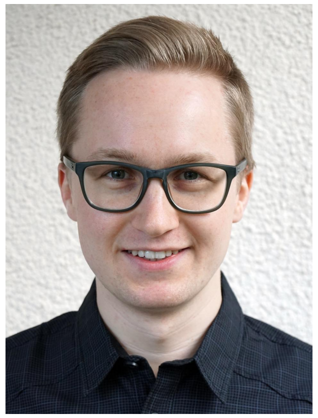
Thirty-seventh International Conference on Machine Learning (ICML 2020)

Training Binary Neural Networks Using the Bayesian Learning Rule



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(EPFL)

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(RIKEN AIP)

Binary Neural Networks (BiNN)

- BiNN: Neural Networks with binary weights
- Much faster and much smaller [1,2]
- Difficult to optimize in theory (discrete optimization)
- But easy in practice: Just use SGD with "Straight-through estimator (STE)"!
- It is mysterious as to why this works [3]
- Are there any principled approaches to explain this?

1. Courbariaux et al., Training deep neural networks with binary weights during propagations. NeurIPS 2015.
2. Courbariaux et al., . Binarized neural networks.… arXiv:1602.02830, 2016.
3. Yin, P. et al., Understanding straight-through estimator in training activation quantized neural nets. arXiv, 2019.

Our Contribution: Training BiNN using Bayes

- We show that by using the Bayesian Learning Rule [1,2] (natural-gradient variational inference), we can justify such previous approaches

  - Main point: optimize the parameter of a Bernoulli distribution (a continuous optimization problem)

- The Bayesian approach gives us an estimate of uncertainty which can be used for continual learning [3]

1. Khan, M. E. and Rue, H. Learning-algorithms from bayesian principles. ArXiv. 2019.
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Training BiNN is a Discrete Optimization problem!

Binary weights

Output

Input

$$\min_{\boldsymbol{w}\in\{-1,1\}^W} \sum_{i\in\mathcal{D}} \ell(y_i, f_{\boldsymbol{w}}(\boldsymbol{x}_i))$$

Loss

Neural Network

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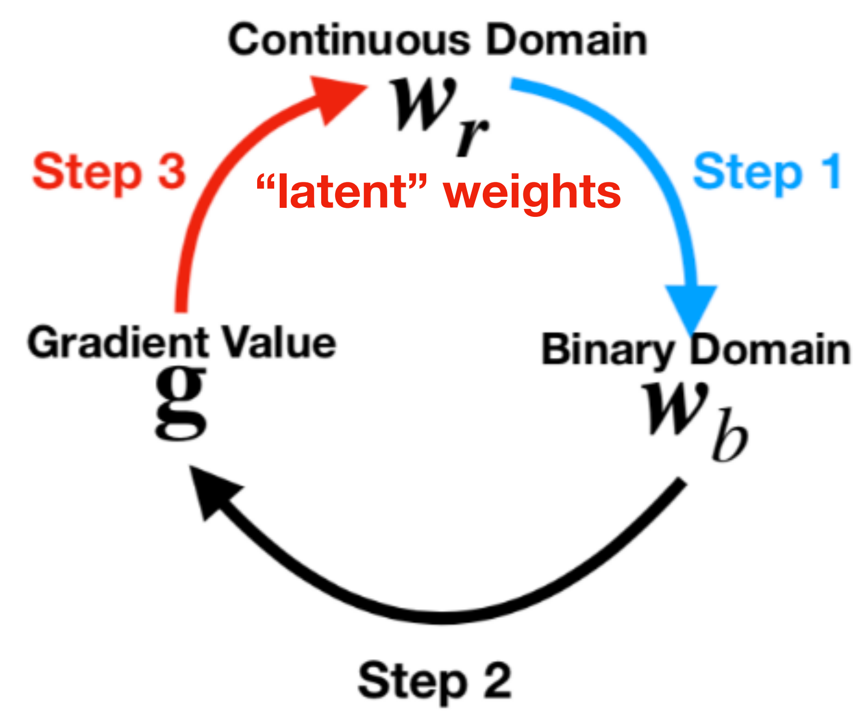
Loss Neural Network

- Easy in practice: SGD with "Straight-through estimator (STE)" [1]



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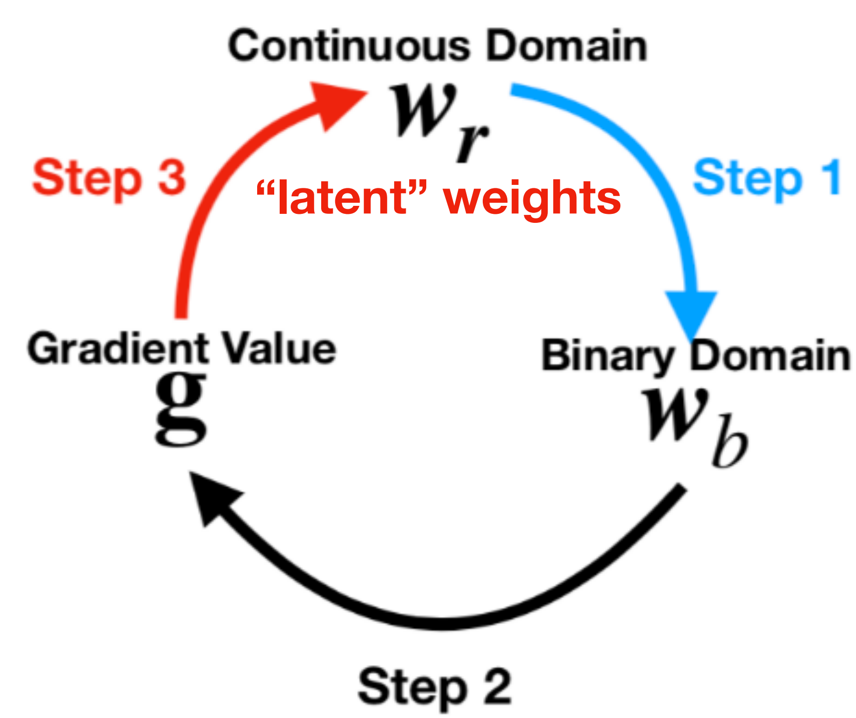
  → Binary Optimizer (Bop)



