EVALUATING DROPOUT PLACEMENTS IN BAYESIAN REGRESSION RESNET

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Abstract

Deep Neural Networks (DNNs) have shown great success in many fields. Various network architectures have been developed for different applications. Regardless of the complexities of the networks, DNNs do not provide model uncertainty. Bayesian Neural Networks (BNNs), on the other hand, is able to make probabilistic inference. Among various types of BNNs, Dropout as a Bayesian Approximation converts a Neural Network (NN) to a BNN by adding a dropout layer after each weight layer in the NN. This technique provides a simple transformation from a NN to a BNN. However, for DNNs, adding a dropout layer to each weight layer would lead to a strong regularization due to the deep architecture. Previous researches [1, 2, 3] have shown that adding a dropout layer after each weight layer in a DNN is unnecessary. However, how to place dropout layers in a ResNet for regression tasks are less explored. In this work, we perform an empirical study on how different dropout placements would affect the performance of a Bayesian DNN. We use a regression model modified from ResNet as the DNN and place the dropout layers at different places in the regression ResNet. Our experimental results show that it is not necessary to add a dropout layer after every weight layer in the Regression ResNet to let it be able to make Bayesian Inference. Placing Dropout layers between the stacked blocks i.e. Dense+Identity+Identity blocks has the best performance in Predictive Interval Coverage Probability (PICP). Placing a dropout layer after each stacked block has the best performance in Root Mean Square Error (RMSE).

Keywords: Regression, Bayesian Neural Network, MC Dropout

1 Introduction

Deep learning has shown great success in the field of computer vision. Various networks have shown high capabilities in image recognition [4, 5, 6, 7]. Based on these networks, more work have been applied for tasks such as object detection [8, 9, 10], semantic segmentation [11, 12, 13], pose estimation [14, 15, 16], gaze estimation [17, 18, 19] and so on. In general, these networks use convolutional neural networks (CNN) to extract fea-

tures and apply different functions for different types of tasks. For classification tasks such as image classification, SoftMax + Fully Connected (FC) layers are usually used to get class probabilities. For regression tasks such as pose estimation, FC layers are normally applied to obtain output vector(s). ResNet [7] uses shortcut connections to overcome the vanishing gradient problem when the layers going deeper. In addition to its use classification tasks, ResNet is used a lot in regression tasks [20, 21, 22, 23]. An empirical study [24] is performed to analyze the VGG-16 [5] and ResNet-50 networks for regression task. The inputs of these works are images hence CNNs are used to extract features.

The regression task in computer vision takes images as the input to the network. In other applications besides computer vision, the input data are often in the form of vectors. Common machine learning based regression techniques include Decision Tree Regression (DTR) [25], Support Vector Regression (SVR)[26] and Neural Network (NN). DNNs are also used for regression tasks when the input data is a vector. In these cases, the DNNs used in computer vision need to be modified. One common solution is replacing the convolutional layers with FC layers [27, 28, 29]. In [28], a modified ResNet, we refer it as Regression ResNet (RRN), is used for the regression. The convolutional layers and pooling layers in ResNet are replaced with FC layers. The authors of [28] show that RRN has better performance than the DTR, SVR and NN. IRNet and SRNet [27] are similar to [28], the main difference is the strategy of residual connections and the number of hidden units. The authors compare IRNet with 10 other machine learning algorithms (including Random Forest, DTR, SVR and so on). Their results show that the IRNet outperforms the 10 machine learning algorithms. In [29], Multi-Layer Perceptron (MLP) is adopted in the Encoder-Decoder architecture. Residual shortcut connections are added between Encoders and Decoders. Adding shortcut connections can increase the performance of regression. The proposed model also has better performance than MLP.

Despite the huge success of DNN, it does not provide weight uncertainty of the model thus it is not able to make probabilistic inference. Bayesian Neural Network (BNN) can capture model uncertainty [30]. A modern technique used in BNNs is Variational Inference (VI), which learns approximate posterior distributions [31]. VI based BNN models include Bayes by Backprop [32], Dropout as a Bayesian Approximation [33] and Bayesian Hypernetwork [34, 35].

