Bayesian neural networks

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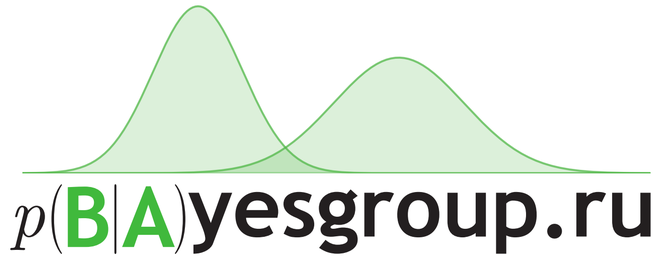
SAMSUNG
Research



Plan

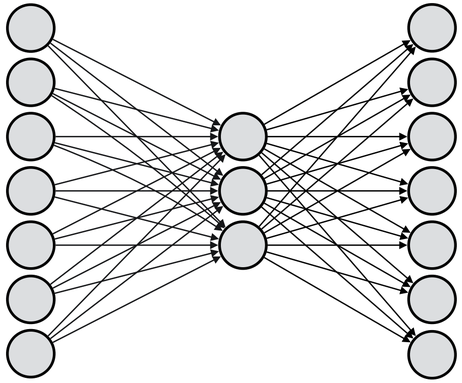
- Advantages of using Bayesian neural networks (30 min)
- Training Bayesian neural networks (30 min)
- Q&A + exercises (30 min)

Plan

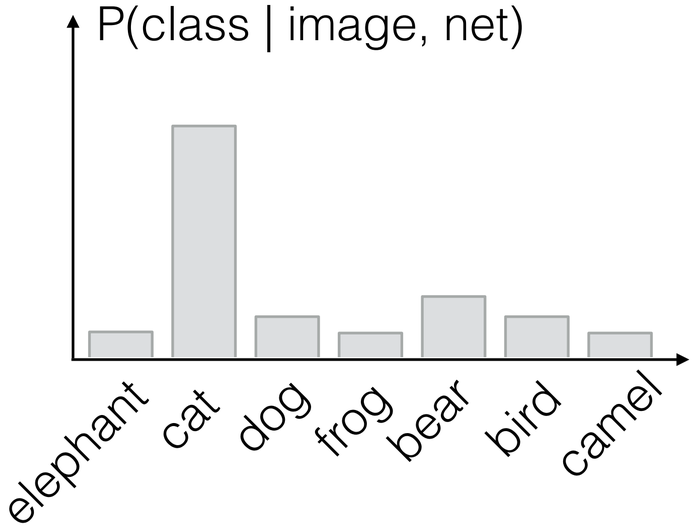
- Advantages of using Bayesian neural networks
- Training Bayesian neural networks
- Q&A + exercises

