# Efficient Variational Inference for Sparse Deep Learning with Theoretical Guarantee

Jincheng Bai, Qifan Song, Guang Cheng

## Introduction

**Motivation:**

- Compress deep learning model for hardware limited devices.
- Recover potential sparsity structure of the target function.
- Variable selection.

**Existing approaches:**

Pruning methods ( no theoretical guarantee on choosing the threshold):

- Frequentist: Zhu and Gupta 2018; Frankle and Carbin 2018, etc.
- Bayesian: Molchanov et al. 2017; Ghosh et al. 2018, etc.

Theoretical work (no efficient implementation):

- Polson and Rockova 2018; Cherief-Abdellatif 2020, etc.

**Our contribution:**

A complete package of both theory and computation for sparse DNN from a Bayesian perspective.

## Model setup

**Nonparametric regression**

Consider a nonparametric regression model with random covariates:

$$Y_i = f_0(X_i) + \epsilon_i, \quad i = 1, \dots, n,$$

where $X_i \sim \mathcal{U}([-1,1]^p)$ and $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$.

**Deep neural network**

The DNN $f_\theta(X)$ is used to approximate $f_0(X)$, where $\theta$ denotes all the coefficients in the neural network. The network configuration includes

- L: number of hidden layers
- N: width of the network (assume equal width)
- s: sparsity level ($\|\theta\|_0 \le s$)

**Optimal sparsity level:**

Define $s^*$ as

$$s^* = \text{argmin}_s\{r_n(L,N,s) + \xi_n(L,N,s)\},$$

such that $s^*$ strikes the balance (trade-off) between the variational error $r_n$ and the approximation error $\xi_n$. Note that $s^*$ is generally unknown, but our modeling is capable of automatically attaining the same rate of convergence as if $s^*$ is known.

## Variational Inference

**Sparse Bayesian deep learning with spike-and-slab prior**

- Prior distribution $\pi(\theta)$:

  $$\theta_i|\gamma_i \sim \gamma_i \mathcal{N}(0, \sigma_0^2) + (1-\gamma_i)\delta_0, \ \gamma_i \sim Bern(\lambda), i = 1, \dots, T,$$

  Note: the theoretical guarantees will be established under proper deterministic choices of hyperparameters $\lambda$ and $\sigma_0$.

- Variational distribution $q(\theta)$:

  $$\theta_i|\gamma_i \sim \gamma_i \mathcal{N}(\mu_i, \sigma_i^2) + (1-\gamma_i)\delta_0, \ \gamma_i \sim Bern(\phi_i), i = 1, \dots, T.$$

  The variational parameters are $(\mu_i, \sigma_i, \phi_i)$, the transformed variational parameters are denoted as $\omega$.

## Theoretical Results

**Conditions:**

The main theorems are under the following conditions.

- The activation function is 1-Lipschitz continuous.
- The hyperparameter $\sigma_0^2$ is set to be some constant, and $\lambda$ satisfies

  $\log(1/\lambda) = O\{(L+1)\log N + \log(p\sqrt{n/s^*})\}$ and

  $\log(1/(1-\lambda)) = O((s^*/T)\{(L+1)\log N + \log(p\sqrt{n/s^*})\})$.
- $max\{s^*\log(p\sqrt{n/s^*}), (L+1)s^*\log N\} = o(n)$ and $r_n(L,N,s^*) \asymp \xi_n(L,N,s^*)$

**Main theorems:**

- $P_0$ and $P_\theta$ are the probability measure corresponding to $f_0$ and $f_\theta$ ; $D$ is the dataset; $l_n(P_0, P_\theta) = \log(p_0(D)/p_\theta(D))$.
- Given some constant $B > 0$, we define

  $$r_n^* \coloneqq r_n(L,N,s^*) = ((L+1)s^*/n)\log N + (s^*/n)\log(p\sqrt{n/s^*})$$
  $$\xi_n^* \coloneqq \xi_n(L,N,s^*) = \inf_{\|\theta\|_\infty \le B} \|f_\theta - f_0\|_\infty^2$$
- The squared Hellinger distance is defined as

  $$d^2(P_\theta, P_0) = E_X(1 - \exp(-(f_\theta(X) - f_0(X))^2/8\sigma_\epsilon^2)$$
- In addition, let $s_n = s^* \log^{2\delta-1} n$ for any $\delta > 1$.