Dropout as a Bayesian Approximation adds Dropout [36] layers to the weight layers. The authors of [33] have shown that it is equivalent to approximating Bayesian inference in deep Gaussian processes. It has the advantage of simple implementation compared to other BNNs. Several works have adopted this technique into existing DNNs. In [1], Dropout as a Bayesian Approximation is applied on PoseNet [15] to make Bayesian inference on camera pose, it uses GoogLeNet [6] as the backbone. In [2], SegNet [12] also uses Dropout as a Bayesian Approximation for semantic segmentation. Segnet uses a Encoder-Decoder frame and VGG-16 as the encoder and the decoder is in the reverse order. In [3], the Bayesian QuickNAT is used for whole-brain segmentation on Magnetic Resonance Imaging (MRI) images. The QuickNAT is based on Fully Convolutional Network (FCN) [11]. Although the Dropout as A Bayesian Approximation is easy to implement, adding a Dropout layer after each convolutional layer will make the regularization too strong [2] in DNNs. It will lead to a long training process. In all the works [1, 2, 3] mentioned above, a reduced number of dropout layers are added at different places in the networks to avoid the strong regularization. All the results show that not adding a dropout layer after each convolutional layer is a better option. Notwithstanding there are numerous DNN architectures proposed in various fields of researches, there is no analytical solution showing the optimal locations to put dropout layers in a certain type of network architecture. Moreover, placing dropout in DNNs for regression and in ResNet is less explored.

In this work, we conduct an empirical study to analyze the BRRN by Applying Dropout as a Bayesian Approximation to the RRN. We place dropout layers at the different locations in the network architecture and see the impacts of these different placements for regression tasks. We observed that placing a Dropout layer after every FC layer in the RRN is not necessary which is consistent with the findings in [2, 12, 3]. Placing dropout layers between the stacked blocks in the RRN has the best performance in Predictive Interval Coverage Probability (PICP). Placing a dropout layer after each stacked block has the best performance in Root Mean Square Error (RMSE). When designing a BRRN using dropout as a Bayesian Approximation, we demonstrate the schemes of dropout placements that can avoid strong regularization and obtain higher accuracy. Our work provides a reference for deploying BRRN in regression applications.

The remainder of the paper is organized as follows, in Section 2, we show the details of the RRN and the methodology of converting a NN to a BNN. In Section 3, we describe the settings for the experiments. We perform two experiments. First, we test different dropout locations in the residual connections in a residual block. Then we test the dropout locations between the residual blocks of the RRN. The experimental results are demonstrated in Section 4. The conclusion is given in Section 5.

2 Methodology

2.1 Regression ResNet

We use the modified ResNet i.e. the RRN in [28] as the DNN. Figure 1 shows the network architecture. The network consists of stacked Dense blocks and Identity blocks. The convolutional layers and pooling layers in ResNet is replaced by FC layers in the RRN. In one stacked block, one Dense block and two Identity blocks are connected sequentially. The network consists of three stacked blocks. A FC layer is used to readout the output. In Dense blocks, the residual connection is fed to a FC layer and Batch Normalization (BN)[37]. In Identity blocks, the residual connection is directly added to the feedforward output. In both types of blocks, the FC layer is followed by BN and non-linear activation i.e. Rectified Linear Uni (ReLU)[38] except the residual connection in the Dense block.

2.2 MC Dropout

For a Neural Network (NN) with weights **W**, bias **b**, adding Dropout layers after each weight layer equivalent to approximate Bayesian inference in deep Gaussian processes [33]. This technique can be referred as MC Dropout [34]. We shortly describe the MC Dropout from [33].