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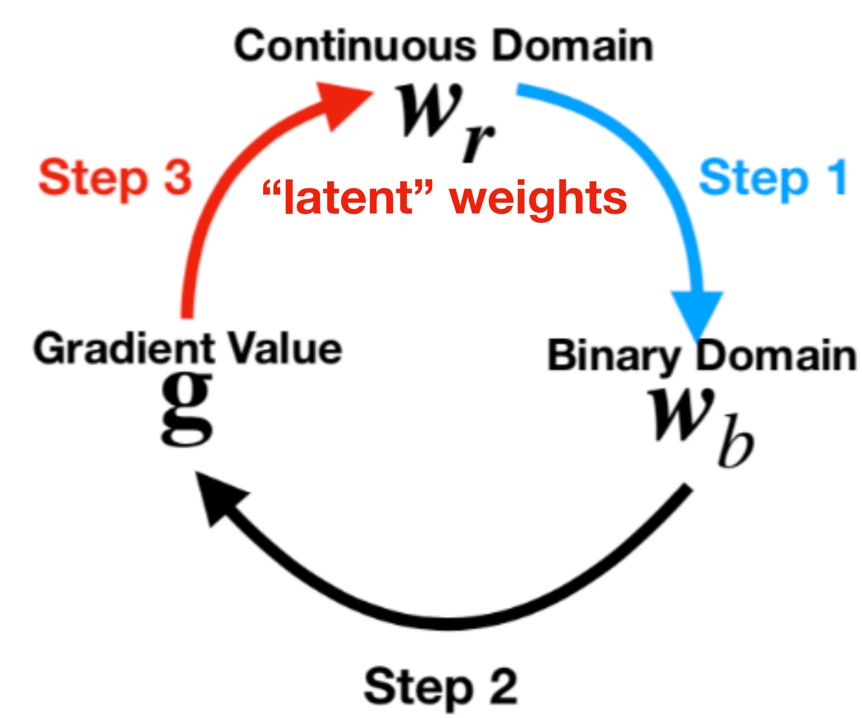
- Easy in practice: SGD with "Straight-through estimator (STE)" [1]
- Helwegen et al. [2] argued "latent" weights are not weights but "Inertia"
  - → Binary Optimizer (Bop)
- Open question: Why does this work?[3]



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BayesBiNN

- Main point: optimize the parameters of Bernoulli distribution (a continuous optimization problem)
- Problem reformulation: Optimize distribution over weights[1,2]

Loss

$$\min_{q(\boldsymbol{w})} \quad \mathbb{E}_{q(\boldsymbol{w})}\left[\sum_{i=1}^{N} \ell(y_i, f_{\boldsymbol{w}}(\boldsymbol{x}_i))\right] + \mathbb{D}_{KL}[q(\boldsymbol{w}) \,\|\, p(\boldsymbol{w})]$$

Posterior approximation over weights

KL Divergence

Prior Distribution

1. Zellner, A. Optimal information processing and Bayes's theorem. The American Statistician, 42(4):278–280, 1988.
2. Bissiri et al.. A general framework for updating belief distributions. Journal of the Royal Statistical Society, 78(5):1103–1130, 2016.

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$$\min_{q(\boldsymbol{w})} \quad \underbrace{\mathbb{E}_{q(\boldsymbol{w})}}_{\text{Posterior approximation over weights}} \left[\sum_{i=1}^{N} \overbrace{\ell}^{\text{Loss}}(y_i, f_{\boldsymbol{w}}(\boldsymbol{x}_i)) \right] + \underbrace{\mathbb{D}_{KL}}_{\text{KL Divergence}}[q(\boldsymbol{w}) \,\|\, \underbrace{p(\boldsymbol{w})}_{\text{Prior Distribution}}]$$

- $q(\boldsymbol{w})$ is chosen to be mean-field Bernoulli distribution

$$q(\boldsymbol{w}) = \prod_{i=1}^{D} \underbrace{p_i}_{\text{Probability of } w_i = +1}^{\frac{1+w_i}{2}} (1 - p_i)^{\frac{1-w_i}{2}} \qquad w_i \in \{-1, +1\}$$

$$\Leftrightarrow$$

$$q(\boldsymbol{w}) = \prod_{i=1}^{D} \exp\left[\lambda_i \phi(w_i) - A(\lambda_i) \right]$$

Natural parameters: $\lambda_i := \frac{1}{2} \log \frac{p_i}{1 - p_i}$

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BayesBiNN

- The Bayesian learning rule[1] (natural-gradient variational inference)

Learning rate

$$\boldsymbol{\lambda} \leftarrow (1-\alpha)\boldsymbol{\lambda} - \alpha \left\{ \nabla_{\boldsymbol{\mu}} \mathbb{E}_{q(\boldsymbol{w})} \left[\sum_{i=1}^{N} \ell(y_i, f_{\boldsymbol{w}}(\boldsymbol{x}_i)) \right] - \boldsymbol{\lambda}_0 \right\}$$

Natural parameter of $q(\boldsymbol{w})$

Expectation parameter of $q(\boldsymbol{w})$

Natural parameter of $p(\boldsymbol{w})$

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How to compute?

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How to compute?

