Bayesian Deep Learning

Extending Probabilistic Backpropagation and Transfer Learning

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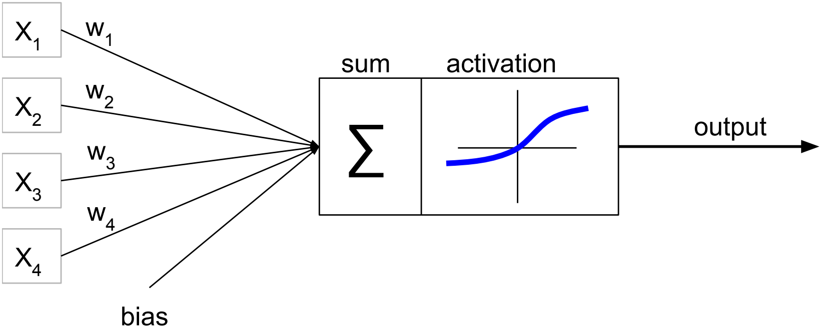
Overview

- Neural Networks
- Bayesian Neural Networks
  - Laplace Approximation
  - Variational Inference
  - Assumed Density Filtering
  - Probabilistic Backpropagation
- Preliminary Work
- Planned Contributions

Perceptron

Basic unit of neural network, described by:

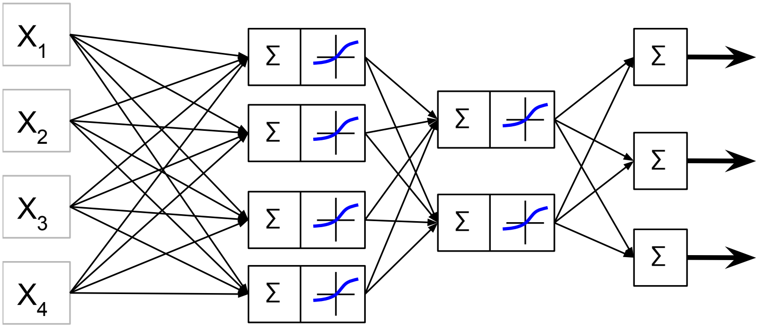
$$f(\mathbf{x}) = \sigma(\mathbf{x}^\top \omega)$$



Frank Rosenblatt. *The Perceptron, a Perceiving and Recognizing Automaton*. Tech. rep. Cornell Aeronautical Laboratory, 1957.

Multi-layer Perceptron

Many perceptrons arranged in layers



Backpropagation (BP)

- BP minimizes a cost function:

  Regression $\|Y - \texttt{NN}(\mathbf{x};\mathcal{W})\|_2^2$

  Classification $-\sum_{k=1}^{K} Y_k \log(\texttt{NN}_k(\mathbf{x};\mathcal{W}))$

- Optional regularization:

  L1 $\lambda \sum_{l,i,j} |W_{lij}|$

  L2 $\lambda \sum_{l,i,j} W_{lij}^2$

- Cleverly applies chain rule of derivatives

$$Z = e^{-Y}, \qquad Y = \frac{1}{1+e^{-X}}$$

$$\frac{dZ}{dY} = -Z, \qquad \frac{dZ}{dX} = \frac{dZ}{dY}\frac{dY}{dX} = -ZY(1-Y)$$

Deep Neural Networks

Advantages:

- Flexible, fast to train (e.g., SGD with backpropagation)
- Can achieve high accuracy/precision/recall
  - Identifying objects in images (Szegedy et al. 2015)
  - Melanoma detection from images (Esteva et al. 2017)
  - Tuberculosis detection from chest x-rays (Lakhani and Sundaram 2017)

Drawbacks:

- Typically, only provides point estimates
- Tendency for overfitting
- Unclear choice of structure

Christian Szegedy et al. Going Deeper with Convolutions. In: *Computer Vision and Pattern Recognition*. 2015.

Andre Esteva et al. Dermatologist-level Classification of Skin Cancer with Deep Neural Networks. In: *Nature* 542.7639 (2017), p. 115.

Paras Lakhani and Baskaran Sundaram. Deep Learning at Chest Radiography: Automated Classification of Pulmonary Tuberculosis by using Convolutional Neural Networks. In: *Radiology* 284.2 (2017), pp. 574–582.