Neural networks

input x

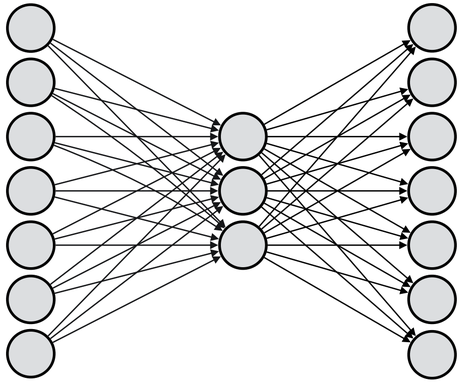


neural network
with weights w



Neural networks

input x



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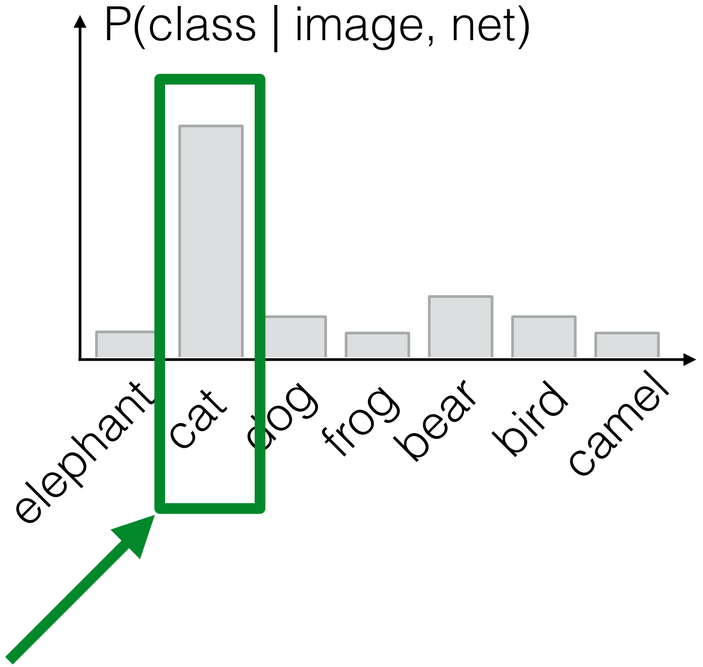
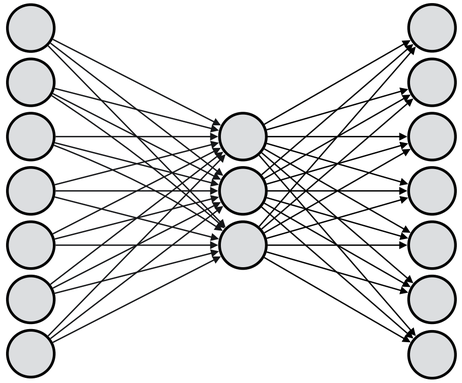


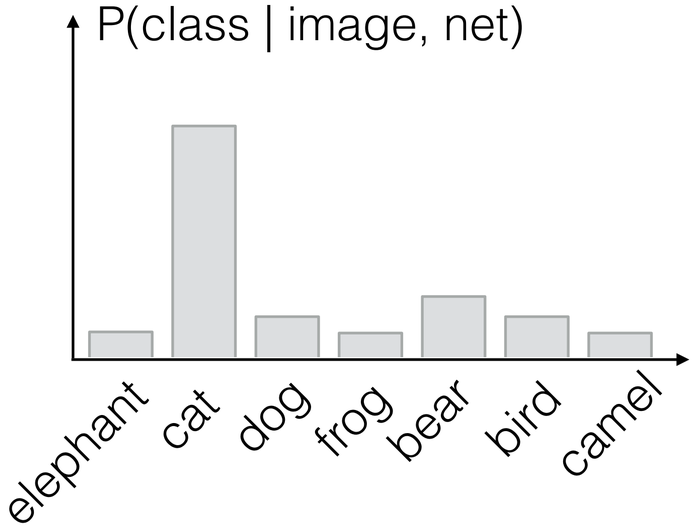
$$p(y = \text{“}cat\text{”} \,|\, x, w)$$

Neural networks

input x



neural network
with weights w

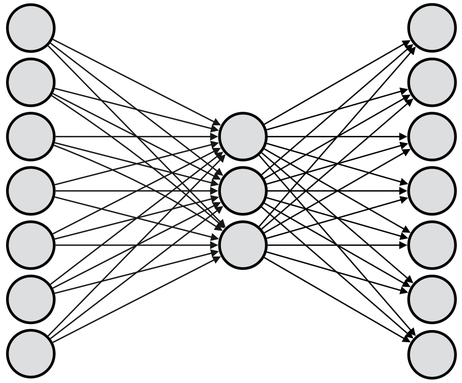


Training — optimization
over weights w
using stochastic
gradient descend:

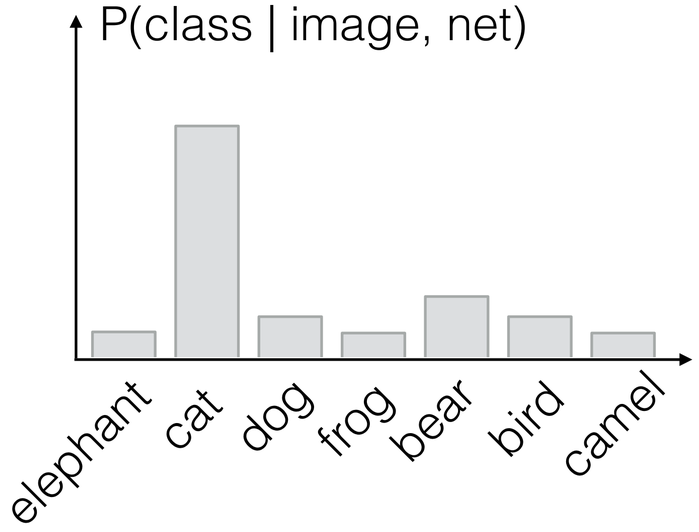
$$-DataLoss(X, Y, w) \to \max_w$$

Neural networks

input x



neural network
with weights w



Training — optimization over weights w using stochastic gradient descend:

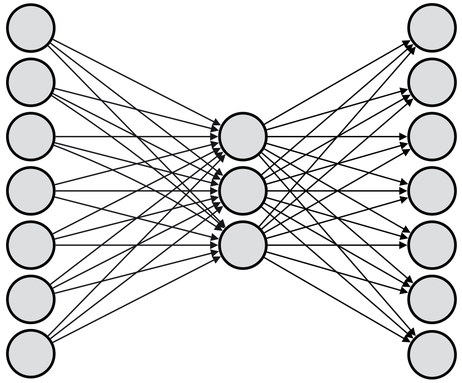
$$\sum_{i=1}^{N} \log p(y^i | x^i, w) \to \max_w$$

sum over objects (images)

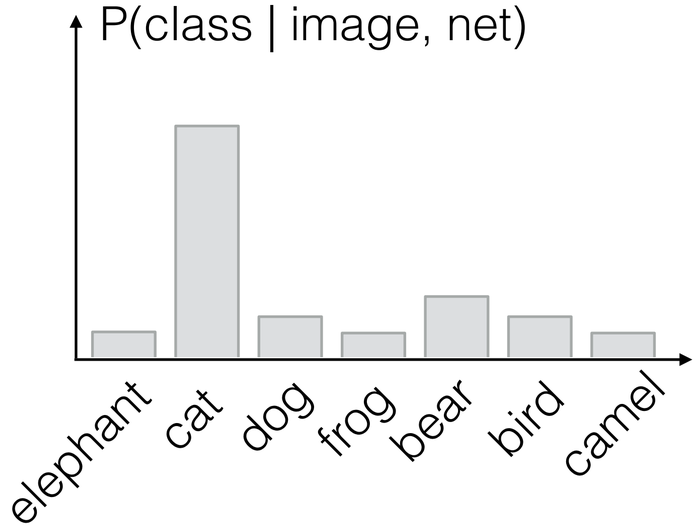
probability of true class

Neural networks

input x



neural network
with weights w



Training — optimization over weights w using stochastic gradient descend:

$$w^{new} = w^{old} + \eta \frac{\partial}{\partial w} \sum_{j=1}^{m} \log p(y^{i_j} | x^{i_j}, w^{old})$$

$$i_j \sim \text{Unif}(1, \ldots, N)$$

m — mini-batch size η — learning rate

Regularization by noise

- Traditional regularization: add some penalty for model complexity
  - L_2, L_1 - regularization, max norm constraint

$$Objective = DataLoss(X, Y, w) + Regularizer(w)$$

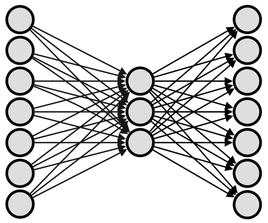
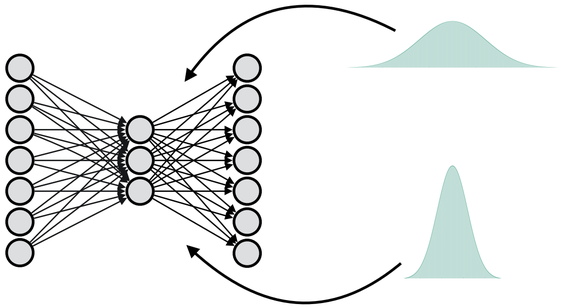
- More recent approaches: regularization by noise
  - Data augmentation, dropout, gradient noise

$$Objective = \mathbb{E}_{p(\Omega)} DataLoss(X, Y, w, \Omega)$$

Bayesian framework provides a principled approach to training with noise!