Natural parameter of $q(\boldsymbol{w})$

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Natural parameter of $p(\boldsymbol{w})$

- Using the Gumbel Softmax trick[2,3], we can approximate the natural gradient by using the mini-batch gradient

$$\nabla_{\boldsymbol{\mu}}\mathbb{E}_{q(\boldsymbol{w})}\left[\sum_{i=1}^{N}\ell(y_i, f_{\boldsymbol{w}}(\boldsymbol{x}_i))\right] \approx \mathbf{s}\odot\mathbf{g}$$

Minibatch Gradient, easy to compute!

Scale vector

$$\mathbf{g} := \frac{1}{m}\sum_{i\in\mathcal{M}}\nabla_{\boldsymbol{w}_b}\ell(y_i, f_{\boldsymbol{w}_b}(\boldsymbol{x}_i)) \qquad \mathbf{s} := \frac{N(1-\boldsymbol{w}_b^2)}{\tau(1-\tanh(\boldsymbol{\lambda})^2)}$$

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BayesBiNN Justifies Some Previous Methods

STE	Our BayesBiNN method	Bop
$\boldsymbol{w}_b \leftarrow \mathrm{sign}(\boldsymbol{w}_r)$ $\mathbf{g} \leftarrow \nabla_{\boldsymbol{w}_b}\ell(y, f_{\boldsymbol{w}_b}(\boldsymbol{x}))$ $\boldsymbol{w}_r \leftarrow \boldsymbol{w}_r - \alpha\mathbf{g}$	$\boldsymbol{w}_b \leftarrow \tanh\left((\boldsymbol{w}_r + \boldsymbol{\delta})/\tau\right)$ $\mathbf{g} \leftarrow \nabla_{\boldsymbol{w}_b}\ell(y, f_{\boldsymbol{w}_b}(\boldsymbol{x}))$ $\boldsymbol{w}_r \leftarrow (1-\alpha)\boldsymbol{w}_r - \alpha\mathbf{s}\odot\mathbf{g}$	$\boldsymbol{w}_b \leftarrow \mathrm{hyst}(\boldsymbol{w}_r, \boldsymbol{w}_b, \gamma)$ $\mathbf{g} \leftarrow \nabla_{\boldsymbol{w}_b}\ell(y, f_{\boldsymbol{w}_b}(\boldsymbol{x}))$ $\boldsymbol{w}_r \leftarrow (1-\alpha)\boldsymbol{w}_r - \alpha\mathbf{g}$

Note that $\boldsymbol{w}_r$ in BayesBiNN corresponds to $\boldsymbol{\lambda}$

- Main point 1: STE works as a special case of BayesBiNN as $\tau \to 0$

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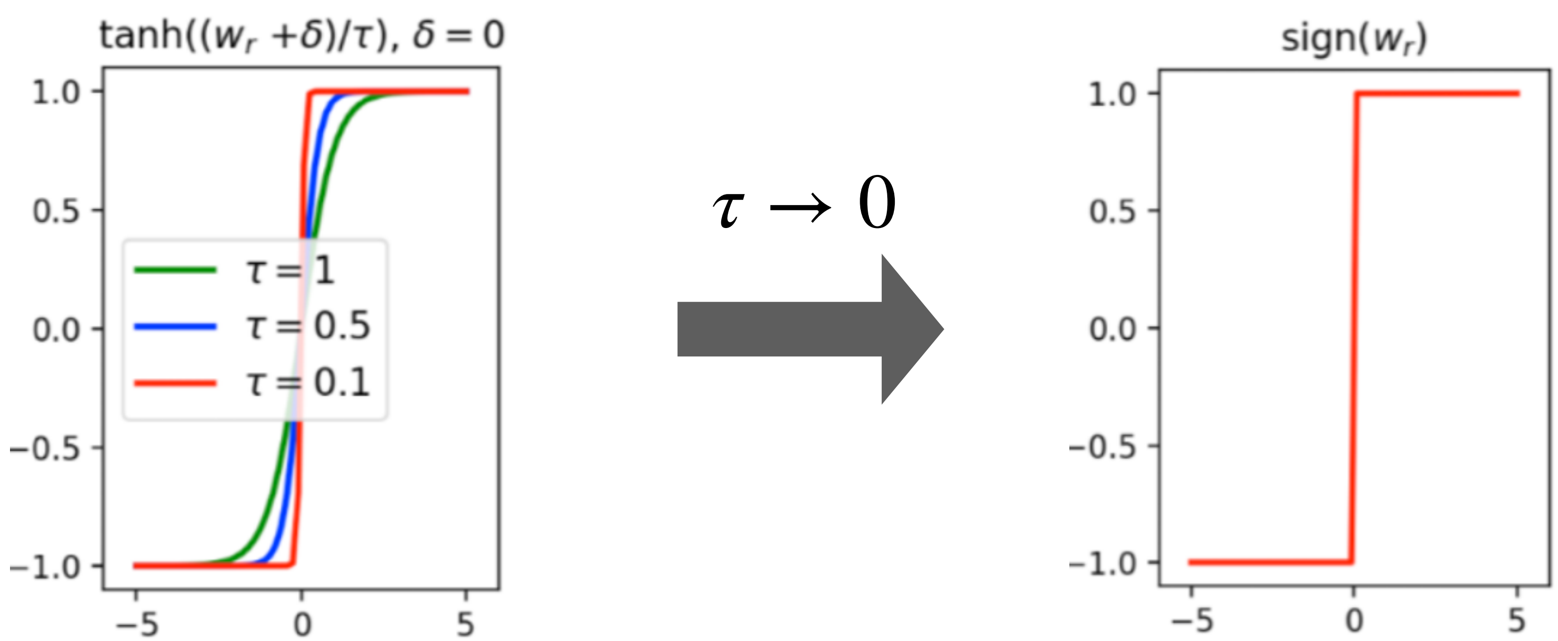

