Bayesian Neural Networks

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Project goal

Goal

Estimate posterior distributions 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.

Related work

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

Inference problem

Bayes' theorem states: $\mathbb{P}(\boldsymbol{\theta} \mid \mathbf{X}) = \dfrac{\mathbb{P}(\mathbf{X} \mid \boldsymbol{\theta})\mathbb{P}(\boldsymbol{\theta})}{\mathbb{P}(\mathbf{X})}$

Maximum A Posteriori (MAP) estimation

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \left[\ln \mathbb{P}(\boldsymbol{\theta} \mid \mathbf{X})\right] = \arg\max_{\boldsymbol{\theta}} \left[\ln \mathbb{P}(\mathbf{X} \mid \boldsymbol{\theta}) + \ln \mathbb{P}(\boldsymbol{\theta})\right]$$

Monte Carlo approach:

- Metropolis-Hastings sampling;
- Gibbs sampling;
- No-U-Turn Sampling (NUTS).

Variational Inference

Goal

Approximate posterior distribution $p(X, \theta)$ by function $q(\theta)$ from parametric family.

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

$$\Updownarrow \qquad\qquad \Updownarrow$$

$$\int q(\boldsymbol{\theta}) \ln \frac{q(\boldsymbol{\theta})}{p(\boldsymbol{\theta}|\mathbf{X})} \mathrm{d}\boldsymbol{\theta} \qquad \int q(\boldsymbol{\theta}) \ln \frac{p(\mathbf{X}, \boldsymbol{\theta})}{q(\boldsymbol{\theta})} \mathrm{d}\boldsymbol{\theta}$$

Minimization of $\mathbf{KL(q||p)}$ $\Leftrightarrow$ Maximization of $\mathbf{ELBO(q)}$

Automatic Differentiation Variational Inference (ADVI)

- Automatic transformation of constrained variables $\boldsymbol{\zeta} = T(\boldsymbol{\theta})$;
  Example: $\theta \in \mathbb{R}_+ \Rightarrow \zeta = T(\theta) = \log \theta$, then $\zeta \in \mathbb{R}$.
- $q(\boldsymbol{\zeta}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, where $\boldsymbol{\Sigma}$ is diagonal;

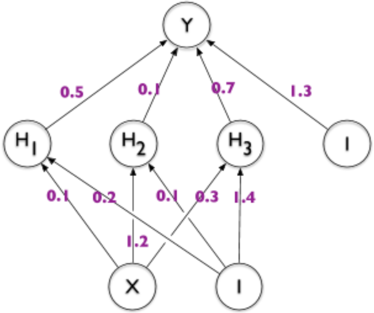
$$\boldsymbol{\mu}^*, \boldsymbol{\Sigma}^* = \arg\max_{\boldsymbol{\mu}, \boldsymbol{\Sigma}} \mathrm{ELBO}(q)$$

- Stochastic optimization;
- Reparametrization trick to apply automatic differentiation;
- Adaptive step-size.

Difference

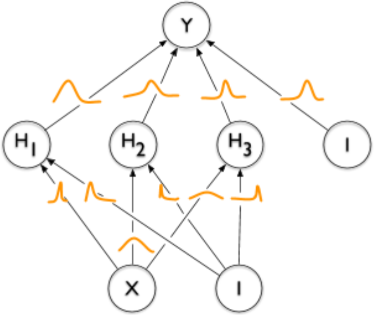
Neural Networks

Predict values of parameters by fitting complex model on the huge dataset



Bayesian Neural Networks

Predict the parameters of the weights distributions from the dataset



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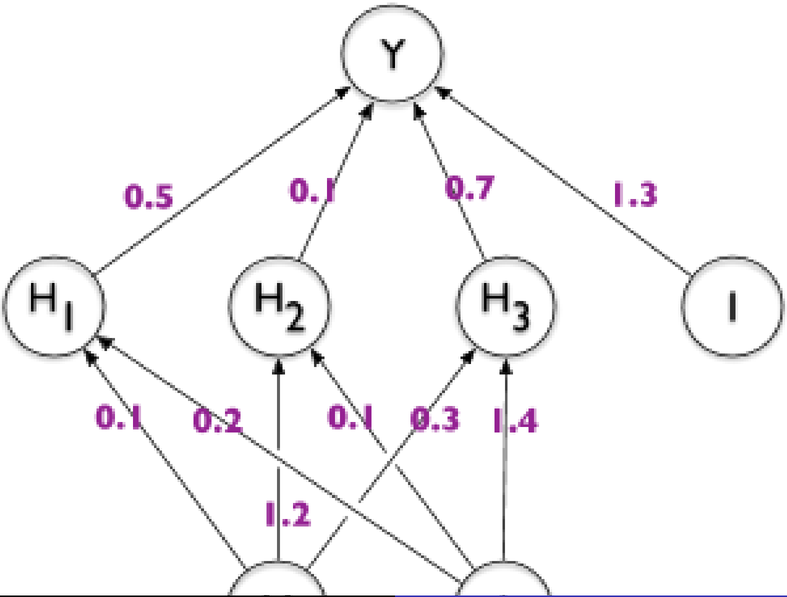
http://bit.ly/2rMQuDq

Deep Learning



Experiments

- Synthetic datasets: moons, circles
- Real data: MNIST

Goals:

- investigate influence of different priors on the predictions
- visualize uncertainties in predictions
- analyze the model behaviour

Experiments

Experiments