Slide From Dmitry Molchanov's presentation, deepbayes.ru/2018

Bayesian neural networks

	Deterministic neural network	Bayesian neural network
Weights:	deterministic weights 	stochastic weights 
Training:	Data X, Y → point estimate w_{MP}	Prior $p(w)$ + Data X, Y → Posterior $p(w\|X, Y)$
Prediction on new object x_*:	$p(y_*\|x_*, w_{MP})$	$\mathbb{E}_{p(w\|X,Y)} p(y_*\|x_*, w)$

Bayesian neural networks

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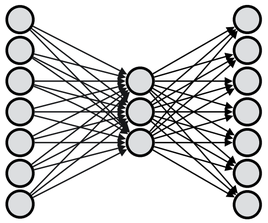
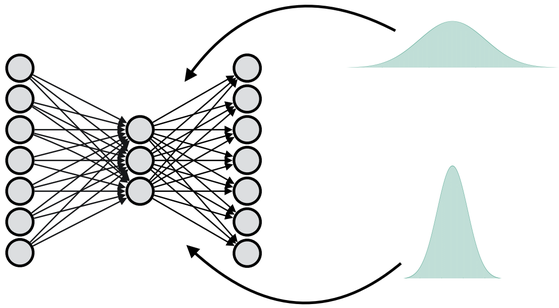
Weights:	deterministic weights 	stochastic weights 
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BNN as an ensemble of neural networks

Prediction on a new object x_*:

$$\mathbb{E}_{p(w|X,Y)} p(y_*|x_*, w) \approx \frac{1}{K} \sum_{k=1}^{K} p(y_*|x_*, w^k), \quad w^k \sim p(w|X, Y)$$

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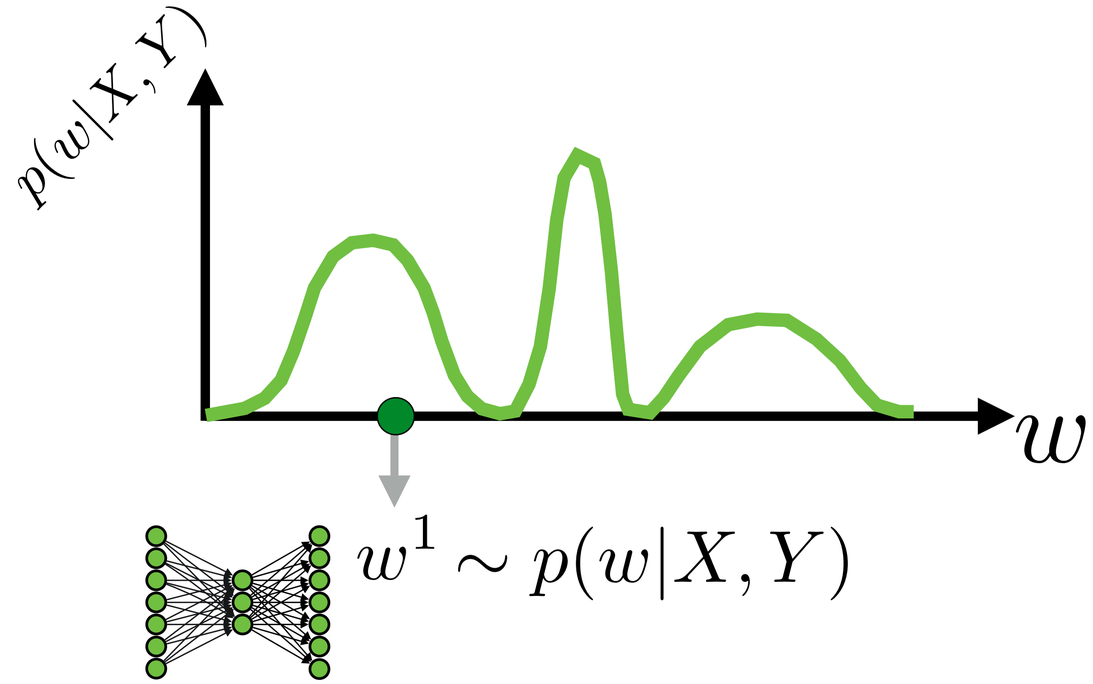

