methods [23], with the uncertainty encoded in the posterior distribution of model prediction. The Bayesian probabilistic approach model the parameter of neural network with probabilistic distributions, based on which uncertainties are analytically computed [27]. Simplification and approximation is needed to make the computation tractable in the process [26][27]. The approach require modification of the network optimization process, and additional efforts is needed to integrate them into existing deep neural network architectures. Probabilistic light weight neural network [28] simplifies the previous models by adopting a partial probabilistic approach. The model requires minimal modification on existing networks, and proved effective for data uncertainty modeling while disregarding model uncertainty.

Monte-Carlo based approaches is another major trend for uncertainty estimation. Researchers have found existing techniques such as dropout [6] and ensemble models [23] could imply useful information on prediction uncertainty. Dropout base approaches [6][29] adopt dropout operation during test time for uncertainty estimation, which can be seen as modeling parameters in network to be Bernoulli distributed. Ensemble based approaches [23][30][31] estimates the posterior of model predictions by sampling on the differently trained neural networks. These Monte-Carlo based approaches effectively capture the uncertainty lies in model parameters.

These models have been used recently for uncertainty estimation in fields such as gravitational lensing of astrophysics [32], biomarker quantification [33] and diagnosis of kidney injury [34].

3 Method

The proposed model performs dropout operation on top of light weight probabilistic neural network to provide an accurate uncertainty estimation considering both uncertainty from signal and uncertainty from model parameters. We first introduce the modeling of each type of uncertainty below, then we derive the composition of overall decoding uncertainty from these two sources.

3.1 Uncertainty propagated from input signal

We take a probabilistic modeling approach of input uncertainty, and propagate the uncertainty through the neural decoder with assumed density filtering (ADF) [35][28]. We denote the underlying noise free signal with $\bar{x}$, and the noise corrupted input as $x$, which can be modeled with distribution

$$p(x|\bar{x}) = \text{normal}(\bar{x}; u)$$

where $u$ is variance depicting uncertainty in source signal.

The joint distribution of the hidden states in intermediate layers of decoder can be represented as

$$p(z^{(1:l)}) = \int_x p(x) \prod_{i=1}^{l} p(z^i|z^{i-1}) dx$$

with $z^0 = x$.

In assumed density filtering, the conditional probability is approximated as

$$p(z^i|z^{i-1}) = \text{normal}(\mu^i, v^i)$$

where the moments of the distribution are

$$\mu^i = \mathbb{E}_{p(z^{i-1})}[f(i)(z^{i-1})]$$

$$v^i = \nabla_{p(z^{i-1})}[f(i)(z^{i-1})]$$

where $f(i)$ is the function performed with the $i$th layer of the neural network. $\mathbb{E}_{p(z^{i-1})}$ and $\nabla_{p(z^{i-1})}$ are the first and second moments of the underlying distribution. Forward propagating with this recursive conditional probabilistic rule produces $\mu^i$ and $v^i$ for the final decoding layer, which corresponds to the network prediction and its corresponding variance.

The probabilistic propagation can be performed on common neural network structures such as convolutional layer, Relu activation layer, batchnorm layer and pooling layer etc., corresponding to the different $f(z)$ functions. The propagation rule outlined in eq. 4 and
eq. [5] can either be exactly derived or through probabilistic approximation. The convolutional layer performs linear operations in which \( \mu^i \) and \( \nu^i \) don’t correlate with each other, allowing straightforward calculation of the two terms in closed form. The Relu layer, although nonlinear in nature, also leads to closed form solutions as derived in [36]. Other types of operations, e.g. max pooling, requires probabilistic approximation for tractable computation, as detailed in [37][38]. Please note this ADF propagation don’t impose additional modification on the network structure. The number of parameters in the network also remains the same as its non-probabilistic counterpart. The only difference is that each layer receives the paired values (mean and variance) as input and also output the paired value to the next layer.