From Backpropagation to Bayesian Neural Networks

Introduce joint probability model:

- Likelihood: $p(Y|\theta)$

  Regression $p(Y|\mathcal{W}, \sigma^2, \mathbf{x}) = N(Y; \mathtt{NN}(\mathbf{x}; \mathcal{W}), \sigma^2)$
  Classification $p(Y|\mathcal{W}, \mathbf{x}) = \text{Categorical}(Y; \mathtt{NN}(\mathbf{x}; \mathcal{W}))$

- Prior distribution: $p(\theta)$

  Independent $w_{lij} \overset{\text{iid}}{\sim} N(0, \tau)$
  Correlated $w_l \sim MN(M, R, C)$, see (Louizos and Welling 2016)

- Posterior distribution:

$$p(\theta|Y) = \frac{p(Y|\theta)p(\theta)}{\int p(Y|\theta)p(\theta)d\theta}$$

Christos Louizos and Max Welling. Structured and Efficient Variational Deep Learning with Matrix Gaussian Posteriors. In: *International Conference on Machine Learning*. 2016, pp. 1708–1716.

Bayesian Neural Networks (BNNs)

The problem:

- Posterior (or posterior predictive, etc.) is intractable
- MCMC possible for small networks (Neal 1993)

Methods used for BNN inference:

- **Assumed density filtering**
- Dropout as deep GP (Gal and Ghahramani 2016)
- Expectation propagation (Soudry et al. 2014)
- **Laplace approximation**
- **Variational inference**

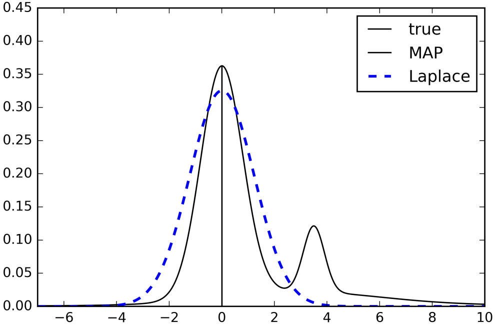
Radford M Neal. Bayesian Learning via Stochastic Dynamics. In: *Advances in Neural Information Processing Systems*. 1993, pp. 475–482.

Yarin Gal and Zoubin Ghahramani. Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. In: *International Conference on Machine Learning*. 2016, pp. 1050–1059.

Daniel Soudry et al. Expectation Backpropagation: Parameter-free Training of Multilayer Neural Networks with Continuous or Discrete Weights. In: *Advances in Neural Information Processing Systems*. 2014, pp. 963–971.

Laplace Approximation

- Approximate posterior introduced by (MacKay 1992)
- Identify MAP estimate by standard backpropagation
- Locally-quadratic approximation to form a Gaussian



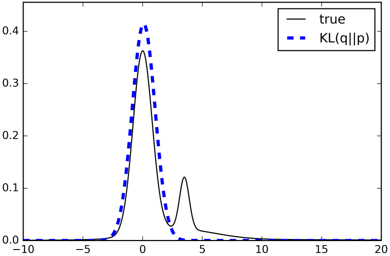
David JC MacKay. A Practical Bayesian Framework for Backpropagation Networks. In: *Neural Computation* 4.3 (1992), pp. 448–472.

Variational Inference

- Posit variational family $\mathcal{Q}$ to approximate $p(W|\mathcal{D})$
- Identify $q(W) \in \mathcal{Q}$ that minimizes

$$KL(q(W)\|p(W|\mathcal{D})) = \int_{\mathcal{W}} q(W) \log\left(\frac{q(W)}{p(W|\mathcal{D})}\right) dW$$

- Applied to BNNs by (Graves 2011) with MCMC likelihood



Alex Graves. Practical Variational Inference for Neural Networks. In: *Advances in Neural Information Processing Systems*. 2011, pp. 2348–2356.

Assumed Density Filtering

Approximate Bayesian approach to online learning (Opper and Winther 1998)

- Approximate posterior $q(\theta|\gamma_t)$ at iteration t with parameters γ_t
  - For example, if q is Gaussian, $\gamma_t = (\mu_t, \sigma_t^2)$
- Given new data y_{t+1}:

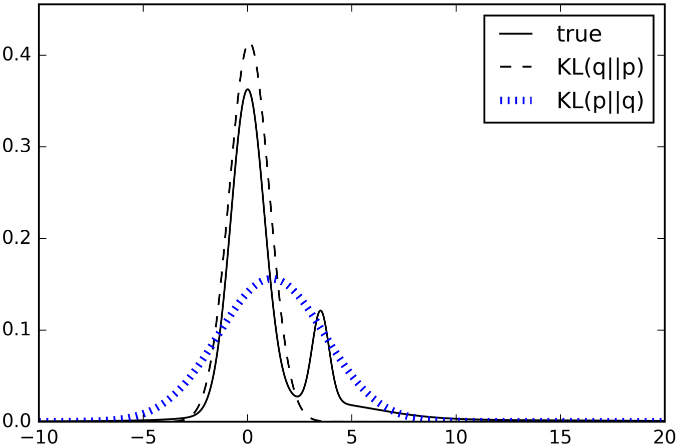
  Update Update "exact" posterior:

$$p(\theta|y_{t+1}, \gamma_t) = \frac{p(y_{t+1}|\theta)q(\theta|\gamma_t)}{\int p(y_{t+1}|\theta)q(\theta|\gamma_t)d\theta}$$