When a dropout operation is applied, some weights are removed and they follow the Bernoulli distribution. For the *i*th layer in a NN, the output is

$$\hat{\mathbf{y}}_{i+1} = \mathbf{\sigma}(\mathbf{x}_i(\mathbf{z}_i \mathbf{W}_i) + \mathbf{b}_i)(\mathbf{z}_{i+1} \mathbf{W}_{i+1}), \qquad (1)$$

where σ is the non-linear activation i.e. ReLU operation and z is the probability distribution for dropout operation. The cost function \mathcal{L} of a NN is

$$\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} E(\mathbf{y}_i, \hat{\mathbf{y}}_i) + \lambda \sum_{i=1}^{L} (||\mathbf{W}_i||_2^2 + ||\mathbf{b}_i||_2^2), \quad (2)$$

where $E(\cdot, \cdot)$ is the loss function, **y** and $\hat{\mathbf{y}}$ are the ground truth and the prediction of the model respectively, *N* is the length of the training data. The second term is a L_2 regularization term with decay factor λ . For approximating the Gaussian process model, the variational inference is used and Monte Carlo integration is used for minimizing KL divergence. The cost function is proportional to

$$\mathcal{L}_{GP-MC} \propto \frac{1}{2N} \sum_{i=1}^{N} E(\mathbf{y}_i, \hat{\mathbf{y}}_i) + \lambda \sum_{i=1}^{L} (\frac{(1-p_i)l^2}{2\tau N} ||\mathbf{W}_i||_2^2 + \frac{l^2}{2\tau N} ||\mathbf{b}_i||_2^2), \quad (3)$$

where p_i is the dropout rate in *i*th layer, τ is model precision and *l* is prior length scale. The predictive mean and predictive variance can be obtained by iterating the NN forward process *T* times,

$$\mathbb{E}(\mathbf{y}^*) \approx \frac{1}{T} \sum_{i=1}^{T} \hat{\mathbf{y}}^*(\mathbf{x}^*, \mathbf{W}_1^i, ..., \mathbf{W}_L^i), \qquad (4)$$

$$Var((\mathbf{y}^{*T})(\mathbf{y})) \approx \frac{1}{T} \sum_{i=1}^{T} \mathbf{\hat{y}}^{*}(\mathbf{x}^{*}, \mathbf{W}_{1}^{i}, ..., \mathbf{W}_{L}^{i})^{T} \mathbf{\hat{y}}^{*}(\mathbf{x}^{*}, \mathbf{W}_{1}^{i}, ..., \mathbf{W}_{L}^{i}), \quad (5)$$

where \mathbb{E} is the predictive mean and *Var* is predictive variance, \mathbf{x}^* and $\hat{\mathbf{y}}^*$ is the new entry data for inference and the new prediction. The weight decay λ is calculated by

$$\lambda = \frac{pl^2}{2N\tau},\tag{6}$$

2.3 Bayesian Regression ResNet

Combining the RRN and MC Dropout, the algorithm for the inference of BRRN is shown below, where **f** is the BRRN network and **P** is the predictions of the BRRN. Give the dropout rate p, the model precision *tau* and the length scale *l*, the weight decay λ can be calculated from Equation 6. To make Bayesian inference for a trained BRRN, simply put a new data entry to the model for *T* times. The mean prediction and the variance of the



Figure 1. Architecture of the Regression ResNet and the Dense block and the Identity block.

predication can be calculated from T predictions.

Algorithm 1: Bayesian Regression ResNet
Inference
Input: λ, p, T
Output: E , <i>Var</i>
Data: Test dataset x [*]
Enable dropout;
$\mathbf{P}=0;$
$\mathbf{f}(\lambda, \mathbf{p});$
for $i \leftarrow 0$ to T do
$\mathbf{y}^* = \mathbf{f}(\mathbf{x}^*);$
$\mathbf{P} = \mathbf{P} \bigcup \mathbf{y}^*;$
end
$\mathbb{E}(\mathbf{P}); Var(\mathbf{P});$

3 Experiment Settings

We perform two experiments, *Dropout Placements in Residual Blocks* and *Dropout Placements in Bayesian Regression ResNet*. In *Dropout Placements in Bayesian Regression ResNet*, we evaluate the performance of placing a dropout layer after each weight layer. However, the residual connection will lead to a few dropout placement variants within the Dense block and the Identity block. We test and select the best dropout placement variant in this experiment. In *Dropout Placements in Bayesian Regression ResNet*, Wee use the result from the previous experiment as the baseline i.e. placing a dropout layer after each weight layer. We evaluate different dropout locations in the stacked blocks and compare the performances with the performance of placing a dropout layer after each weight layer.