### 3.2 Uncertainty from model parameters

Given the randomness in the initialization and the training process of neural decoders, especially when amount of training data is limited, another source of uncertainty is brought in by the variation lying in model parameters. We model this source of uncertainty by performing dropout during testing, which is computationally efficient and easy to integrate into existing neural decoders.

Dropout can be seen as the sampling process with parameters are approximated as Bernoulli distributed. Denoting parameter distribution after training as \( P(W|X, Y) \), this approximation can be represented as

\[
P(W|X, Y) = \text{Bernoulli}(W; \phi) \tag{6}
\]

where \( \phi \) is the dropout rate. Binary variables are sampled out for each node in the network (except nodes of output layer). Each variable is 1 with probability \( \phi \), corresponding to the nodes retained during dropout. This process is performed during testing to estimate the resulting uncertainty on model output \( y^* \).

\[
v_m = \mathbb{E}_{p(y^*|x^*)}(y^*)^2 - (\mathbb{E}_{p(y^*|x^*)}(y^*))^2 \tag{7}
\]

where \( (x^*, y^*) \) is testing data and

\[
\mathbb{E}_{p(y^*|x^*)}(y^*)^2 = \frac{1}{T} \sum_{t=1}^{T} y^*(x^*, W^t) \tag{8}
\]

\[
\mathbb{E}_{p(y^*|x^*)}(y^*)^2 = \frac{1}{T} \sum_{t=1}^{T} y^*(x^*, W^t) \tag{9}
\]

\( T \) is the number of stochastic dropout forward passes for each test data point. The optimal dropout rate \( \phi \) minimizes the KL divergence between the approximated Bernoulli distribution and the underlying parameter distribution, previous work [25] has shown this is equivalent to maximizing the log likelihood when input and hidden states are normal distributed. We perform a grid search for \( \phi \) in the range of \([0, 1]\) in our experiment.

### 3.3 Estimating total uncertainty

The variance from model parameter becomes independent of variance from source signal with post-training parameter distribution \( p(W|X, Y) \) modeled as Bernoulli distributed \( q(W) \)

\[
v_{p(y|x)}(y) = \mathbb{E}_{p(y|x)}(yy^T) - \mathbb{E}_{p(y|x)}(y)\mathbb{E}_{p(y|x)}(y)^T
\]

\[
= \frac{1}{N} \sum_{n=1}^{N} v_n + \frac{1}{N} \sum_{n=1}^{N} \mu_n^2 - \bar{\mu}^2
\]

\[
= \frac{1}{N} \sum_{n=1}^{N} v_n + \frac{1}{N} \sum_{n=1}^{N} (\mu_n - \bar{\mu})^2
\]

\[
= v^d_{p(y|x)}(y) + v^m_{p(y|x)}(y) \tag{10}
\]

where \( N \) is the number of samples during test, \( \mu_n \) and \( v_n \) are from the ADF output, and \( \bar{\mu} = \frac{1}{N} \sum_{n=1}^{N} \mu_n \). The total uncertainty is derived as above when we use dropout for parameter variance estimation.

The overall workflow for estimating output uncertainty on an EEG classifier can be summarized into three steps:

(1) Train the classifier on EEG signals the same way as normal EEG neural decoders.

(2) Change the network into ADF propagation setting during test, and collect \( N \) samples \( \{\mu_i, v_i\}_{i \in [1...N]} \) with dropout rate \( \phi \).

