Supplementary Material: Variational Bayesian Dropout with a Hierarchical Prior

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1. The derivation of Variational Bayesian Dropout

With the proposed hierarchical prior $p(\mathbf{W}, \gamma) = p(\mathbf{W}|\gamma)p(\gamma)$, variational posterior distribution $q(\mathbf{W}, \gamma) = q(\mathbf{W})q(\gamma)$, and the original objective:

$$D_{KL}(q(\mathbf{W})||p(\mathbf{W},\gamma|\mathcal{D})),$$
 (1)

we have:

$$\min_{\alpha,\theta,\gamma} D_{KL}(q(\mathbf{W},\gamma)||p(\mathbf{W},\gamma|\mathcal{D}))
= \min_{\alpha,\theta,\gamma} \int q(\mathbf{W},\gamma) \log \frac{q(\mathbf{W},\gamma)}{p(\mathbf{W},\gamma|\mathcal{D})}
= \min_{\alpha,\theta,\gamma} \int q(\mathbf{W},\gamma) \log q(\mathbf{W},\gamma) - \int q(\mathbf{W},\gamma) \log p(\mathbf{W},\gamma|\mathcal{D})
= \max_{\alpha,\theta,\gamma} \int q(\mathbf{W},\gamma) \log p(\mathbf{W},\gamma|\mathcal{D}) - \int q(\mathbf{W},\gamma) \log q(\mathbf{W},\gamma)
= \max_{\alpha,\theta,\gamma} \int q(\mathbf{W},\gamma) \log p(\mathbf{W},\gamma)p(\mathcal{D}|\mathbf{W}) - \int q(\mathbf{W},\gamma) \log p(\mathcal{D}) - \int q(\mathbf{W},\gamma) \log q(\mathbf{W},\gamma)
= \max_{\alpha,\theta,\gamma} \int q(\mathbf{W},\gamma) \log p(\mathcal{D}|\mathbf{W}) + \int q(\mathbf{W},\gamma) \log p(\mathbf{W},\gamma) - \int q(\mathbf{W},\gamma) \log q(\mathbf{W},\gamma)
= \max_{\alpha,\theta,\gamma} \int q(\mathbf{W},\gamma) \log p(\mathcal{D}|\mathbf{W}) - \int q(\mathbf{W},\gamma) \log \frac{q(\mathbf{W},\gamma)}{p(\mathbf{W},\gamma)}
= \max_{\alpha,\theta,\gamma} \int q(\mathbf{W},\gamma) \log p(\mathcal{D}|\mathbf{W}) - \int q(\mathbf{W},\gamma) \log \frac{q(\mathbf{W},\gamma)}{p(\mathbf{W},\gamma)}$$

As mentioned in the manuscript, we assume that $q(\mathbf{W}, \gamma) = q(\mathbf{W})q(\gamma)$, hence we have:

$$\max_{\alpha,\theta,\gamma} \int q(\mathbf{W},\gamma) \log p(\mathcal{D}|\mathbf{W}) - \int q(\mathbf{W},\gamma) \log \frac{q(\mathbf{W},\gamma)}{p(\mathbf{W},\gamma)} \\
= \max_{\alpha,\theta,\gamma} \int q(\mathbf{W}) q(\gamma) \log p(\mathcal{D}|\mathbf{W}) - \int q(\mathbf{W}) q(\gamma) \log \frac{q(\mathbf{W}) q(\gamma)}{p(\mathbf{W}|\gamma) p(\gamma)} \\
= \max_{\alpha,\theta,\gamma} \int q(\mathbf{W}) \log p(\mathcal{D}|\mathbf{W}) - \int q(\mathbf{W}) q(\gamma) \log \frac{q(\mathbf{W})}{p(\mathbf{W}|\gamma)} - \int q(\mathbf{W}) q(\gamma) \log \frac{q(\gamma)}{p(\gamma)} \\
= \max_{\alpha,\theta,\gamma} L_{\mathcal{D}}(\alpha,\theta) - D_{KL}(q(\mathbf{W})||p(\mathbf{W}|\gamma)) - D_{KL}(q(\gamma)||p(\gamma))$$
(3)

2. The proof of Proposition 2

To proof **Proposition 2**, we only need to proof that $D_{KL}(q(\gamma)||p(\gamma))$ becomes a constant and can be neglected during optimization. To this end, we employ mean-field variational approximation viz., $q(\gamma) = \prod_{k=1}^K \prod_{d=1}^D q(\gamma_{k,d})$, to gather with $p(\gamma) = \prod_{k=1}^K \prod_{d=1}^D p(\gamma_{k,d}) = \prod_{k=1}^K \prod_{d=1}^D \mathcal{U}(\gamma_{k,d}|a,b)$, we have:

$$D_{KL}(q(\gamma)||p(\gamma)) = \prod_{k=1}^{K} \prod_{d=1}^{D} D_{KL}(q(\gamma_{k,d})||p(\gamma_{k,d})), \tag{4}$$