3.1 Dataset

We use 10 datasets for our experiments. The details of the datasets are indicated in Table 1. The datasets are from various fields. The SafeVS dataset is from [39], the rest datasets are the same as in [33]. The SafeVS dataset collects the hand positions and robot TCP positions and predicts repulsive TCP positions for hand collision avoidance. All the data is not pre-processed except for the normalization. We apply Z Normalization to all datasets. The Z-Normalization is defined as,

$$\mathbf{X}' = \frac{\mathbf{X} - \boldsymbol{\mu}_x}{\boldsymbol{\sigma}_x},\tag{7}$$

where μ_x and σ_x are the mean and standard deviation of the training data **X**.

3.2 Evaluation Metrics

The evaluation metrics are RMSE and PICP [40]. The PICP is calculated as follows,

$$P(\hat{y}_{L_i} \le y_i \le \hat{y}_{U_i}) > 0.95, \tag{8}$$

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	No. of Sample	Input Dimension	Output Dimension				
SafeVS	500000	6	3				
Kin8nm	8192	8	1				
Boston	506	13	1				
Concrete	1030	8	1				
Energy	768	8	1				
Naval	11934	16	1				
Power	9568	4	1				
Protein	45730	9	1				
Wine	1599	11	1				
Yacht	308	6	1				

Table 1. Datasets details.

where \hat{y}_{L_i} and \hat{y}_{U_i} is the lower bound and the upper bound of the prediction interval. We select the confidence as 95%. A boolean vector **b** summarizes if y_i is captured by the prediction interval,

$$b_i = \begin{cases} 1 & \text{if } \hat{y}_{L_i} \le y_i \le \hat{y}_{U_i} \\ 0 & \text{else} \end{cases}, \tag{9}$$

The PICP is calculated as,

$$PICP = \frac{1}{n} \sum_{i=1}^{n} b_i.$$
(10)

We also use the mean rank to compare the performances of the models in datasets. The mean rank R is calculated as,

$$R = \frac{1}{K} \sum_{i=1}^{K} rank_i, \qquad (11)$$

where *K* is the number of datasets. We calculate rank R_{RMSE} in RMSE and the rank R_{PICP} in PICP as well as R_{MEAN} which is the mean of R_{RMSE} and R_{PICP} .

4 **Results**

We demonstrate the experimental results of dropout Placements in Residual Blocks and dropout Placements in Bayesian Regression ResNet in this Section.

4.1 Dropout Placements in Residual Blocks

4.1.1 Baseline

In this experiment, we evaluate the dropout placements in the Dense block and the Identity block. The architecture of the baseline model is shown in Figure 2. The number (N) of the stacked block Dense+Identity+Identity is one. The dropout layer is added after the residual connection and nonlinear activation. The experiment is performed on Boston Housing, Concrete Compressive Strength, Energy Efficiency, Naval Propulsion Plants, Combined Cycle Power Plant, Wine Quality and Yacht Hydrodynamics. The loss function is Mean Square Error (MSE) loss and the optimizer is Adam. After every training epoch, a validation is performed. The final model is the one with the least validation loss. The hyper-parameters for training the baseline model are shown in Table 2.

4.1.2 Dropout Placement Variants

We evaluate three dropout placement variants in the Dense block and two variants in the Identity block. Figure 3 shows the detailed configuration of the variants. Since the model consists of the stacked block combination Dense+Identity+Identity. We name the variant as Di-Ij where *i* is the index in the Dense block configuration and *j* is the index in the Identity block configuration. For instance, D1-I1 represents that the Dense block in the network uses the Dropout-Dense-1 (Figure 3) configuration and the Identity blocks use the Dropout-Iden-1 (Figure 3) configuration. The baseline variant is D3-I0.