(3) Compute predicted uncertainty based on eq. [10]

Different ways exist to estimate the noise level \( u \) in the input signal. Previously works either uses a user-defined constant [6] or estimate the noise level from the data [5]. Using a constant is computationally efficient,
but in general it is not easy to accurately get the prior information of input noise characteristics. Learning the input noise from data is able to reflect the change from different input sources and increases the model’s adaptation ability. However, its implementation requires tailored modification on the network architecture and hinders its application on existing classifiers. For applications in EEG signal analysis, the signal to noise ratio (SNR) is either available or can be readily computed with well developed techniques [14] [39], allowing us to make an accurate estimation on input variance $u$

4 Experiments

4.1 Dataset

We used two public BCI datasets in our experiment, which are BCI competition IV dataset 2a (abbreviated as BCI IV-2a below) [40] and high gamma dataset [18]. BCI IV-2a is relatively small and high gamma dataset contains a larger number of trials per subject. Details for each dataset is introduced below.

BCI IV-2a involves 9 subjects performing 4 class motor imaginary tasks. Each subject taking part in two sessions and each session consists of 288 trials. The tasks includes movement of left hand, right hand, both feet and tongue. Signals are recorded with 22 electrodes at 250Hz sampling rate. A training phase and an evaluation phase were recorded on different days for each subject.

High gamma dataset is originally recorded with 128 electrodes, and in our experiment, we used the 44 channels covering the motor cortex region, in accordance with [18]. 880 trials are performed on 14 subjects of balanced gender, with each trial consists of 4 seconds of recording on 4 classes of movement: left hand, right hand, both feet and tongue. The signal is recorded with a BCI2000 device and then downsampled to 250 Hz, which is the same as BCI IV-2a dataset and allows the same hyper parameter setting for both datasets.

4.2 Settings

We evaluated our uncertainty estimation model for both intra subject classification and cross subject classification. For intra subject classification, recording from the same subject are split between training and testing, and for the cross subject setting, we leave one subject out each time and model is trained on the remaining subjects. For recording of each trial, we break it down to segments with window size of 400, and a stride size of 50 between adjacent segments. The models are implemented with Pytorch [5] and runs on a single TITAN-V GPU. The models are fully trained for 40 epochs before evaluation, and we used Adam optimizer with learning rate set to 0.001. We performed dropout during testing to estimate the model uncertainty, and the dropout rate $\phi = 0.1$ is determined by grid search on 40 log range uniformly distributed rates lying between $[0, 1]$.

The EEG neural decoder used in our experiment is a 3 layer CNN network similar to EEGNet [17]. The first layer consists temporal convolution filters to learn frequency information, followed by batch normalization. The second layer involves depthwise convolutions with temporal specific spatial filters. Zero padding is done to maintain the original data dimension, after which batch normalization and dropout are applied. The third layer performs pointwise convolution. Its post processing is the same as the second layer. The prediction layer is a single fully connected layer followed by softmax operation.

4.3 Metrics and Baselines

We evaluated the model in terms of three different aspects: the quality of estimated variance, calibration and performance.

The quality of estimated variance is reflected by the Negative log likelihood (NLL) on the prediction, which is defined as $\text{NLL} = \frac{1}{2} \log(v) + \frac{1}{2b}(y - \bar{y})^2$. It is a major metric for measuring uncertainty [23] [6]. Higher values of NLL depicts lower confidence of capturing the ground truth based on predicted output, and vice versa.

Calibration metrics such as Brier score [41] and ECE score [24] measures the confidence of model output for classification tasks and is reported here in complement of NLL. Brier score computes the squared error between predicted logits and one hot label encoding, defined as $\text{BS} = K^{-1} \sum_{k=1}^{K} (t_k - p(y_k))^2$, where $K$ is the number of classes, $t_k$ are elements of one hot label encoding and $p(y_k)$ are the predicted logits. ECE
score is $L^1\ norm$ of the difference between predicted logits and accuracy. Please note the evaluation of Brier score and ECE score only depend on the predicted logits and don’t involve the estimated variance. Both Brier score and ECE score are proper scoring rules as defined in [42]. We also reported the accuracy and AUC-ROC score in our experiments to evaluate on the model’s prediction and study the relationship between the model’s performance and its predicted uncertainty.