  Projection $\gamma_{t+1} := \arg\min_{\gamma} D\left(p(\cdot|y_{t+1}, \gamma_t) \parallel q(\cdot|\gamma)\right)$

Manfred Opper and Ole Winther. A Bayesian Approach to On-line Learning. In: *On-line Learning in Neural Networks, ed. D. Saad* (1998), pp. 363–378.

Assumed Density Filtering



Probabilistic Backpropagation (PBP)

ADF algorithm for BNNs (Hernández-Lobato and Adams 2015)

- Normal prior on all weights:

$$w_{lij} \overset{\text{iid}}{\sim} N(0, \tau)$$

- Independent normal approximate posterior on each weight:

$$q(w_{lij}) = N(w_{lij} | m_{lij}, v_{lij})$$

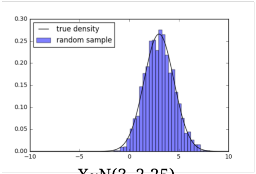
- Regression likelihood: $Y | \mathbf{x}, \mathcal{W} \sim N(\mathtt{NN}(\mathbf{x}; \mathcal{W}), \gamma^{-1})$
- Sequential closed-form approximation for normalization constant, posterior predictive

José Miguel Hernández-Lobato and Ryan Adams. Probabilistic Backpropagation for Scalable Learning of Bayesian Neural Networks. In: *International Conference on Machine Learning*. 2015, pp. 1861–1869.

Probabilistic Backpropagation (PBP)

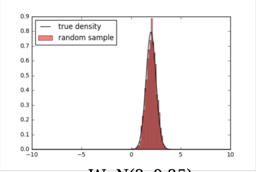
Closed-form approximations match moments to a Gaussian

Illustration with simulated data:



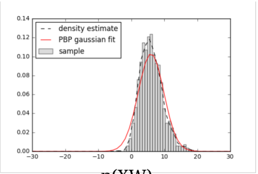
X~N(3, 2.25)

X

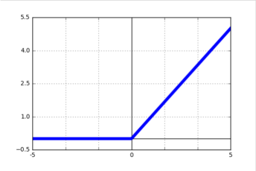


W~N(2, 0.25)

=

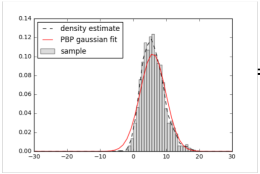


p(XW)



f(z)=max(0, z)

O



p(XW)

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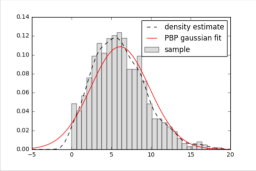
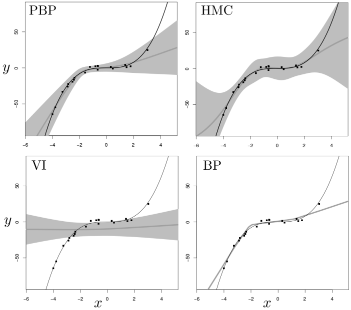


p(f(XW))

PBP Properties

- Trains like standard MLP, so it's fast
- Only given for regression with ReLU activation
- Extended by (Ghosh et al. 2016) to binary classification (probit) and multiclass via MCMC step



Soumya Ghosh et al. Assumed Density Filtering Methods for Learning Bayesian Neural Networks. In: *AAAI Conference on Artificial Intelligence*. 2016, pp. 1589–1595.

Hernández-Lobato and Adams 2015, Figure 1.

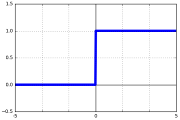
Comparison

	MCMC	**VI**	**PBP**
Object	w	$q(w)$	$q(w)$
Strategy	Simulation	Optimization	Optimization
Integrals	Sample MCMC chain	Sample $q(w)$	Closed-form approximations
Scale	?	Y	Y
Speed	N	?	Y
Papers	(Neal 1993)	(Graves 2011)	(Hernández-Lobato and Adams 2015)

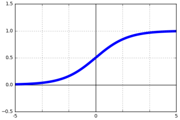
Preliminary Work

Exploring other activation functions

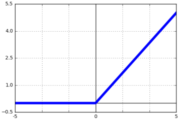
Step $\sigma(z) = \mathbb{1}\{z \geq 0\}$