Table 3 shows the results of Dropout placement variants in the Dense block and the Identity block.



Figure 2. The baseline of the dropout placements. A dropout layer is placed after each weight layer.

 Table 2. Hyper parameters of the baseline model for the experiment Dropout Placements in Residual Blocks.

	Boston	Concrete	Energy	Naval	Power	Wine	Yacht
Epoch	130	200	200	150	200	200	200
Hidden Unit	32	16	16	32	16	16	16
Batch Size	32	8	64	128	128	32	16
Learning Rate	0.001	1e-4	0.001	1e-4	0.001	1e-4	1e-4
Tau	5e-4	0.03	0.15	0.5	0.05	2	0.01
Dropout Rate	0.1	0.005	0.05	0.005	0.005	0.1	0.005

The baseline model i.e. D3-I0 performs best on the Boston Housing and Naval Propulsion datasets, the ranks are within two. D0-I0 performs best on Energy Efficiency and Yacht Hydrodynamics datasets. The performance on Naval Propulsion is slightly lower. For D1-I1, the performances on Concrete Compressive Strength and Power Plant are the best. D3-I1 also performs well on Boston Housing. Regarding to the ranks of the model variants, we use $R_{RMSE},\,R_{PICP}$ and R_{MEAN} for the evaluation. Considering the RMSE rank, D2-I1 has the best RMSE mean rank score. D1-I0 has the best PICP mean rank. Considering both RMSE and PICP, D1-I0 and D0-I0 are the only two variants with the rand score below 4 and D1-I0 is around 0.3 better than D0-I0. Overall, D1-I0 has the best PICP mean rank score and the second best RMSE mean rank score.

4.2 Dropout Placements in Bayesian Regression ResNet

4.2.1 Baseline

We evaluate the dropout placement in the BRR. The baseline model for this experiment is similar to the one in Figure 2. The N is set to three, which is the same as the RR. A dropout layer is placed after each weight layer. In the case of residual connection, we adapt the D1-I0 variant configuration in each of the Dense+Identity+Identity stacked blocks. We refer the baseline model as *DO-Dense*. We applied the same baseline model to Kin8nm dataset, Protein dataset and SafeVS dataset. The loss function and the optimizer is the same as in the previous experiment. The hyper-parameters for the baseline model in the datasets are shown in Table 4.

Table 4. Hyper parameters of the baseline modelfor the experiment Dropout Placements inBayesian Regression ResNet.

	Kin8nm	SafeVS	Protein
Epoch	200	200	250
Hidden Unit	16	32	16
Batch Size	16	5000	512
Learning Rate	0.005	0.001	0.001
Tau	2	1e-5	0.5
Dropout Rate	5e-4	0.1	0.005

4.2.2 Dropout Placement Variants

We evaluate five Dropout placement variants, DO-Inter, DO-InterD, DO-Before, DO-After and DO-SE in the Regression ResNet. The details of the variants are indicated in Figure 4. In DO-Inter, all three stacked Dense+Identity+Identity blocks are separated by Dropout layers. In DO-InterD, one Dropout layer is added after each Dense block and Identity block. In DO-Before and DO-After configurations, the one Dropout layer is added before and after each stacked block. The DO-SE only places Dropout layers at the start and the end of the stacked blocks.

Table 5 shows the RMSEs and PICPs of the dropout placement variants on SafeVS dataset. DO-After obtains the best RMSE among all variant configurations. DO-Before, DO-After and DO-SE generally perform well than DO-Dense, DO-Inter and DO-InterD in RMSE. The differences are clearly observable. For PICP (1), all other variants perform better than the baseline model. For PICP (2) and PICP (3), DO-Before has comparable results with the baseline model, the rest variant configurations have obvious better results than the baseline. Considering the RMSE and PICPs together, all the tested dropout placement variants outperform the baseline i.e. DO-Dense. DO-InterD has extremely well performance on PICP (2) and PICP (3) but it only performs better than the baseline on PICP (1). DO-Inter and DO-SE have similar results on PICP (2) and PICP (3), however DO-SE has higher PICP (1) than DO-Inter. In addition, The RMSE of DO-SE is lower than DO-Inter. The difference is around 6. In total, DO-SE has the best performance in PICP among all dropout Placement Variants and DO-After has the least RMSE.