We compared the UE-EEG model with several other models applicable to EEG uncertainty analysis. The method of Gal et al. [6] is the dropout oriented uncertainty estimation approach. The model of Kendall et al. [5] compute output uncertainty utilizing Bayesian neural network. The model proposed in [23] is a robust uncertainty estimation model based on ensemble method.

Table 1: Comparison of different uncertainty estimation methods for intra subject classification on BCI-IV 2a dataset. The reported results are averaged across 10 runs. The highest performance are bolded and the runner up method are marked with †. Quality of estimated variance are measured with NLL, on which the proposed model outperformed comparison methods by at least 28%. The model achieved either better or comparable result compared to other models in terms of calibration and prediction performance.

| Method         | Variance Estimation | Calibration | Performance |
|----------------|---------------------|-------------|-------------|
|                | NLL(↓)             | Brier(↓)    | ECE(↓)      | Acc(↑)      | ROC-AUC(↑) |
| Ensemble[23]   | 12.4               | 0.108       | 0.276       | 0.705       | 0.832      |
| BayesNet[5]    | 32.4               | 0.117       | 0.295       | 0.661       | 0.813      |
| Dropout[6]     | 7.45†              | 0.105†      | 0.271†      | 0.687       | 0.817      |
| UE-EEG (ours)  | 5.39               | 0.092       | 0.268       | 0.692†      | 0.824†     |

4.4 Results

We evaluate the uncertainty estimation model for both intra subject classification and cross subject classification on the two public datasets, with BCI-IV 2a dataset being relatively small and high gamma dataset considerably larger. Cross subject classification is a more challenging task compared to intra subject classification given the significant variability lies in the EEG signal across different subjects.

Table 2 shows the result for intra subject classification on BCI-IV 2a dataset. The proposed model outperformed comparison methods by at least 28% on NLL, which is the major metric to evaluate the quality of estimated variance. The proposed model achieved comparable performance on Brier score and ECE score compared to other models, which shows the model’s calibration is not significantly influenced by the different uncertainty estimation approaches. Ensemble oriented method [23] achieved slightly better result on accuracy and ROC-AUC, which can be attributed to the joint decision making of the mixture of models. The result on high gamma dataset with intra subject setting is reported in table 2 where the proposed model achieved a 44.8% improvement in terms of NLL. The models are better calibrated on high gamma dataset compared to BCI-IV 2a dataset, as reflected from the Brier score and ECE score. This is attributed to the lower noise level in its signal and also its larger dataset size allowing more thorough training.

We further evaluated the model performance under cross subject classification settings, and the results on BCI-IV 2a and high gamma dataset are reported respectively in Table 2 and Table 2. The accuracy and ROC-AUC sees a significant drop compared to their intra subject counterparts, as cross subject classification is a more challenging setting compared to intra subject classification. We also observed calibration error increase with the adoption of a more challenging task setting. NLL sees an evident increase compared to intra subject settings with the longer tailed output distribution yields reduced likelihood. For both datasets, the proposed model performs consistently better than the comparison methods in terms of variance estimation while calibrating to a similar degree as the other comparison models.

Table 2: Comparison of different uncertainty estimation methods for intra subject classification on high gamma dataset. Other experiment settings are kept the same as table 1.

| Method         | Variance Estimation | Calibration | Performance |
|----------------|---------------------|-------------|-------------|
|                | NLL(↓)             | Brier(↓)    | ECE(↓)      | Acc(↑)      | ROC-AUC(↑) |
| Ensemble[23]   | 1.16                | 0.069       | 0.205       | 0.873†      | 0.922†     |
| BayesNet[5]    | 2.75                | 0.074       | 0.217       | 0.865       | 0.908      |
| Dropout[6]     | 1.48                | 0.062†      | 0.179†      | 0.871       | 0.919      |
| UE-EEG (ours)  | 0.64                | 0.053       | 0.144       | 0.881       | 0.927      |

We explore the influence of individual channels towards the output uncertainty and compares it to the channel level influence on the prediction. The influence is quantified by adopting the occlusion based in-
Figure 1: Scalp topography heat maps visualizing the influence of individual channels on output prediction and uncertainty. The columns from left to right correspond to left hand, right hand, foot and tongue. Top row shows the influence on prediction and bottom row reveals the influence on uncertainty. Given the dynamic and volatile nature of EEG signals, the result is averaged across 20 runs.