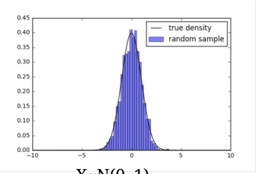
Sigmoid $\sigma(z) = 1/(1 + e^{-z})$



ReLU $\sigma(z) = \max(0, z)$

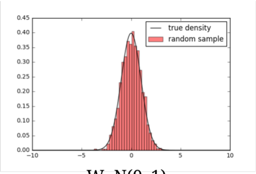


Preliminary Work



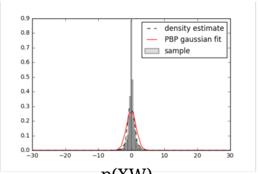
X~N(0, 1)

X

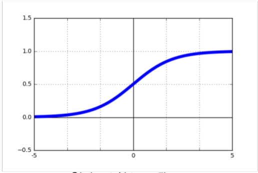


W~N(0, 1)

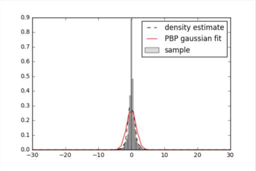
=



p(XW)

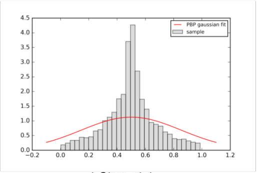

$f(z)=1/(1+e^{-z})$

O



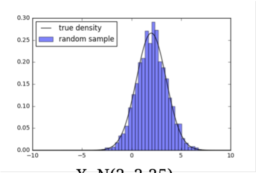
p(XW)

=



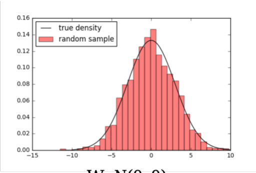
p(f(XW))

Preliminary Work



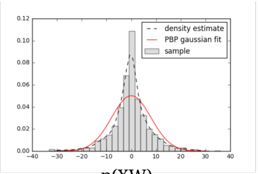
X~N(2, 2.25)

X

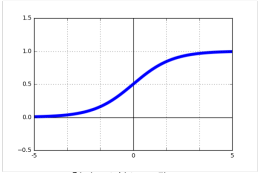


W~N(0, 9)

=

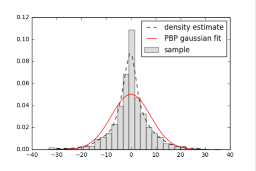


p(XW)



$f(z)=1/(1+e^{-z})$

O



p(XW)

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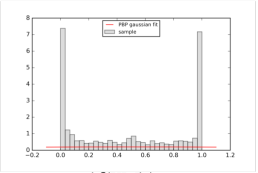
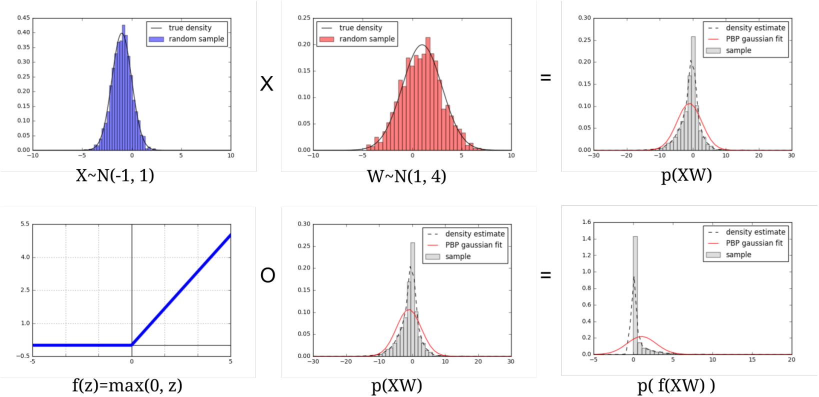


p(f(XW))

Current and Past Work



Led to questions about Gaussian approximation - replace with spike and slab?

$$q(w) = (1 - \pi)\delta_0(w) + \pi N(w; \mu, \sigma^2)$$

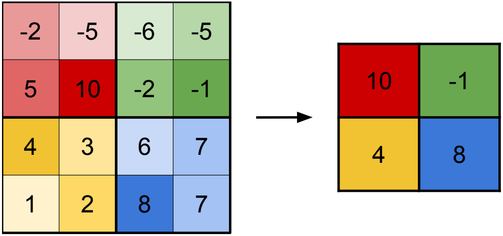
Planned Contributions

Classification Alternative to softmax without MCMC?