Table 6 shows the RMSEs and PICPs of the dropout placement variants on Kin8nm and Protein dataset. The RMSEs of all variants on Kin8nm dataset are comparable. DO-After has the least RMSE. Except for DO-SE, the RMSEs of all other variants are around 0.25. The PICP of DO-Inter is the highest among all variants on Kin8nm. For the Protein dataset, DO-After also has the least RMSE and highest PICP. For the baseline model, the performance in PICP is only better than DO-SE for Kin8nm and DO-Before for Protein. Although the RMSE for Kin8nm is the second best, the score is not obviously better than other Dropout variants.



Figure 3. Different Dropout placement variants in the Dense block and the Identity block.

	Baseline(D3-I0)	D0-I0	D1-I0	D2-I0	D0-I1	D1-I1	D2-I1	D3-I1
RMSE	2.4978	2.6249	2.6039	2.5165	3.065	3.318	2.8683	2.2879
PICP	0.902	0.8325	0.8039	0.7647	0.7255	0.7451	0.8431	0.8627
RMSE	18.0635	18.2892	17.6064	18.1651	18.0433	17.789	18.0225	18.1268
PICP	0.5	0.5577	0.5288	0.5192	0.5192	0.5577	0.5288	0.5481
RMSE	1.7527	1.631	1.6541	3.1067	3.5543	2.0553	1.5758	3.6017
PICP	0.9539	0.9231	0.9359	0.8333	0.8718	0.8205	0.8974	0.8846
RMSE	0.001	0.0011	0.0029	0.0027	0.003	0.003	0.001	0.0028
PICP	0.8728	0.8861	0.788	0.7714	0.7714	0.8362	0.8362	0.8188
RMSE	5.0471	5.0156	5.0402	5.0686	5.0524	4.9525	5.0687	4.9886
PICP	0.6415	0.6269	0.6674	0.6508	0.6321	0.6601	0.6259	0.6259
RMSE	0.8543	0.8659	0.8481	0.8656	0.8441	0.8656	0.8437	0.8482
PICP	0.8148	0.8395	0.8395	0.8519	0.8642	0.8333	0.8272	0.8519
RMSE	5.8718	5.4153	5.8387	5.6126	5.9612	5.8003	5.638	5.4224
PICP	0.6875	0.7812	0.8125	0.6875	0.7188	0.75	0.5625	0.7188
R _{RMSE}	4.1429	4.2857	3.8571	5.1429	5.8571	4.8571	3.4286	4
R _{PICP}	4.8257	3.1429	3	5.5714	5.1429	4.2857	5.2857	4.2857
R _{MEAN}	4.2143	3.7143	3.4286	5.3571	5.5	4.5714	4.3571	4.1429
	RMSE PICP RMSE PICP RMSE PICP RMSE PICP RMSE PICP RMSE PICP RMSE PICP RMSE RRMSE RPICP RMEAN	Baseline(D3-I0) RMSE 2.4978 PICP 0.902 RMSE 18.0635 PICP 0.5 RMSE 1.7527 PICP 0.9539 RMSE 0.001 PICP 0.8728 RMSE 5.0471 PICP 0.8543 PICP 0.8148 RMSE 5.8718 PICP 0.6875 RMSE 4.1429 RPICP 4.8257 RMEAN 4.2143	Baseline(D3-I0) D0-I0 RMSE 2.4978 2.6249 PICP 0.902 0.8325 RMSE 18.0635 18.2892 PICP 0.5 0.5577 RMSE 1.7527 1.631 PICP 0.9039 0.9231 RMSE 0.001 0.0011 PICP 0.8728 0.8861 RMSE 5.0471 5.0156 PICP 0.6415 0.6269 RMSE 0.8543 0.8659 PICP 0.8148 0.8395 RMSE 5.8718 5.4153 PICP 0.6875 0.7812 R _{RMSE} 4.1429 4.2857 R _{PICP} 4.8257 3.1429 R _{MEAN} 4.2143 3.7143	Baseline(D3-I0) D0-I0 D1-I0 RMSE 2.4978 2.6249 2.6039 PICP 0.902 0.8325 0.8039 RMSE 18.0635 18.2892 17.6064 PICP 0.5 0.5577 0.5288 RMSE 1.7527 1.631 1.6541 PICP 0.9539 0.9231 0.9359 RMSE 0.001 0.0011 0.0029 PICP 0.8728 