Table 3: Comparison of different uncertainty estimation methods for cross subject classification on BCI-IV 2a dataset. Other experiment settings are kept the same as table 1.

| Method       | Variance Estimation | Calibration | Performance       |
|--------------|---------------------|-------------|-------------------|
|              | NLL(↓)  | Brier(↓) | ECE(↓) | Acc.(↑) | ROC-AUC(↑) |
| Ensemble[23] | 76.8      | 0.158      | 0.340   | 0.523   | 0.715     |
| BayesNet[5]  | 130.1     | 0.162      | 0.343   | 0.487   | 0.692     |
| Dropout[6]   | 68.7      | 0.153      | 0.331†  | 0.494‡  | 0.688     |
| UE-EEG (ours)| 46.5      | 0.156†     | 0.317   | 0.506†  | 0.695‡    |

Table 4: Comparison of different uncertainty estimation methods for cross subject classification on high gamma dataset. Other experiment settings are kept the same as table 1.

| Method       | Variance Estimation | Calibration | Performance       |
|--------------|---------------------|-------------|-------------------|
|              | NLL(↓)  | Brier(↓) | ECE(↓) | Acc.(↑) | ROC-AUC(↑) |
| Ensemble[23] | 1.66†    | 0.102     | 0.307   | 0.771   | 0.888†    |
| BayesNet[5]  | 2.87      | 0.107     | 0.284   | 0.768   | 0.879     |
| Dropout[6]   | 1.92      | 0.095†    | 0.267†  | 0.774‡  | 0.883     |
| UE-EEG (ours)| 1.24      | 0.086     | 0.251   | 0.796   | 0.894     |

To reveal the relationship between calibration and output uncertainty, we empirically analyzed the correlation between calibration error and negative log-likelihood (NLL). The relationship between NLL and Brier score are revealed in fig. 2a and fig. 2c for
Figure 2: The correlation between calibration and output uncertainty. The relationship of NLL and Brier score are revealed in fig. 2a and fig. 2c for BCI-IV 2a and high gamma dataset respectively. Fig. 2b and fig. 2d shows correlation between NLL and ECE score.

BCI-IV 2a and high gamma dataset respectively. The two metrics sees a positive correlation in general. Intuitively, lower Brier score indicates predicted $\hat{y}$ and ground truth $\bar{y}$ being closer to each other, contributing to NLL decrease. Fig. 2b and fig. 2d shows NLL and ECE score are largely uncorrelated.

The input noise of EEG source signal can be estimated based on signal to noise ratio (SNR) of the BCI system. Here we adopt a more accurate approach and estimate it by performing a grid search on a range of noise values, as previous study [25] proved NLL is minimized when the magnitude of assumed input noise matches the underlying ground truth. Result on the grid research for BCI-IV 2a and high gamma dataset is provided in Table 5 and Table 6 respectively. The input noise of BCI-IV 2a is estimated to have a magnitude of 0.1, and high gamma dataset is endowed with smaller noise magnitude of 0.01.

Table 5: Estimation of BCI-IV 2a input noise level through NLL

| Estimated Input Noise | 0.02 | 0.05 | 0.1  | 0.2  |
|-----------------------|------|------|------|------|
| NLL                   | 6.4  | 6.19 | 6.11 | 6.31 |

We further explores on the influence of number of samples collected during dropout on NLL. The result is shown in Table 7 for each of the experiment settings. The estimated NLL tend to converge with 150 samples for both BCI-IV 2a and high gamma dataset.

