

Bayesian Neural Networks

ROY team: Ilya Zharikov,
Roman Isachenko,
Artem Bochkarev

Skolkovo Institute of Science and Technology
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Project goal

Aim

Estimate posterior distribution of the model parameters from data

Problem

Monte Carlo sampling is very slow for high-dimensional data

Probabilistic Programming

- Uncertainty in predictions
- Uncertainty in representations
- Regularizations with priors
- Transfer learning
- Hierarchical Neural Networks

- 1 Salvatier J, Wiecki T. V., Fonnesbeck C. Probabilistic programming in Python using PyMC3. // *PeerJ Computer Science*. 2016.
- 2 Blundell C. et al. Weight Uncertainty in Neural Network // *Proceedings of The 32nd International Conference on Machine Learning*. 2015.
- 3 Kucukelbir A. et al. Automatic Differentiation Variational Inference // *arXiv preprint arXiv:1603.00788*. – 2017.

Problem Statement

Bayes Theorem

$$p(\theta|X) = \frac{p(X|\theta)p(\theta)}{p(X)}$$

Frequentist approach

$$\theta^* = \arg \max_{\theta} p(\theta|X) = \arg \max_{\theta} p(X|\theta) + p(\theta)$$

Monte Carlo approach

- Metropolis Hasting
- Gibbs sampling
- No-U-Turn Sampling (NUTS)

$$\ln p(X) = \text{KL}(q||p) + \text{ELBO}(q)$$

$$\text{KL}(q||p) = \int q(\theta) \ln \frac{q(\theta)}{p(\theta|X)} d\theta; \quad \text{ELBO}(q) = \int q(\theta) \ln \frac{p(X, \theta)}{q(\theta)} d\theta$$

Problem

minimization of $\text{KL}(q||p) \Leftrightarrow$ maximization of $\text{ELBO}(q)$

ADVI

- Transformation of constrained variables
- $q(\theta)$ comes from parametric family (usually $\mathcal{N}(\mu, \text{diag}(\sigma^2))$)
- Stochastic optimization
- Integral differentiation \Rightarrow reparametrization trick

Neural Networks

- **Neural networks** predict values of parameters by fitting complex model on the huge dataset
- **Bayesian Neural Networks** predict the parameters distributions