$$\hat{p}_i = \mathrm{Softmax}_i(\mathbf{x}) = \frac{e^{x_i}}{\sum_j e^{x_j}}$$

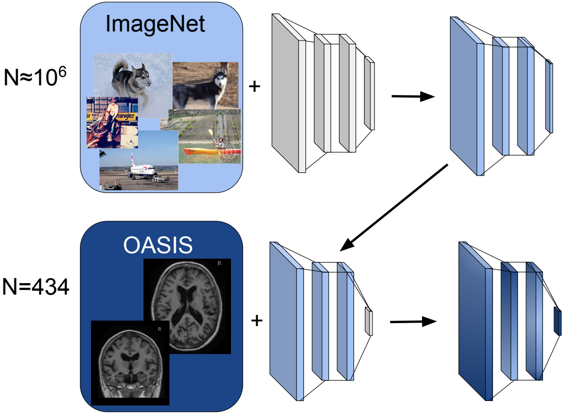
$$\tilde{p}_i = p(\mathtt{NN}(\mathbf{x}; \mathcal{W}) \in \mathcal{A}_i)$$

Pooling Need approximation for $p\left(\max\left(X_1, X_2, \ldots, X_k\right)\right)$



Planned Contributions

Bayesian version of transfer learning



Olga Russakovsky et al. ImageNet Large Scale Visual Recognition Challenge. In: *International Journal of Computer Vision* 115.3 (2015), pp. 211–252.

Daniel S Marcus et al. Open Access Series of Imaging Studies: Longitudinal MRI Data in Nondemented and Demented Older Adults. In: *Journal of Cognitive Neuroscience* 22.12 (2010), pp. 2677–2684.

Summary

- Deep neural networks in real-world problems
- Quantifying uncertainty critical for decision-making
- PBP as scalable, flexible BNN framework
- Need Bayesian analogues for deep learning practices

Thanks

Questions?

This presentation:
https://www.evanott.com/research/Oral_Exam.pdf

References I

- Esteva, Andre, Brett Kuprel, Roberto A Novoa, Justin Ko, Susan M Swetter, Helen M Blau, and Sebastian Thrun. Dermatologist-level Classification of Skin Cancer with Deep Neural Networks. In: *Nature* 542.7639 (2017), p. 115.
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- Graves, Alex. Practical Variational Inference for Neural Networks. In: *Advances in Neural Information Processing Systems*. 2011, pp. 2348–2356.

References II

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References III

Marcus, Daniel S, Anthony F Fotenos, John G Csernansky, John C Morris, and Randy L Buckner. Open Access Series of Imaging Studies: Longitudinal MRI Data in Nondemented and Demented Older Adults. In: *Journal of Cognitive Neuroscience* 22.12 (2010), pp. 2677–2684.

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Rosenblatt, Frank. *The Perceptron, a Perceiving and Recognizing Automaton*. Tech. rep. Cornell Aeronautical Laboratory, 1957.

References IV

Russakovsky, Olga, Jia Deng, Hao Su, Jonathan Krause, Sanjeev Satheesh, Sean Ma, Zhiheng Huang, Andrej Karpathy, Aditya Khosla, Michael Bernstein, Alexander C. Berg, and Li Fei-Fei. ImageNet Large Scale Visual Recognition Challenge. In: *International Journal of Computer Vision* 115.3 (2015), pp. 211–252.

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References V

Szegedy, Christian, Wei Liu, Yangqing Jia, Pierre Sermanet, Scott Reed, Dragomir Anguelov, Dumitru Erhan, Vincent Vanhoucke, and Andrew Rabinovich. Going Deeper with Convolutions. In: *Computer Vision and Pattern Recognition*. 2015.

Hamiltonian Monte Carlo

- Let q be the parameters of our distribution $P(q)$
- Define potential energy $E(q)$ as $P(q) \propto \exp(-E(q))$
- Augment space to include momentum vector p, same dimension as q
- Define Hamiltonian $H(q,p) = E(q) + \frac{1}{2}\|p\|_2^2$
- Use Hamiltonian dynamics for equal-energy trajectories:

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} = p \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q} = -\nabla E(q)$$

- Use log posterior
  $-\log P(q) = -\log f(X|q) - \log \pi(q) + \log p(X)$
- Find valid state, give it a kick, follow trajectory, move via Metropolis-Hastings.

Dropout as Variational Inference

(Gal and Ghahramani 2016)

- Stochastically set nodes in network to 0
- Connection to deep Gaussian process
- Really, dropout is a regularizer
- Matt Taddy and others: variational dropout provides poor variance estimates

Gal and Ghahramani 2016.