5 Conclusion

In this work, we proposed an effective method to estimate the uncertainty lying in EEG neural decoders. The proposed method considers both the noise from input electrodes and also the randomness lying in model parameters, allowing accurate modeling of the uncertainty in decoding decision. We performed detailed experiment on two motor imagery classification tasks, where it outperforms current state of the arts in terms of uncertainty estimation, and at the same time maintains predictive accuracy on par with the other models. The method can be readily integrated into existing BCI systems and helps gain knowledge on the reliability of the system.

References

[1] N. Padfield, J. Zabalza, H. Zhao, V. Masero, and J. Ren, “Eeg-based brain-computer interfaces using motor-imagery: Techniques and challenges,” Sensors, vol. 19, no. 6, 2019. [Online]. Available: https://www.mdpi.com/1424-8220/19/6/1423

[2] M. Tariq, P. M. Trivailo, and M. Simic, “Eeg-based bci control schemes for lower-limb assistive-robots,” Frontiers in Human Neuroscience, vol. 12, p. 312, 2018. [Online]. Available: https://www.frontiersin.org/article/10.3389/fnhum.2018.00312

[3] J. Cantillo-Negrete, R. I. Carino-Escobar, P. Carrillo-Mora, D. Elias-Vinas, and J. Gutierrez-Martinez, “Motor imagery-based brain-computer interface coupled to a robotic hand orthosis aimed for neurorehabilitation of stroke patients,” Journal of Healthcare Engineering, vol. 2018,
Table 7: Influence of different number of samples collected during dropout on NLL, the estimated NLL converges with 150 samples for both BCI-IV 2a and high gamma dataset.

| Num Samples | 25   | 50   | 75   | 100  | 125  | 150  | 175  | 200  |
|--------------|------|------|------|------|------|------|------|------|
| BCI-IV 2a intra | 174.7 | 75.9 | 27.4 | 7.09 | 5.97 | 5.74 | 5.66 | 5.39 |
| BCI-IV 2a cross | 2586.3 | 583.2 | 211.8 | 124.3 | 109.5 | 74.6 | 51.9 | 46.5 |
| High gamma intra | 323.2 | 24.6 | 2.71 | 1.86 | 1.22 | 1.03 | 0.71 | 0.64 |
| High gamma cross | 856.8 | 71.5 | 6.83 | 2.72 | 1.91 | 1.58 | 1.39 | 1.24 |

[Accession information for Table 7 and other relevant references]
[15] M. Hassani and M. R. Karami, “Noise estimation in electroencephalogram signal by using volterra series coefficients,” *Journal of medical signals and sensors*, vol. 5, no. 3, pp. 192–200, 2015, 26284176[pmid]. [Online]. Available: https://pubmed.ncbi.nlm.nih.gov/26284176

[16] N. Li, Y. Nie, and W. Zhu, “The application of fpga-based discrete wavelet transform system in eeg analysis,” in *2012 Second International Conference on Intelligent System Design and Engineering Application*, 2012, pp. 1306–1309.

[17] V. J. Lawhern, A. J. Solon, N. R. Waytowich, S. M. Gordon, C. P. Hung, and B. J. Lance, “EEG-Net: a compact convolutional neural network for EEG-based brain–computer interfaces,” *Journal of Neural Engineering*, vol. 15, no. 5, p. 056013, jul 2018.

[18] R. T. Schirrmeister, J. T. Springenberg, L. D. J. Fiederer, M. Glasstetter, K. Eggensperger, M. Tangermann, F. Hutter, W. Burgard, and T. Ball, “Deep learning with convolutional neural networks for eeg decoding and visualization,” *Human Brain Mapping*, vol. 38, no. 11, pp. 5391–5420, 2017. [Online]. Available: https://onlinelibrary.wiley.com/doi/abs/10.1002/hbm.23730

[19] D. Zhang, L. Yao, X. Zhang, S. Wang, W. Chen, R. Boots, and B. Benatallah, “Cascade and parallel convolutional recurrent neural networks on eeg-based intention recognition for brain computer interface,” in *AAAI*, 2018.