**Lemma 1**

With dominating probability,

$$\inf_{q(\theta)\in\mathcal{Q}} \left\{ KL(q(\theta)\|\pi(\theta|\lambda)) + \int_\Theta l_n(P_0, P_\theta) q(\theta) d\theta \right\} \le C' n (r_n^* + \xi_n^*),$$

where $C'$ is any diverging sequence.

**Lemma 2**

If $\sigma_0^2$ is set to be constant and $\lambda \le T^{-1}\exp\{-Mnr_n^*/s_n\}$ for any positive diverging sequence $M$, then with dominating probability,

$$\int_\Theta d^2(P_\theta, P_0)\hat{q}(\theta) \le C\varepsilon_n^{*2} + \frac{3}{n} \inf_{q(\theta)\in\mathcal{Q}} \left\{ KL(q(\theta)\|\pi(\theta|\lambda)) + \int_\Theta l_n(P_0, P_\theta) q(\theta) d\theta \right\},$$

where C is some constant and the estimation error is

$$\varepsilon_n^* \coloneqq \varepsilon_n(L,N,s^*) = \sqrt{r_n(L,N,s^*)}\log^\delta n \text{ , for any } \delta > 1.$$

Lemma 1 and Lemma 2 together imply the following guarantee for VB posterior:

**Theorem 1**

Let $\sigma_0^2$ be a constant and $-\log\lambda = \log T + \delta[(L+1)\log N + \log\sqrt{n}\,p]$ for any constant $\delta > 0$, we have with high probability

$$\int_\Theta d^2(P_\theta, P_0)\hat{q}(\theta) \le C\varepsilon_n^{*2} + C'(r_n^* + \xi_n^*),$$

where $C$ is some positive constant and $C'$ is any diverging sequence.

## Implementation

Since it is impossible to reparameterize the discrete variable $\gamma$ by a continuous system, we apply the Gumbel-softmax approximation (Maddison et al. 2017), and $\gamma_i \sim \text{Bern}(\phi_i)$ is approximated by $\widetilde{\gamma}_i \sim \text{Gumbel-softmax}(\phi_i, \tau)$, where

$$\widetilde{\gamma}_i = (1 + \exp(-\eta_i/\tau))^{-1}, \quad \eta_i = \log\frac{\phi_i}{1-\phi_i} + \log\frac{u_i}{1-u_i},$$
$$u_i \sim \mathcal{U}(0,1), \quad \tau > 0 \text{ is the temperature.}$$