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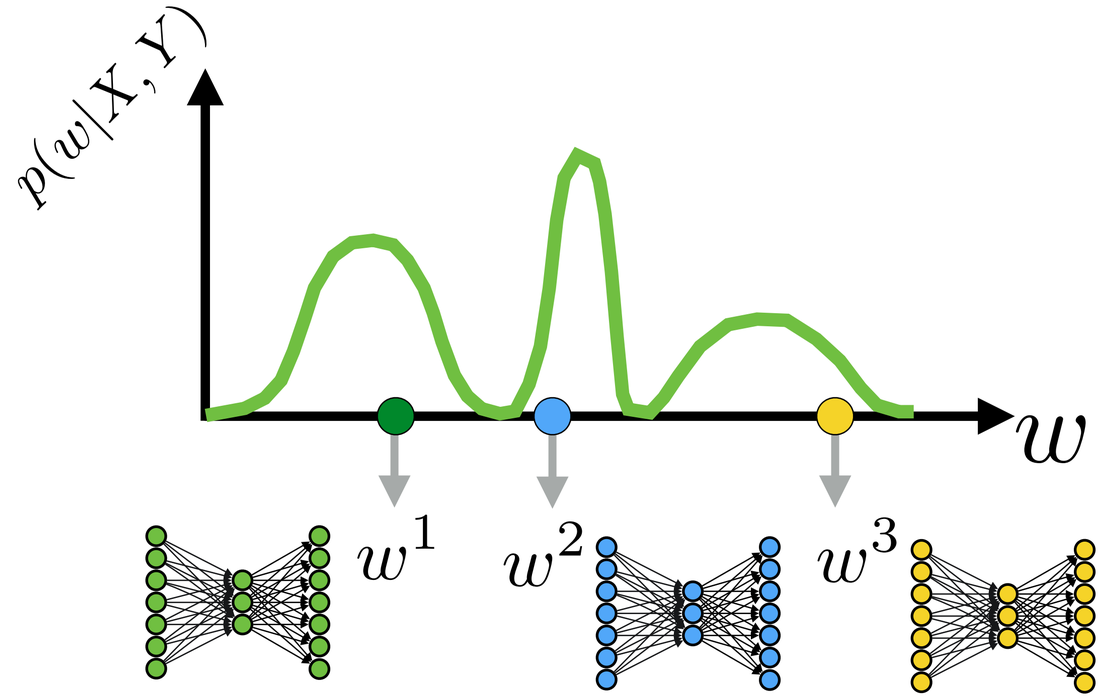