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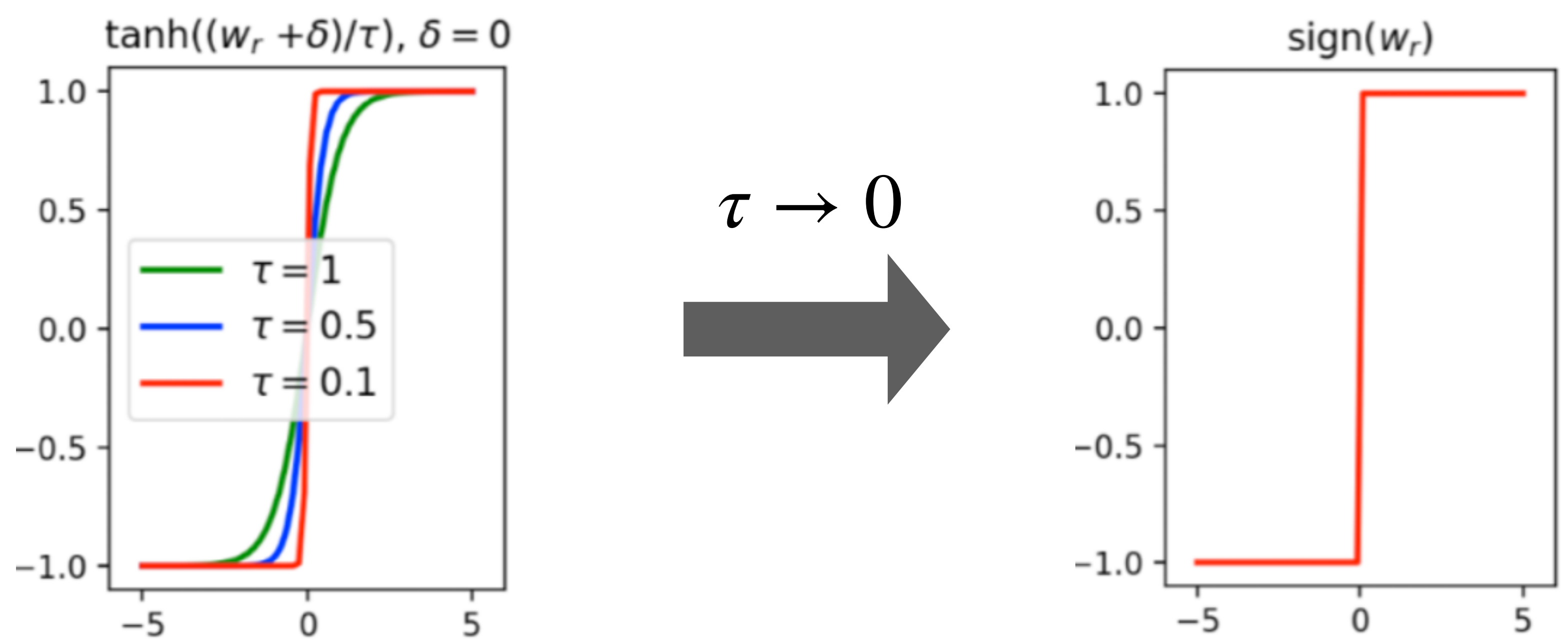
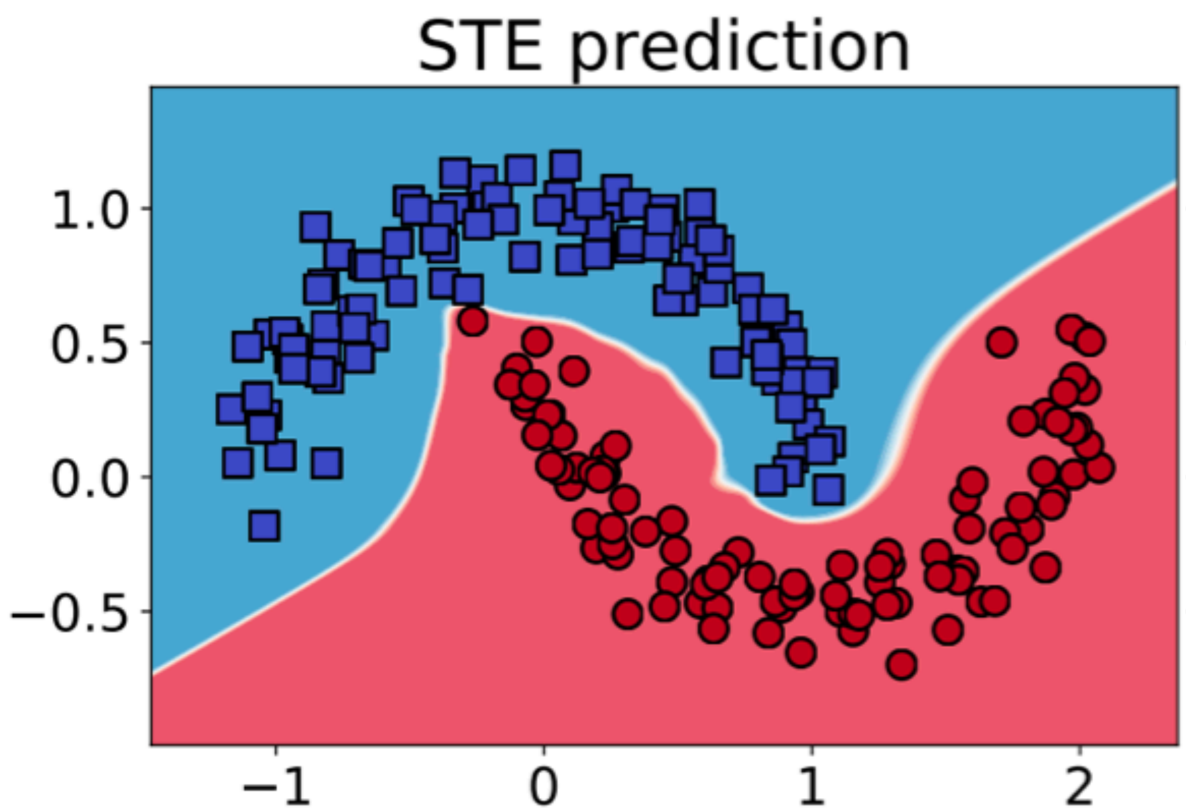
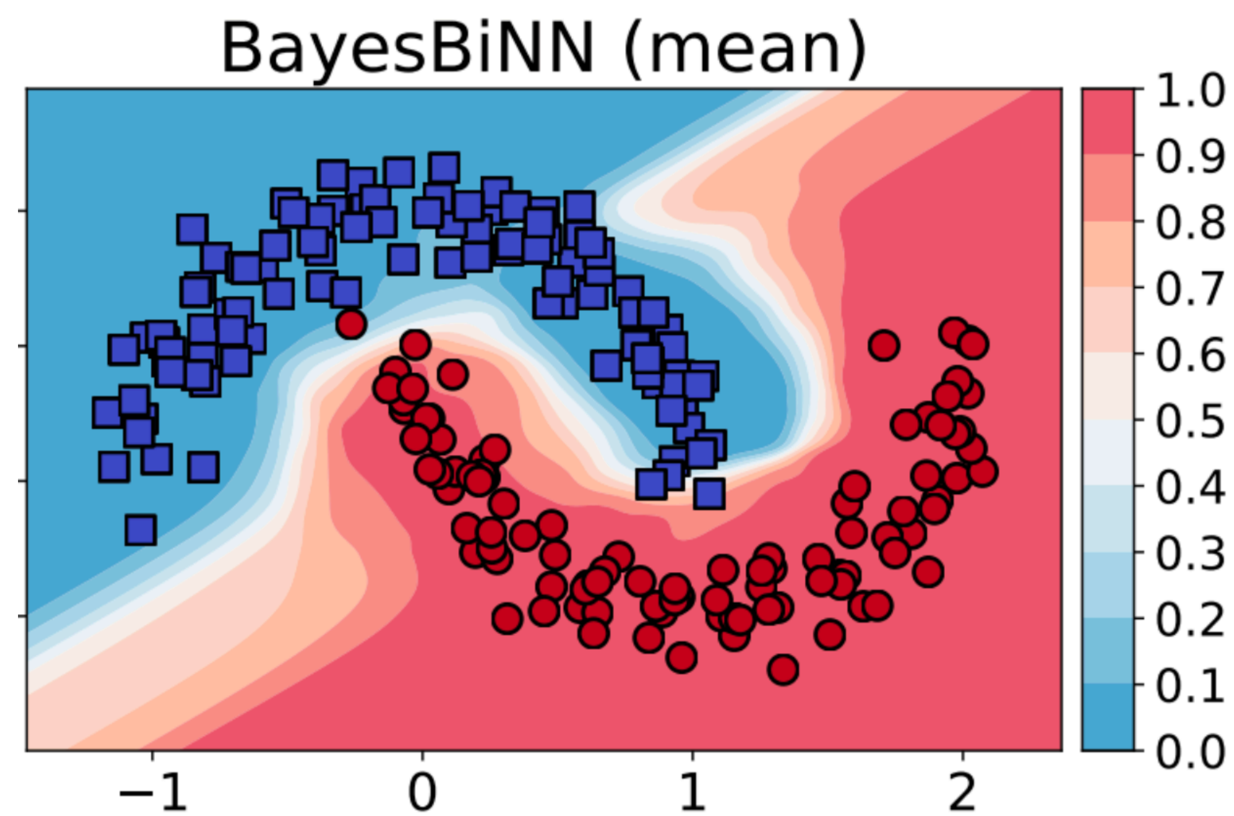


