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 θ 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 ($\|\theta\|_0 \le s$)

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 λ and σ_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 ω.

Stochastic estimator of negative ELBO and its gradient

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

where $D_i's$ are randomly sampled data points and $g(\omega, \nu_k)$ are the reparameterized version of θ with some auxiliary noise ν_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 ξ_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 σ_0^2 is set to be some constant, and λ 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_θ 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

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

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* $\limsup n(r_n^* + \xi_n^*) \ne \infty$.

Lemma

If σ_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,*

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

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 σ_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*

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

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

Implementation

Since it is impossible to reparameterize the discrete variable γ 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 $\widetilde{\gamma}_i \sim$ Gumbel-softmax(ϕ_i, τ), 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.

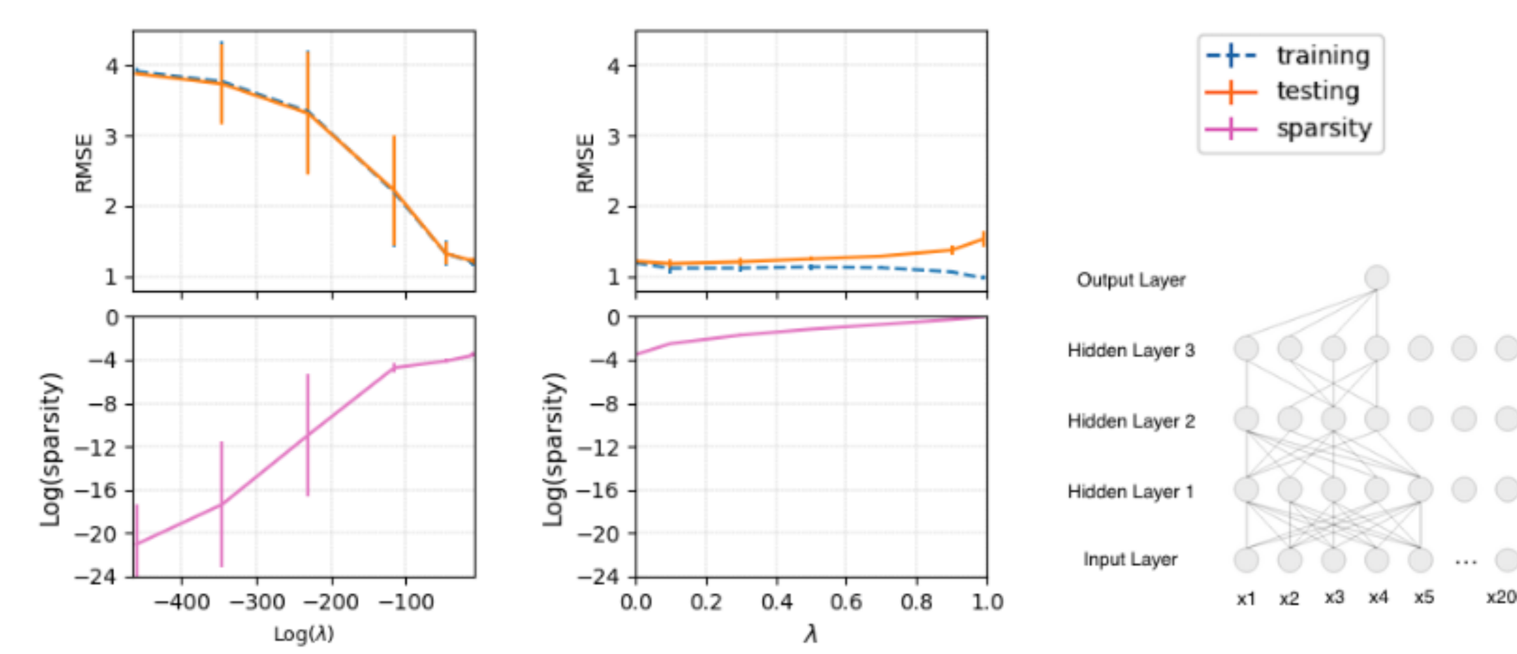
parameters: $\omega = (\mu, \sigma', \phi')$,
where $\sigma_i = \log(1 + \exp(\sigma_i'))$, $\phi_i = (1 + \exp(\phi_i'))^{-1}$, for $i = 1, \dots, T$
repeat
  $D^m \leftarrow$ Randomly draw a minibatch of size m from D
  $\epsilon_i, u_i \leftarrow$ Randomly draw K samples from $\mathcal{N}(0,1)$ and $\mathcal{U}(0,1)$
  $\widetilde{\Omega}^m(\omega) \leftarrow$ Use (1) with $(D^m, \omega, \epsilon, u)$; Use γ 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 ω

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 λ_{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 λ_{opt} is a reasonable choice and a possible network structure is provided in 1(c).

Selected references

Ghosh, S., Yao, J., and Doshi-Velez, F. (2018). Structured variational learning of Bayesian neuralnetworks with horseshoe priors. In ICML 2018.

Maddison, C., Mnih, A., and Teh, Y. W. (2017). The concrete distribution: A continuous relaxation ofdiscrete random variables. In ICLR 2017.

Polson, N. and Rockova, V. (2018). Posterior concentration for sparse deep learning. In NeurIPS 2018.

Zhu, M. and Gupta, S. (2018). To prune, or not to prune: Exploring the efficacy of pruning for model compression. In ICLR 2018