Bayesian Neural Networks

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Deep Learning course

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Project goal

Goal

Estimate posterior distributions of the model parameters from data

Probabilistic Programming:

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

Problem

Monte Carlo sampling is very slow for high-dimensional data

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: $\mathbb{P}(\boldsymbol{\theta} \,|\, \mathbf{X}) = \dfrac{\mathbb{P}(\mathbf{X} \,|\, \boldsymbol{\theta})\mathbb{P}(\boldsymbol{\theta})}{\mathbb{P}(\mathbf{X})}$

Maximum A Posteriori (MAP) estimation

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\arg\max}\,[\ln \mathbb{P}(\boldsymbol{\theta} \,|\, \mathbf{X})] = \underset{\boldsymbol{\theta}}{\arg\max}\,[\ln \mathbb{P}(\mathbf{X} \,|\, \boldsymbol{\theta}) + \ln \mathbb{P}(\boldsymbol{\theta})]$$

Monte Carlo approach:

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

Variational Inference

Goal

Approximate posterior distribution $p(\boldsymbol{\theta}|\boldsymbol{X})$ by function $q(\boldsymbol{\theta})$ from parametric family.

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

$$\Updownarrow \qquad \Updownarrow$$

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

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;

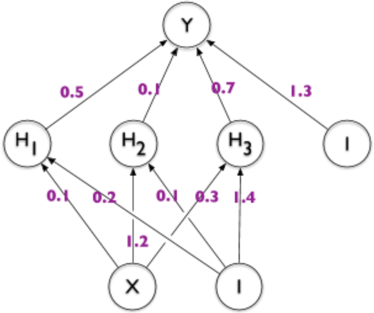
$$\boldsymbol{\mu}^*, \boldsymbol{\Sigma}^* = \arg\max_{\boldsymbol{\mu}, \boldsymbol{\Sigma}} \mathrm{ELBO}(q)$$

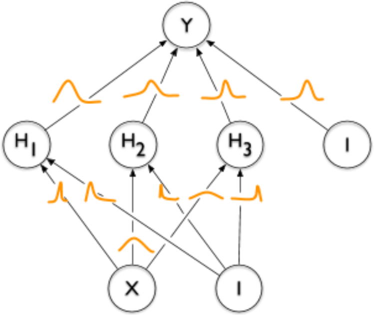
- Stochastic optimization;
- Reparametrization trick to apply automatic differentiation;
- Adaptive step-size.

Deep Learning

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





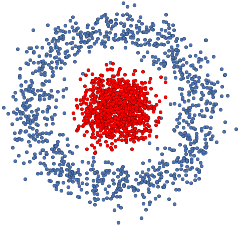
http://bit.ly/2rMQuDq

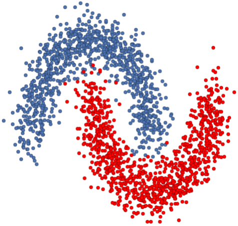
Experiments

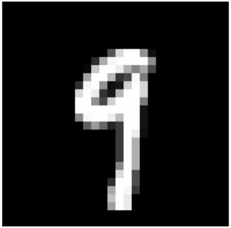
Goals:

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

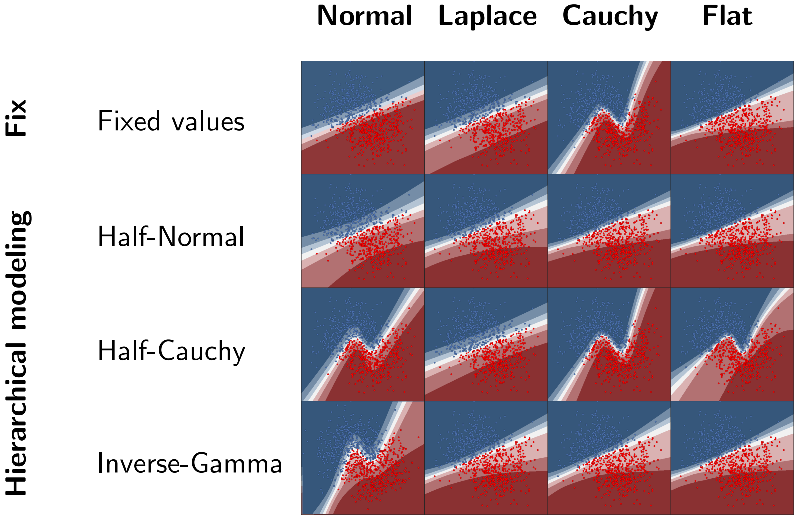
Datasets:







Course of work

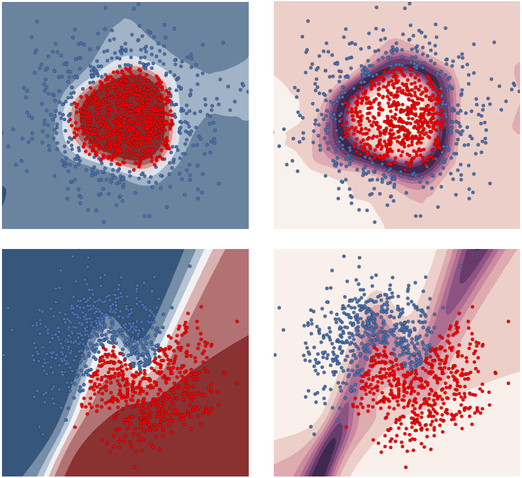


Synthetic data

Posterior Probability | **Uncertainty**

Prior: Cauchy
Hyperprior: Inverse-Gamma
Accuracy: 0.735

Prior: Normal
Hyperprior: Inverse-Gamma
Accuracy: 0.851

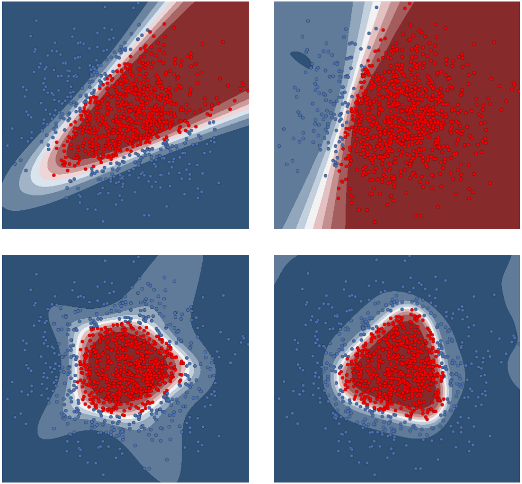


Hierarchical modelling

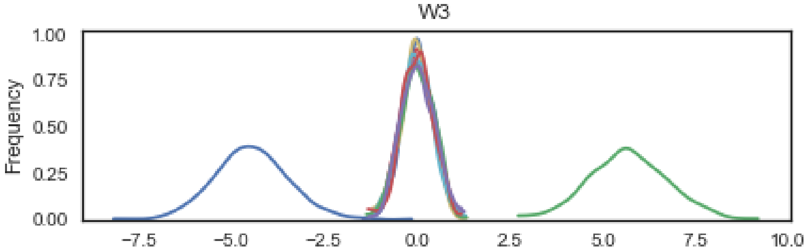
Prior: Normal | **Prior:** Laplace

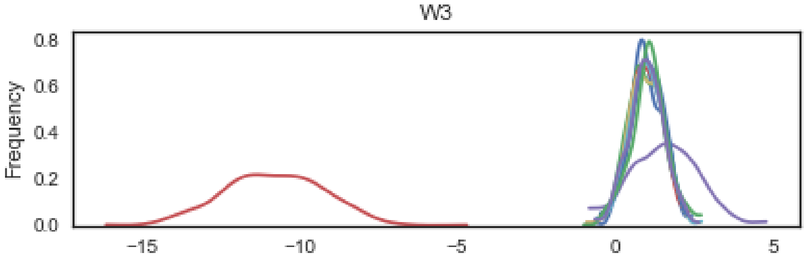
Hyperprior: Fixed values

Hyperprior: Inverse-Gamma

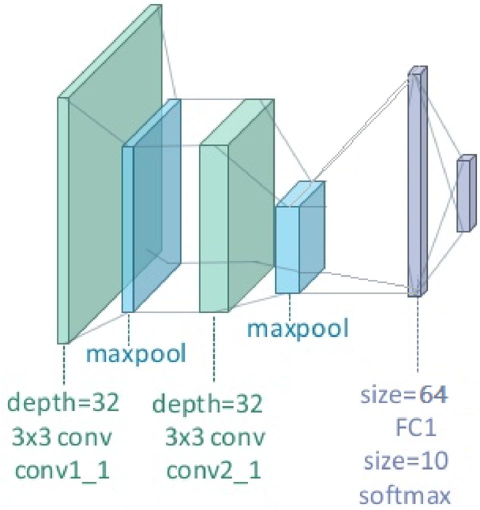


Laplace sparsity



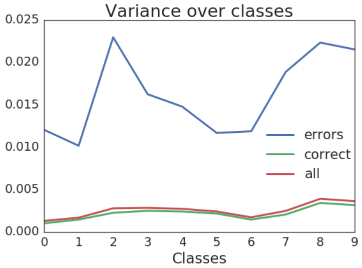


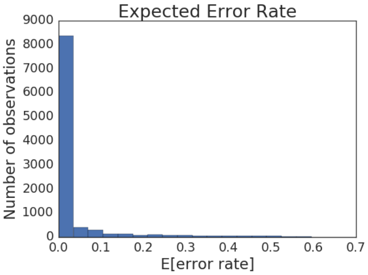
MNIST



maxpool
maxpool
depth=32
3x3 conv
conv1_1
depth=32
3x3 conv
conv2_1
size=64
FC1
size=10
softmax

MNIST





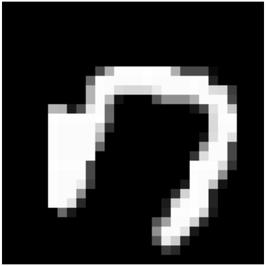