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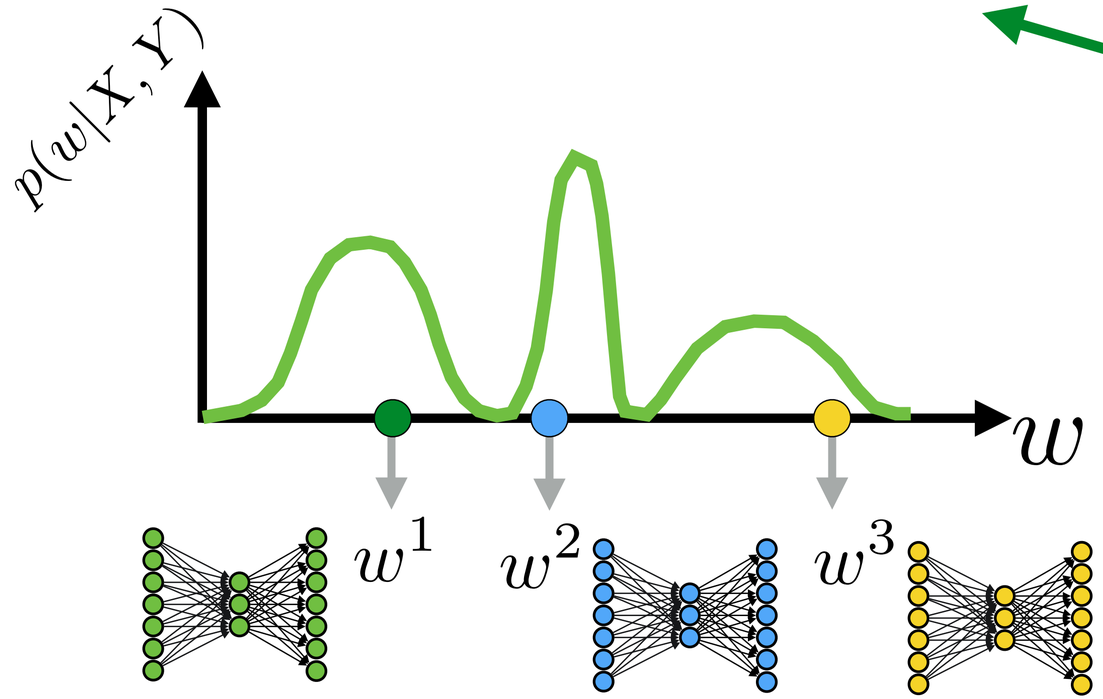

average net's output across several weight samples

BNN as an ensemble of neural networks

input x

$w^1 \sim p(w|X,Y)$

$w^2 \sim p(w|X,Y)$

$w^3 \sim p(w|X,Y)$

$$\frac{1}{K}\sum_{k=1}^{K}$$

$p(y = \text{“}cat\text{”}|x)$

BNN as an ensemble of neural networks

Prediction on a new object x_*:

$$\mathbb{E}_{p(w|X,Y)} p(y_*|x_*, w) \approx \frac{1}{K} \sum_{k=1}^{K} p(y_*|x_*, w^k), \quad w^k \sim p(w|X, Y)$$

- Higher quality (models compensate each other's errors)
- Better uncertainty estimation

Slide From Dmitry Molchanov's presentation, deepbayes.ru/2018

Questions

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- How many forward passes do we perform to make the prediction in the BNN?

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- If the posterior is a delta function: $p(w|X,,Y) = \delta(w_0)$,
  how will the predictive ensemble look like?

$$w \sim p(w|X,Y) = \delta(w_0) \Leftrightarrow w \equiv w_0 \quad \longrightarrow$$