- Main point 2: Justify the “exponential average” used in Bop

Uncertainty Estimation

- Main point: BayesBiNN obtains uncertainty estimates around the classification boundaries





Classification on two moons dataset

$\hat{p}_k \leftarrow \frac{1}{C}\sum_{c=1}^{C} p\left(y=k \mid \boldsymbol{x}, \boldsymbol{w}^{(c)}\right), C=10 \quad \boldsymbol{w}^{(c)} \sim q(\boldsymbol{w})$

- STE finds a deterministic boundary

- **Open-source Code Available** : https://github.com/team-approx-bayes/BayesBiNN

BayesBiNN $\approx$ STE

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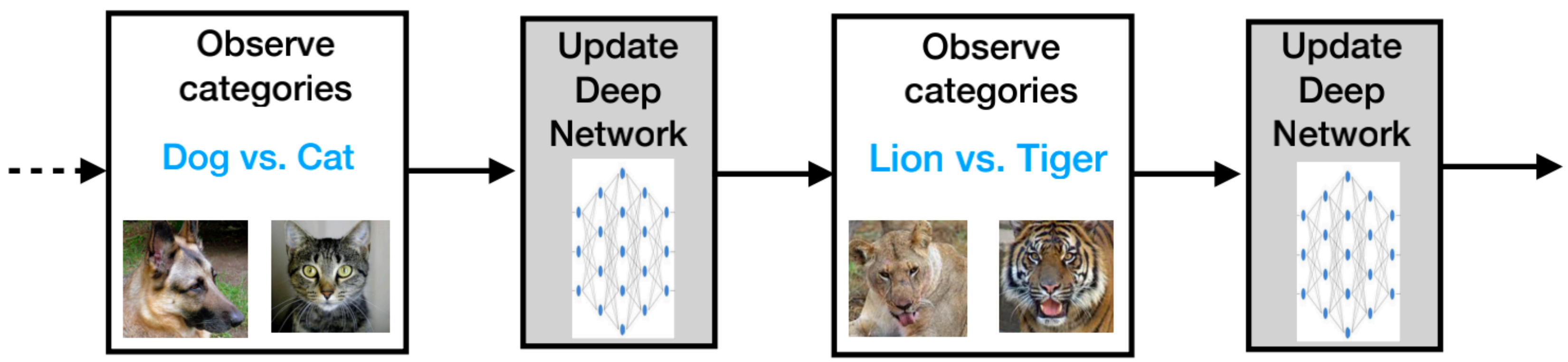
Table 2. Results of different optimizers trained on MNIST, CIFAR-10 and CIFAR-100 (Averaged over 5 runs).