[20] D. Zhang, L. Yao, K. Chen, and J. Monaghan, “A convolutional recurrent attention model for subject-independent eeg signal analysis,” *IEEE Signal Processing Letters*, vol. 26, no. 5, pp. 715–719, May 2019.

[21] Kai Keng Ang, Zheng Yang Chin, Haihong Zhang, and Cuntai Guan, “Filter bank common spatial pattern (fbcps) in brain-computer interface,” in *2008 IEEE International Joint Conference on Neural Networks (IEEE World Congress on Computational Intelligence)*, June 2008, pp. 2390–2397.

[22] N. Jatupai boon, S. Pan-ngum, and P. Israsena, “Real-time eeg-based happiness detection system,” *TheScientificWorldJournal*, vol. 2013, p. 618649, 08 2013.

[23] B. Lakshminarayanan, A. Pritzel, and C. Blundell, “Simple and scalable predictive uncertainty estimation using deep ensembles,” in *Advances in Neural Information Processing Systems 30*, I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, Eds. Curran Associates, Inc., 2017, pp. 6402–6413. [Online]. Available: http://papers.nips.cc/paper/7219-simple-and-scalable-predictive

[24] C. Guo, G. Pleiss, Y. Sun, and K. Q. Weinberger, “On calibration of modern neural networks,” in *Proceedings of the 34th International Conference on Machine Learning - Volume 70*, ser. ICML’17. JMLR.org, 2017, p. 1321–1330.

[25] A. Loquercio, M. Segù, and D. Scaramuzza, “A general framework for uncertainty estimation in deep learning,” *IEEE Robotics and Automation Letters*, vol. 5, pp. 3153–3160, 2020.

[26] J. M. Hernández-Lobato and R. P. Adams, “Probabilistic backpropagation for scalable learning of bayesian neural networks,” in *Proceedings of the 22nd International Conference on International Conference on Machine Learning - Volume 37*, ser. ICML’15. JMLR.org, 2015, p. 1861–1869.

[27] H. Wang, X. Shi, and D.-Y. Yeung, “Natural-parameter networks: A class of probabilistic neural networks,” *ArXiv*, vol. abs/1611.00448, 2016.

[28] J. Gast and S. Roth, “Lightweight probabilistic deep networks,” 2018 IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp. 3369–3378, 2018.

[29] Y. Gal, J. Hron, and A. Kendall, “Concrete dropout,” in *Advances in Neural Information Processing Systems 30*, I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, Eds. Curran Associates, Inc., 2017, pp. 3581–3590. [Online]. Available: http://papers.nips.cc/paper/6949-concrete-dropout.pdf

[30] J. Thurin, R. Brossier, and L. Métilvier, “Ensemble-based uncertainty estimation in
full waveform inversion,” *Geophysical Journal International*, vol. 219, no. 3, pp. 1613–1635, 08 2019. [Online]. Available: https://doi.org/10.1093/gji/ggz384

[31] A. Ashukha, A. Lyzhov, D. Molchanov, and D. Vetrov, “Pitfalls of in-domain uncertainty estimation and ensembling in deep learning,” in *International Conference on Learning Representations*, 2020. [Online]. Available: https://openreview.net/forum?id=BJxI5gHKDr

[32] L. P. Levasseur, Y. D. Hezaveh, and R. H. Wechsler, “Uncertainties in parameters estimated with neural networks: Application to strong gravitational lensing,” *The Astrophysical Journal*, vol. 850, no. 1, p. L7, nov 2017. [Online]. Available: https://doi.org/10.3847%2F2041-8213%2Faa9704

[33] Z. Eaton-Rosen, F. J. S. Bragman, S. Biswas, S. Ourselin, and M. J. Cardoso, “Towards safe deep learning: accurately quantifying biomarker uncertainty in neural network predictions,” in *MICCAI*, 2018.

