# Efficient Variational Inference for Sparse Deep Learning with Theoretical Guarantee

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## 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 ($\|\theta\|_0 \leq s$)

## 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 $\omega$.

**Stochastic estimator of negative ELBO and its gradient**

$$\widetilde{\Omega}^m(\omega) = -\frac{n}{m}\frac{1}{K}\sum_{i=1}^{m}\sum_{k=1}^{K} \log p_{g(\omega,\nu_k)}(D_i) + \mathrm{KL}(q_\omega(\theta)||\pi(\theta)),$$
$$\nabla_\omega \widetilde{\Omega}^m(\omega) = -\frac{n}{m}\frac{1}{K}\sum_{i=1}^{m}\sum_{k=1}^{K} \nabla_\omega \log p_{g(\omega,\nu_k)}(D_i) + \nabla_\omega \mathrm{KL}(q_\omega(\theta)||\pi(\theta)), \quad (1)$$

where $D_i's$ are randomly sampled data points and $g(\omega, \nu_k)$ are the reparameterized version of $\theta$ with some auxiliary noise $\nu_k$ , $m$ and $K$ are minibatch size and Monte Carlo sample size.

## Theoretical Results

**Optimal sparsity level:**

Define $s^*$ as

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

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.

**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:**

Denote the log-likelihood ratio between $p_0$ and $p_\theta$ as $l_n(P_0, P_\theta) = \log(p_0(D)/p_\theta(D)) = \sum_{i=1}^n \log(p_0(D_i)/p_\theta(D_i))$. Given some constant $B > 0$, we define

$$r_n^* := r_n(L,N,s^*) = ((L+1)s^*/n)\log N + (s^*/n)\log(p\sqrt{n/s^*}),$$
$$\xi_n^* := \xi_n(L,N,s^*) = \inf_{\theta \in \Theta(L,\boldsymbol{p},s^*), \|\theta\|_\infty \leq B} ||f_\theta - f_0||_\infty^2.$$

The Hellinger distance is defined as

$$d^2(P_\theta, P_0) = \mathbb{E}_X\left(1 - \exp\{-[f_\theta(X) - f_0(X)]^2/(8\sigma_\epsilon^2)\}\right).$$

In addition, let $s_n = s^* \log^{2\delta-1}(n)$ for any $\delta > 1$.

**Lemma**

*With dominating probability,*

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

*where C is either some positive constant if* $\lim n(r_n^* + \xi_n^*) = \infty$*, or any diverging sequence if* $\limsup n(r_n^* + \xi_n^*) \neq \infty$.

**Lemma**

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

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

*where C is some constant, and*

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

*which is the estimation error from the statistical estimator for* $P_0$.

The above two lemmas together imply the following guarantee for VB posterior:

**Theorem**

*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*

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

*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 $\gamma_i \sim \mathrm{Bern}(\phi_i)$ 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.

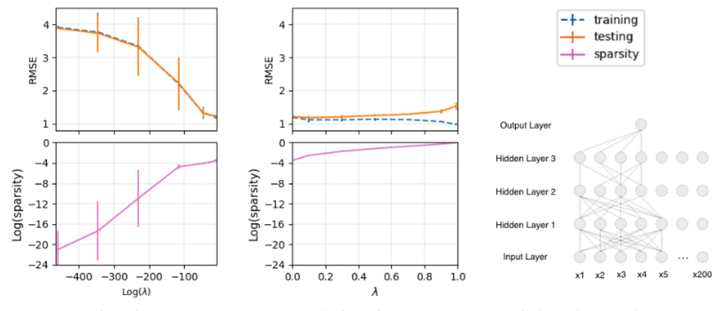
parameters: $\omega = (\mu, \sigma', \phi')$ ,
where $\sigma_i = \log(1+\exp(\sigma_i'))$, $\phi_i = (1+\exp(\phi_i'))^{-1}$, for $i = 1, \dots, T$
**repeat**
  $D^m \leftarrow$ Randomly draw a minibatch of size $m$ from $D$
  $\epsilon_i, u_i \leftarrow$ Randomly draw $K$ samples from $\mathcal{N}(0,1)$ and $\mathcal{U}(0,1)$
  $\widetilde{\Omega}^m(\omega) \leftarrow$ Use (1) with $(D^m, \omega, \epsilon, u)$; Use $\gamma$ in the forward pass
  $\nabla_\omega\widetilde{\Omega}^m(\omega) \leftarrow$ Use (1) with $(D^m, \omega, \epsilon, u)$; Use $\widetilde{\gamma}$ in the backward pass
  $\omega \leftarrow$ Update with $\nabla_\omega\widetilde{\Omega}^m(\omega)$ using gradient descent algorithms (e.g. SGD, RMSprop or Adam)
**until** convergence of $\widetilde{\Omega}^m(\omega)$
**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 the main theorem.




(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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