0.8861 0.788 RMSE 5.0471 5.0156 5.0402 PICP 0.6415 0.6269 0.6674 RMSE 0.8543 0.8659 0.8481 PICP 0.8148 0.8395 0.8395 RMSE 5.8718 5.4153 5.8387 PICP 0.6875 0.7812 0.8125 R _{MSE} 4.1429 4.2857 3.8571 R _{PICP} 4.8257 3.1429 3 R _{MEAN} 4.2143 3.7143 3.4286	Baseline(D3-I0) D0-I0 D1-I0 D2-I0 RMSE 2.4978 2.6249 2.6039 2.5165 PICP 0.902 0.8325 0.8039 0.7647 RMSE 18.0635 18.2892 17.6064 18.1651 PICP 0.5 0.5577 0.5288 0.5192 RMSE 1.7527 1.631 1.6541 3.1067 PICP 0.9539 0.9231 0.9359 0.8333 RMSE 0.001 0.0011 0.0029 0.0027 PICP 0.8728 0.8861 0.788 0.7714 RMSE 5.0471 5.0156 5.0402 5.0686 PICP 0.6415 0.6269 0.6674 0.6508 RMSE 0.8543 0.8659 0.8481 0.8656 PICP 0.8148 0.8395 0.8395 0.8519 RMSE 5.8718 5.4153 5.8387 5.6126 PICP 0.6875 0.7812 0.8125 0.6875	Baseline(D3-I0) D0-I0 D1-I0 D2-I0 D0-I1 RMSE 2.4978 2.6249 2.6039 2.5165 3.065 PICP 0.902 0.8325 0.8039 0.7647 0.7255 RMSE 18.0635 18.2892 17.6064 18.1651 18.0433 PICP 0.5 0.5577 0.5288 0.5192 0.5192 RMSE 1.7527 1.631 1.6541 3.1067 3.5543 PICP 0.9539 0.9231 0.9359 0.8333 0.8718 RMSE 0.001 0.0011 0.0029 0.0027 0.003 PICP 0.8728 0.8861 0.788 0.7714 0.7714 RMSE 5.0471 5.0156 5.0402 5.0686 5.0524 PICP 0.6415 0.6269 0.6674 0.6508 0.6321 RMSE 0.8543 0.8659 0.8481 0.8656 0.8441 PICP 0.6875 0.7812 0.8125 0.6875	Baseline(D3-I0)D0-I0D1-I0D2-I0D0-I1D1-I1RMSE2.49782.62492.60392.51653.0653.318PICP0.9020.83250.80390.76470.72550.7451RMSE18.063518.289217.606418.165118.043317.789PICP0.50.55770.52880.51920.51920.5577RMSE1.75271.6311.65413.10673.55432.0553PICP0.95390.92310.93590.83330.87180.8205RMSE0.0010.00110.00290.00270.0030.003PICP0.87280.88610.7880.77140.77140.8362RMSE5.04715.01565.04025.06865.05244.9525PICP0.64150.62690.66740.65080.63210.6601RMSE0.85430.86590.84810.86560.84410.8656PICP0.81480.83950.83950.85190.86420.8333RMSE5.87185.41535.83875.61265.96125.8003PICP0.68750.78120.81250.68750.71880.75R _{MSE} 4.14294.28573.85715.14295.85714.8571R _{MSE} 4.21433.71433.42865.35715.54.5714	Baseline(D3-I0)D0-I0D1-I0D2-I0D0-I1D1-I1D2-I1RMSE2.49782.62492.60392.51653.0653.3182.8683PICP0.9020.83250.80390.76470.72550.74510.8431RMSE18.063518.289217.606418.165118.043317.78918.0225PICP0.50.55770.52880.51920.51920.55770.5288RMSE1.75271.6311.65413.10673.55432.05531.5758PICP0.95390.92310.93590.83330.87180.82050.8974RMSE0.0010.00110.00290.00270.0030.0030.001PICP0.87280.88610.7880.77140.77140.83620.8362RMSE5.04715.01565.04025.06865.05244.95255.0687PICP0.64150.62690.66740.65080.63210.66010.6259RMSE0.85430.86590.84810.86560.84410.86560.8437PICP0.81480.83950.83950.85190.86420.83330.8272RMSE5.87185.41535.83875.61265.96125.80035.638PICP0.68750.78120.81250.68750.71880.750.5625R _{MSE} 4.14294.28573.85715.14295.85714.85713.4286R _{MSE}