Dataset	Optimizer	Train Accuracy	Validation Accuracy	Test Accuracy
MNIST	STE Adam	99.78 ± 0.10 %	99.02 ± 0.11 %	$\mathbf{98.85} \pm 0.09$ %
	Bop	99.23 ± 0.04 %	98.55 ± 0.05 %	98.47 ± 0.02 %
	PMF		99.06 ± 0.01 %	98.80 ± 0.06 %
	BayesBiNN (mode)	99.85 ± 0.05 %	99.02 ± 0.13 %	$\mathbf{98.86} \pm 0.05$ %
	BayesBiNN (mean)	99.85 ± 0.05 %	99.02 ± 0.13 %	$\mathbf{98.86} \pm 0.05$ %
	Full-precision	99.96 ± 0.02 %	99.15 ± 0.14 %	99.01 ± 0.06 %
CIFAR-10	STE Adam	99.99 ± 0.01 %	94.25 ± 0.42 %	$\mathbf{93.55} \pm 0.15$ %
	Bop	99.79 ± 0.03 %	93.49 ± 0.17 %	93.00 ± 0.11 %
	PMF		91.87 ± 0.10 %	91.43 ± 0.14 %
	BayesBiNN (mode)	99.96 ± 0.01 %	94.23 ± 0.41 %	$\mathbf{93.72} \pm 0.16$ %
	BayesBiNN (mean)	99.96 ± 0.01 %	94.23 ± 0.41 %	$\mathbf{93.72} \pm 0.15$ %
	Full-precision	100.00 ± 0.00 %	94.54 ± 0.29 %	93.90 ± 0.17 %
CIFAR-100	STE Adam	99.06 ± 0.15 %	74.09 ± 0.15 %	72.89 ± 0.21 %
	Bop	90.09 ± 0.57 %	69.97 ± 0.29 %	69.58 ± 0.15 %
	PMF		69.86 ± 0.08 %	70.45 ± 0.25 %
	BayesBiNN (mode)	98.02 ± 0.18 %	74.76 ± 0.41 %	$\mathbf{73.68} \pm 0.31$ %
	BayesBiNN (mean)	98.02 ± 0.18 %	74.76 ± 0.41 %	$\mathbf{73.65} \pm 0.41$ %
	Full-precision	99.89 ± 0.02 %	75.89 ± 0.41 %	74.83 ± 0.26 %

Uncertainty Provided by BayesBiNN Enables Continual Learning

- Main point: BayesBiNN enables continual learning (CL) for BiNN using the intrinsic KL divergence as regularization
- CL: Sequentially learning new tasks without forgetting old ones[1]



Overcoming catastrophic forgetting

Common Method:
Regularizing weights

- But, it is unclear how to regularize binary weights of BiNN using STE/Bop

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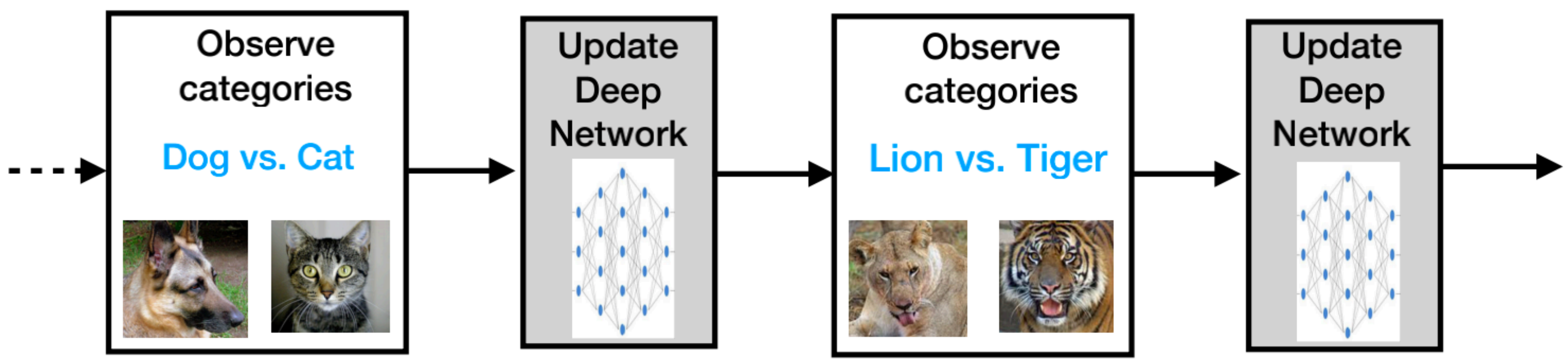

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- In BayesBiNN, there is one natural solution using KL divergence

Independent Learning

$$\min_{q_t(\mathbf{w})} \mathbb{E}_{q_t(\mathbf{w})}\left[\sum_{i\in D^t} \ell(y_i^t, f_{\mathbf{w}}(\mathbf{x}_i^t))\right] + \mathbb{D}_{KL}\left(q_t(\mathbf{w})\,||\,p(\mathbf{w})\right)$$

Prior Distribution (uniform)