**Algorithm 1** Variational inference for sparse BNN with normal slab distribution.

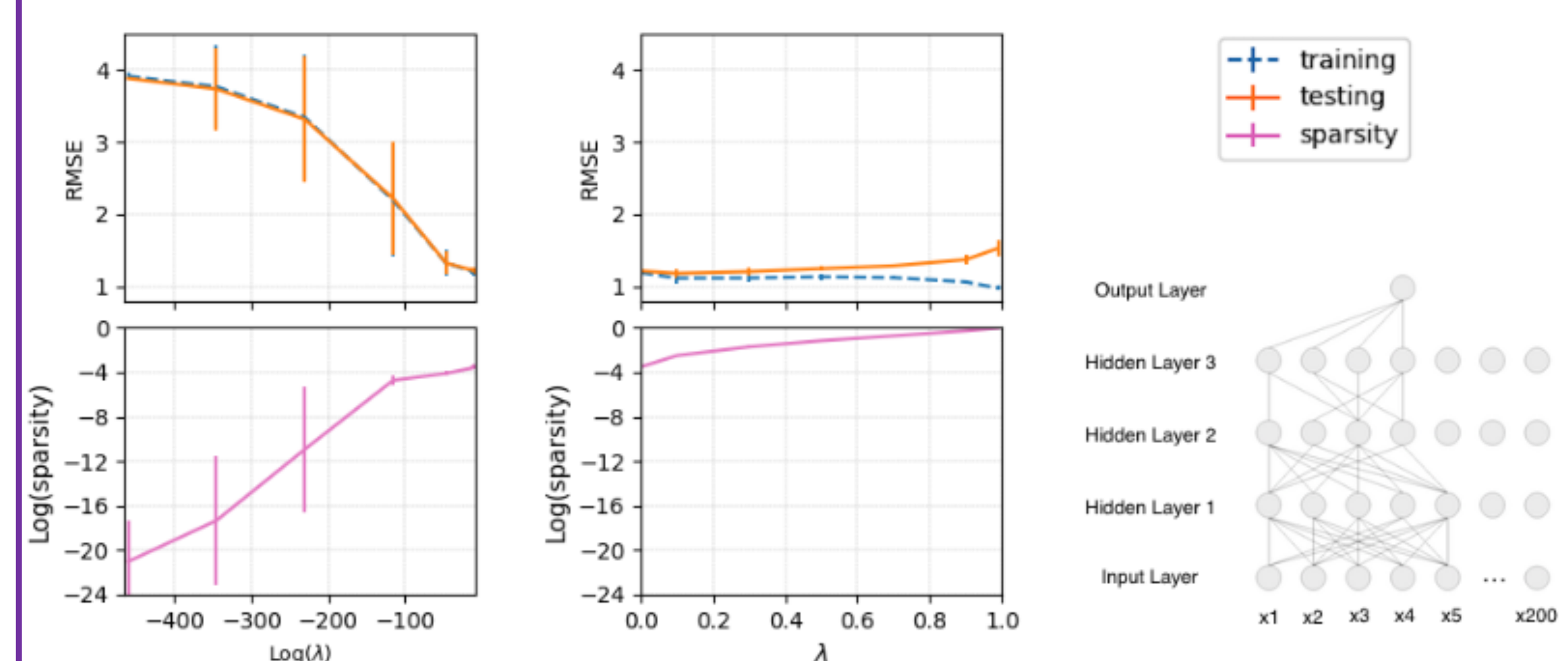
1: parameters: $\omega = (\mu, \sigma', \phi')$ , where $\sigma_i = \log(1+\exp(\sigma_i'))$, $\phi_i = (1+\exp(\phi_i'))^{-1}$
2: objective: negative ELBO $\Omega(\omega)$ ,
3: **repeat**
4: $D^m \leftarrow$ Randomly draw a minibatch of size $m$ from $D$
5: $\epsilon_i, u_i \leftarrow$ Randomly draw $K$ samples from $\mathcal{N}(0,1)$ and $\mathcal{U}(0,1)$
6: $\widetilde{\Omega}^m(\omega) \leftarrow$ Stochastic estimator with ($D^m$, $\omega$, $\epsilon$, $u$); Use $\gamma$ in the forward pass
7: $\nabla_\omega \widetilde{\Omega}^m(\omega) \leftarrow$ Stochastic estimator with ($D^m$, $\omega$, $\epsilon$, $u$); Use $\widetilde{\gamma}$ in the backward pass
8: $\omega \leftarrow$ Update with $\nabla_\omega \widetilde{\Omega}^m(\omega)$ using gradient descent algorithms (e.g. SGD, RMSprop
9: or Adam)
10: **until** convergence of $\widetilde{\Omega}^m(\omega)$
11: **return** $\omega$

## Experiment

Consider the following sparse target function $f_0$:

$$f_0(x_1, \dots, x_{200}) = \frac{7x_2}{1+x_1^2} + 5\sin(x_3x_4) + 2x_5, \ \epsilon \sim \mathcal{N}(0,1)$$

The $\lambda_{opt}$ is chosen according to Theorem 1.




(a) $\lambda \leqslant \lambda_{opt}$. (b) $\lambda \geqslant \lambda_{opt}$. (c) Selected network structure.

Figure 1. Nonlinear regression example.

Figure 1(a) and 1(b) show $\lambda_{opt}$ is a reasonable choice and a possible network structure is provided in 1(c).

**Selected references**

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