Table 3. Dropout placement variants in the Dense block and the Identity block.



Figure 4. Different dropout placements in the Regression ResNet.

	-	-			
	RMSE	PICP (1)	PICP (2)	PICP (3)	Mean PICP
Baseline (DO-Dense)	25.0269	0.6418	0.8357	0.8577	0.7784
DO-Inter	24.8448	0.7742	0.9456	0.963	0.8943
DO-InterD	28.2758	0.6544	0.9969	0.9969	0.8827
DO-Before	19.5191	0.8209	0.8736	0.8466	0.847
DO-After	15.1608	0.8158	0.9049	0.9498	0.8902
DO-SE	18.6065	0.8646	0.937	0.95	0.9172

 Table 5. Result of Dropout position variants on SafeVS dataset.

	Kin	8nm	Protein		
	RMSE	PICP	RMSE	PICP	
Baseline (DO-Dense)	0.2563	0.4872	5.5586	0.5712	
DO-Inter	0.2583	0.6413	5.7376	0.6062	
DO-InterD	0.2583	0.6304	5.7965	0.5926	
DO-Before	0.2572	0.5	5.4146	0.5634	
DO-After	0.2556	0.5761	5.2859	0.5809	
DO-SE	0.2783	0.4239	5.5219	0.575	

Table 6. Result of dropout position variants on Kin8nm and Protein dataset.

Overall, the baseline does not outperform the other Dropout variants, placing a Dropout layer after every weight layer in the RRN is unnecessary. It is consistent with the findings in [2, 12, 3]. Considering RMSE as the criterion for model selection, DO-After has the best performance. Considering PICP as the criterion for model selection, DO-Inter has the best performance on Kin8nm dataset and Protein dataset. Although DO-SE has the best mean PICP in SafeVS dataset, its performances in Kin8nm and Protein can not compete with DO-Inter.

5 Conclusion

In this paper, we perform an empirical study on evaluating the impact of different dropout placements in a modified ResNet for regression tasks. The MC Dropout technique places a dropout layer after each weight layer in a DNN, which is equivalent to an approximation to deep Gaussian process. Using MC Dropout can easily convert a DNN to a Bayesian DNN, however, the regularization will be too strong due to the deep network architecture. This will lead to a very long training process. Adding fewer dropout layers to a DNN has been shown to be effective to convert the DNN to Bayesian DNN. ResNet was developed for computer vision tasks, it can also be modified to be applied in univariate and multivariate regression tasks. We study the impact of different dropout placements in the Regression ResNet. We find out that placing dropout layers after each FC layer does not outperform the other dropout placement variants. Placing dropout layers after and between the residual blocks have the best RMSE and PICP among all tested variants.

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