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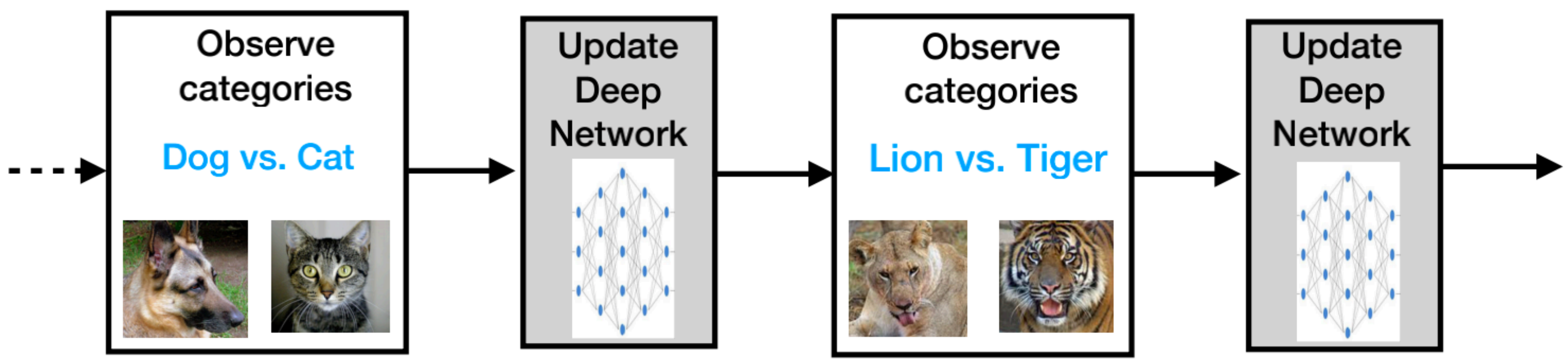

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posterior approximation after task $t-1$

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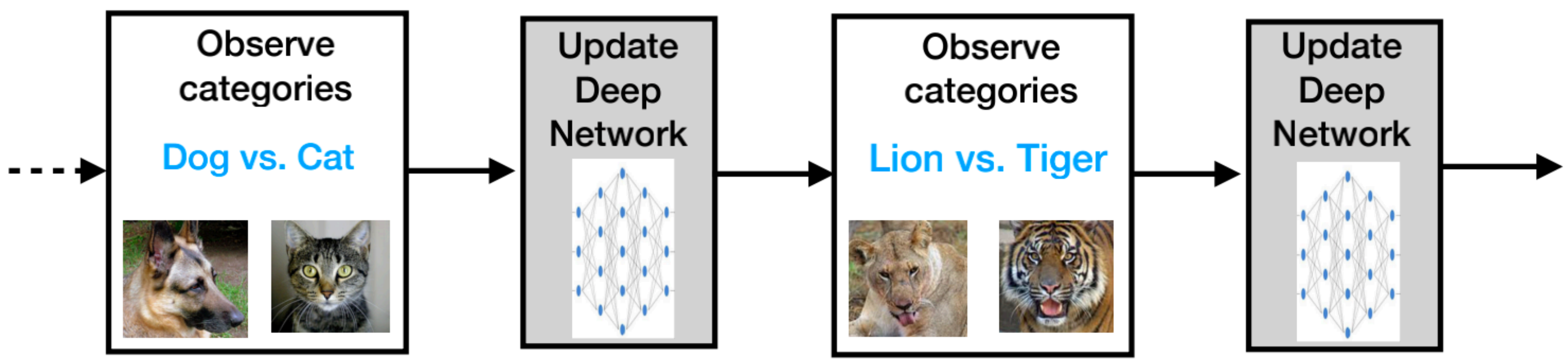

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posterior approximation after task $t-1$

$$\lambda_t \leftarrow (1-\alpha)\lambda_t - \alpha\left[\mathbf{s}\odot\mathbf{g} - \lambda_{t-1}\right]$$

Learned natural parameter after task $t-1$

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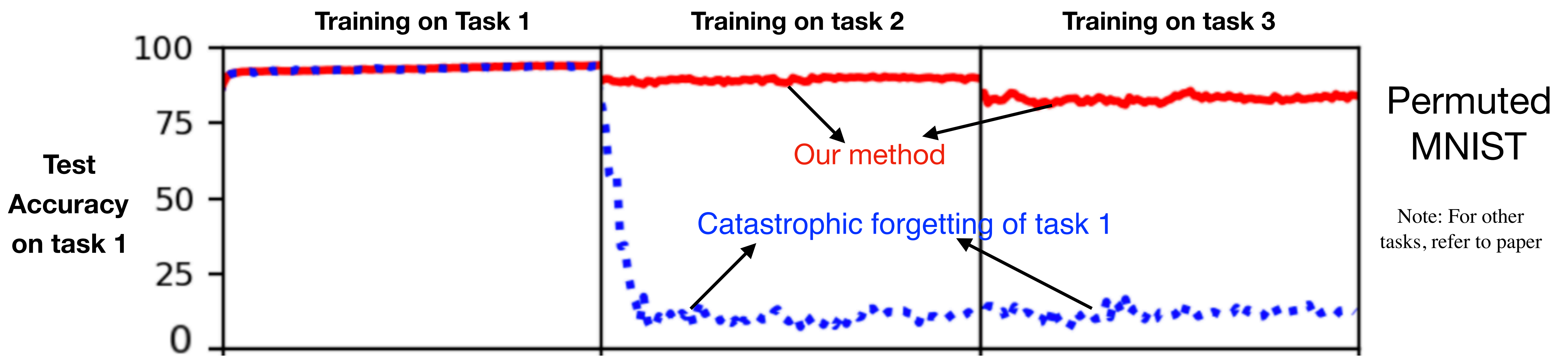
Uncertainty Provided by BayesBiNN Enables Continual Learning