Conclusions:

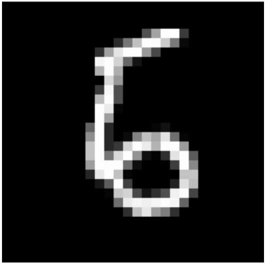
- Accuracy score: 97.7%;
- Variance is much higher for misclassified pictures;
- Model is not always confident.

MNIST

Misclassified pictures with **zero expected error rate**:

True	Prediction	True	Prediction	True	Prediction
7	0	9	7	5	6

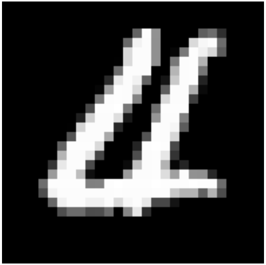


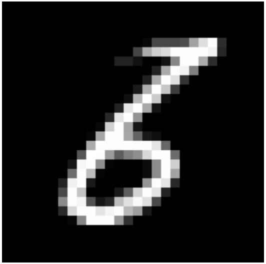


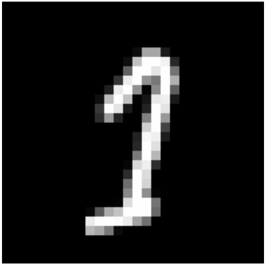
MNIST

Pictures with the **lowest confidence**:

True	Prediction	True	Prediction	True	Prediction
4	0	6	8	1	1







Conclusion

- Posterior distribution helps to make conclusions about uncertainties
- Variational inference allows to approximate posterior distribution for high-dimensional data
- Hierarchical models have more degrees of freedom