[34] N. Tomášev, X. Glorot, J. W. Rae, M. Zielinski, H. Askham, A. Saraiva, A. Mottram, C. Meyer, S. Ravuri, I. Protsyuk, A. Connell, C. O. Hughes, A. Karthikesalingam, J. Cornebise, H. Montgomery, G. Rees, C. Laing, C. R. Baker, K. Peterson, R. Reeves, D. Hassabis, D. King, M. Suleyman, T. Back, C. Nielson, J. R. Ledsam, and S. Mohamed, “A clinically applicable approach to continuous prediction of future acute kidney injury,” *Nature*, vol. 572, no. 7767, pp. 116–119, Aug 2019. [Online]. Available: https://doi.org/10.1038/s41586-019-1390-1

[35] X. Boyen and D. Koller, “Tractable inference for complex stochastic processes,” in *Proceedings of the Fourteenth Conference on Uncertainty in Artificial Intelligence*, ser. UAI’98. San Francisco, CA, USA: Morgan Kaufmann Publishers Inc., 1998, p. 33–42.

[36] B. J. Frey and G. E. Hinton, “Variational learning in nonlinear gaussian belief networks,” *Neural Comput.*, vol. 11, no. 1, p. 193–213, Jan. 1999. [Online]. Available: https://doi.org/10.1162/089976699300016872

[37] E. T. A. F. Jacobs and M. R. C. M. Berkelaar, “Gate sizing using a statistical delay model,” in *Proceedings Design, Automation and Test in Europe Conference and Exhibition 2000 (Cat. No. PR00537)*, 2000, pp. 283–290.

[38] J. Jin, A. Dundar, and E. Culurciello, “Robust convolutional neural networks under adversarial noise,” *ArXiv*, vol. abs/1511.06306, 2015.

[39] A. Suarez-Perez, G. Gabriel, B. Rebollo, X. Illa, A. Guimerà-Brunet, J. Hernández-Ferrer, M. T. Martínez, R. Villa, and M. V. Sanchez-Vives, “Quantification of signal-to-noise ratio in cerebral cortex recordings using flexible mes with co-localized platinum black, carbon nanotubes, and gold electrodes,” *Frontiers in Neuroscience*, vol. 12, p. 862, 2018. [Online]. Available: https://www.frontiersin.org/article/10.3389/fnins.2018.00862

[40] M. Tangermann, K.-R. Müller, A. Aertsen, N. Birbaumer, C. Braun, C. Brunner, R. Lée, C. Mehring, K. Miller, G. Mueller-Putz, G. Nolte, G. Pfurtscheller, H. Preissl, G. Schalk, A. Schlögl, C. Vidaurre, S. Waldert, and B. Blankertz, “Review of the bci competition iv,” *Frontiers in Neuroscience*, vol. 6, p. 55, 2012. [Online]. Available: https://www.frontiersin.org/article/10.3389/fnins.2012.00055

[41] A. A. Bradley, S. S. Schwartz, and T. Hashino, “Sampling Uncertainty and Confidence Intervals for the Brier Score and Brier Skill Score,” *Weather and Forecasting*, vol. 23, no. 5, pp. 992–1006, 10 2008. [Online]. Available: https://doi.org/10.1175/2007WAF2007049.1

[42] T. Gneiting and A. E. Raftery, “Strictly proper scoring rules, prediction, and estimation,” *Journal of the American Statistical Association*, vol. 102, no. 477, pp. 359–378, 2007. [Online]. Available: https://doi.org/10.1198/016214506000001437

[43] M. D. Zeiler and R. Fergus, “Visualizing and understanding convolutional networks,” in *In Computer Vision–ECCV 2014*. Springer, 2014, pp. 818–833.