- Main point: BayesBiNN avoids the catastrophic forgetting problem



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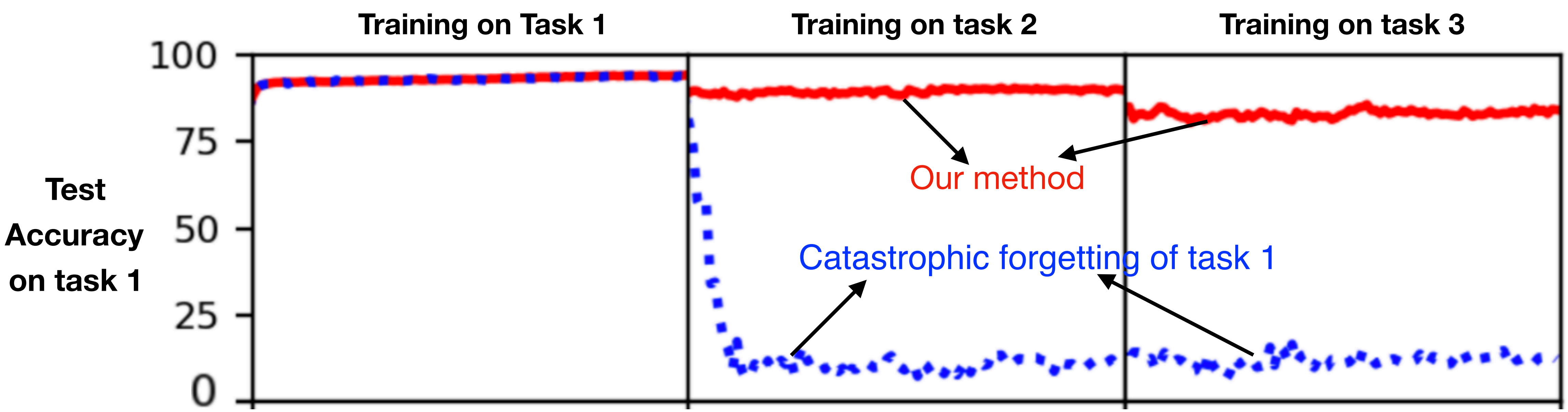
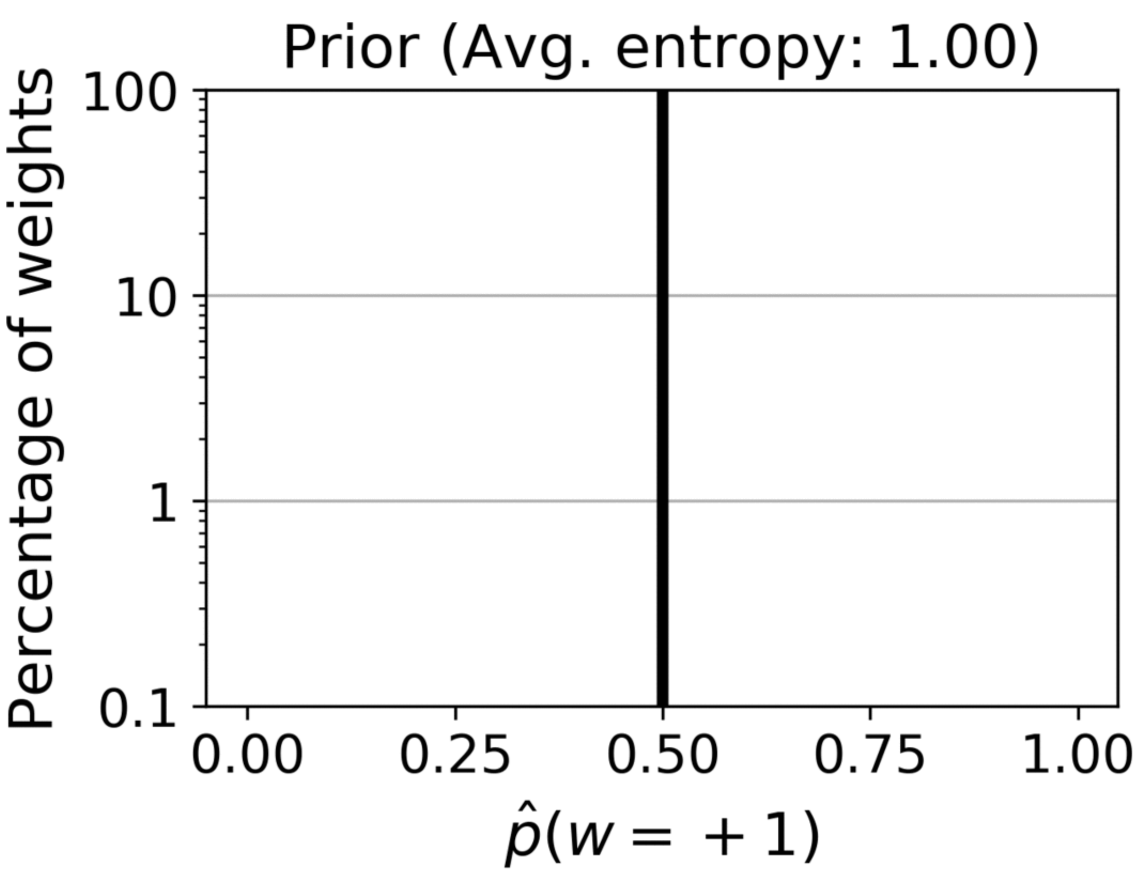


Permuted MNIST

Note: For other tasks, refer to paper



- As the number of tasks increases, the distribution over binary weights become more and more deterministic

- Open-source Code Available : https://github.com/team-approx-bayes/BayesBiNN

Summary

- BiNN: Neural Networks with binary weights
- Much faster and much smaller but difficult to optimize
- Gradient based methods work well but not well understood
- We proposed a principled approach to train BiNN using the Bayesian Learning Rule, which can justify some previous approaches
- The Bayesian approach also gives us estimate of uncertainty which can be used for continual learning

Thank you!
Q&A