Now, we can directly investigate $D_{KL}(q(\gamma_{k,d})||p(\gamma_{k,d}))$,

$$D_{KL}(q(\gamma_{k,d})||p(\gamma_{k,d}))$$

$$= \int q(\gamma_{k,d}) \log \frac{q(\gamma_{k,d})}{p(\gamma_{k,d})}$$

$$= \int q(\gamma_{k,d}) \log q(\gamma_{k,d}) - \int q(\gamma_{k,d}) \log p(\gamma_{k,d})$$

$$= -\mathcal{H}(\gamma_{k,d}) - \int q(\gamma_{k,d}) \log p(\gamma_{k,d}),$$
(5)

where $\mathcal{H}(\gamma_{k,d})$ denotes the entropy of a random variable $\gamma_{k,d}$. As defined in main paper, $q(\gamma_{k,d})$ obeys a delta distribution, hence $\mathcal{H}(\gamma_{k,d}) = 0$ because delta distribution do not provide any uncertainty [4]. As a result, we obtain:

$$D_{KL}(q(\gamma_{k,d})||p(\gamma_{k,d})) = -\int q(\gamma_{k,d})\log p(\gamma_{k,d}),\tag{6}$$

To simplify the problem, assuming the dimension of $\gamma_{k,d}$ is 1, e.g., $p(\gamma_{k,d}) = 1/(b-a)$, thus we have:

$$D_{KL}(q(\gamma_{k,d})||p(\gamma_{k,d}))$$

$$= -\int_{-\infty}^{a} q(\gamma_{k,d}) \log p(\gamma_{k,d}) - \int_{a}^{b} q(\gamma_{k,d}) \log p(\gamma_{k,d}) - \int_{b}^{+\infty} q(\gamma_{k,d}) \log p(\gamma_{k,d})$$

$$= -\log \beta \int_{-\infty}^{a} q(\gamma_{k,d}) - \log(1/(b-a)) \int_{a}^{b} q(\gamma_{k,d}) - \log \beta \int_{b}^{+\infty} q(\gamma_{k,d}),$$
(7)

where $\beta \to 0$ (Strictly speaking, β should be equal to 0, since $p(\gamma_{k,d}) = 0$ in the intervals $(-\infty,a]$ and $[b,+\infty)$). Thus, if $q(\gamma_{k,d})$ as a delta function lies in [a,b], e.g., $\delta(\gamma_{k,d}-\gamma'_{k,d})$ and $\gamma'_{k,d}$ lies in [a,b], then $\int_{-\infty}^a q(\gamma_{k,d})$ and $\int_b^{+\infty} q(\gamma_{k,d})$ is equal to 0, so $D_{KL}(q(\gamma_{k,d})||p(\gamma_{k,d})) = \log(b-a)$, else, $\int_a^b q(\gamma_{k,d})$ is equal to 0, and $D_{KL}(q(\gamma_{k,d})||p(\gamma_{k,d})) = +\infty$. To avoid $D_{KL}(q(\gamma_{k,d})||p(\gamma_{k,d})) = +\infty$, [a,b] is generally regarded as a large enough interval, so the KL is a constant $\log(b-a)$ and can be neglected.

3. The experimental setting on MNIST Dataset

Following the suggestion in [6], we adopt a fully connected neural network consisting of 3 hidden layers and rectified linear units as the basic deep neural network. For the dropout with Bernoulli noise or Gaussian noise, we fix the dropout rate as p=0.5 for the hidden layers and p=0.2 for the input layer as recommended in the references. All networks are trained for 50 epochs with batch size 1000 and Adam optimizer [1] with initial learning rate 0.001. To reduce the influence of random initialization, we train the network for each methods within 5 random runs and report the average results of those 5 trained networks during testing.

4. The experimental setting on Cifar-10 Dataset

Following the setting in [2], the basic neural network for all methods consists of two convolutional layers followed by two fully connected layers. In these two convolutional layer, there are $32 \times scale$ and $64 \times scale$ feature maps, respectively. The

kernels size and stride parameter is 3×3 and 2. Each convolutional layer is further fed into a softplus unit for improving non-linearity. In addition, each fully connected layer contains $128 \times scale$ hidden units. In experiments, we fix the dropout rate as 0.5 for the dropout with Bernoulli noise or Gaussian noise. For each method, the network is trained for 100 epochs with batch size 1000 and Adam optimizer with initial learning rate 0.001. Similarly, we also report the average test result for each method through training the network in 5 random runs.

5. Structured compressing for VGG on Cifar-10 Dataset

To prove that VBD scales to deep architectures, we apply it to a VGG-like network ¹ that was adapted for the CIFAR dataset. The network consists of 13 convolutional and two fully-connected layers, trained with pre-activation batch normalization and Binary Dropout. At the start of the training procedure, we use pre-trained weights for initialization. We compare the proposed method with existing variational dropout based methods, Variational Dropout (VD) [3] and SBP [5]. Table 1 shows the advantage of the proposed VBD in structured compressing for the deep VGG-like architecture, compared with the others.

Table 1. Compressing VGG on Cifar-10 Dataset.

Methods	Error %	Neurons per Layer
Original	7.2	64 - 64 - 128 - 128 - 256 - 256 - 256 - 512 - 512 - 512 - 512 - 512 - 512 - 512
VD	7.2	64 - 62 - 128 - 126 - 234 - 155 - 31 - 81 - 76 - 9 - 138 - 101 - 413 - 373
SBP(a)	7.5	64 - 62 - 128 - 126 - 234 - 155 - 31 - 79 - 73 - 9 - 59 - 73 - 56 - 27
SBP(b)	9.0	44 - 54 - 92 - 115 - 234 - 155 - 31 - 76 - 55 - 9 - 34 - 35 - 21 - 280
Ours	8.8	38 - 62 - 127 - 128 - 229 - 193 - 93 - 32 - 16 - 11 - 5 - 8 - 12 - 12

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