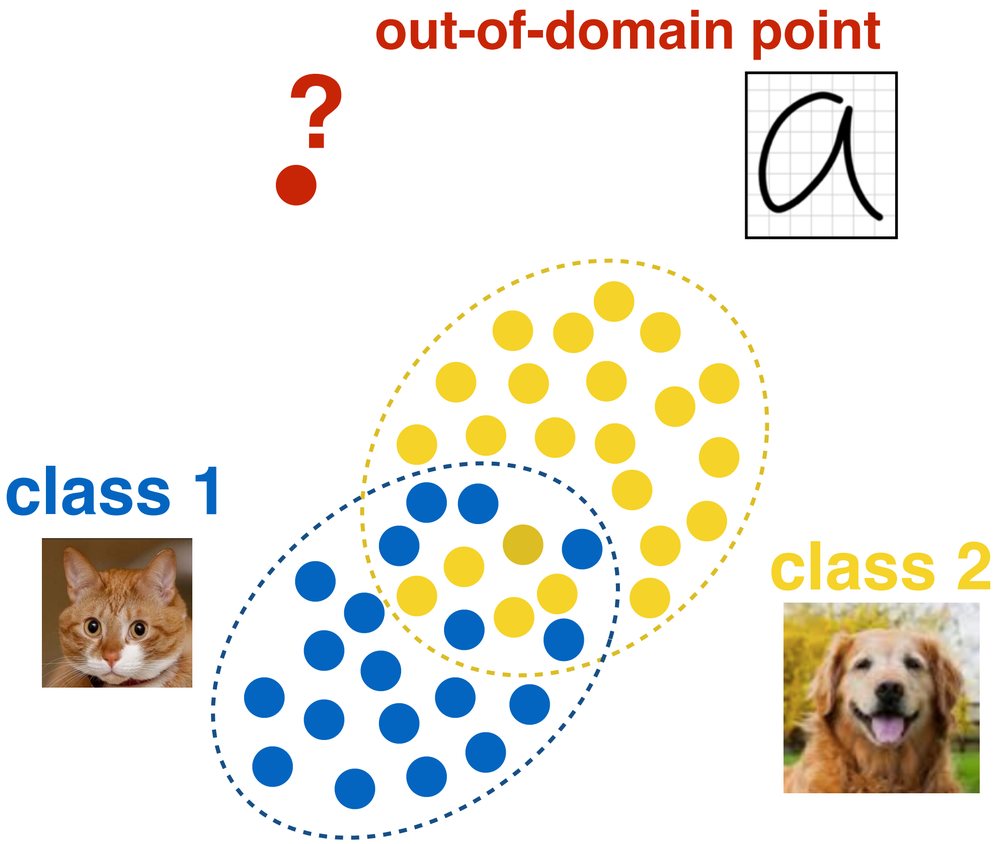
all the samples (networks) are the same

Why go Bayesian?

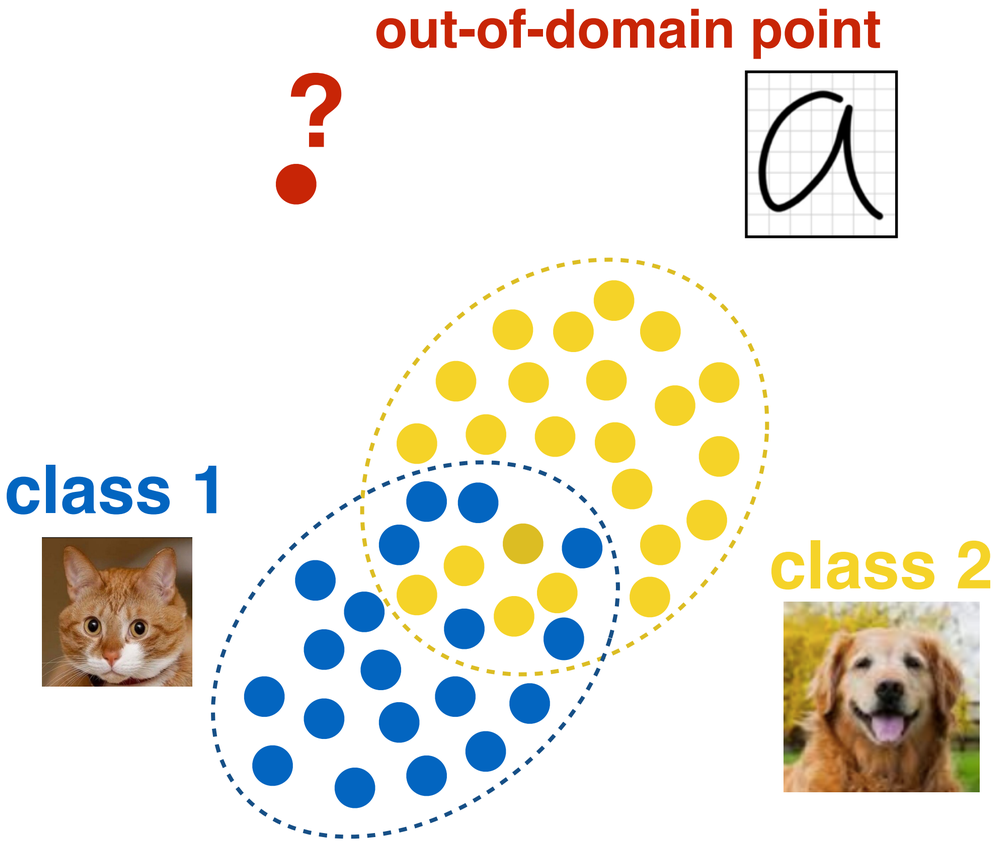
A principled framework with many useful applications

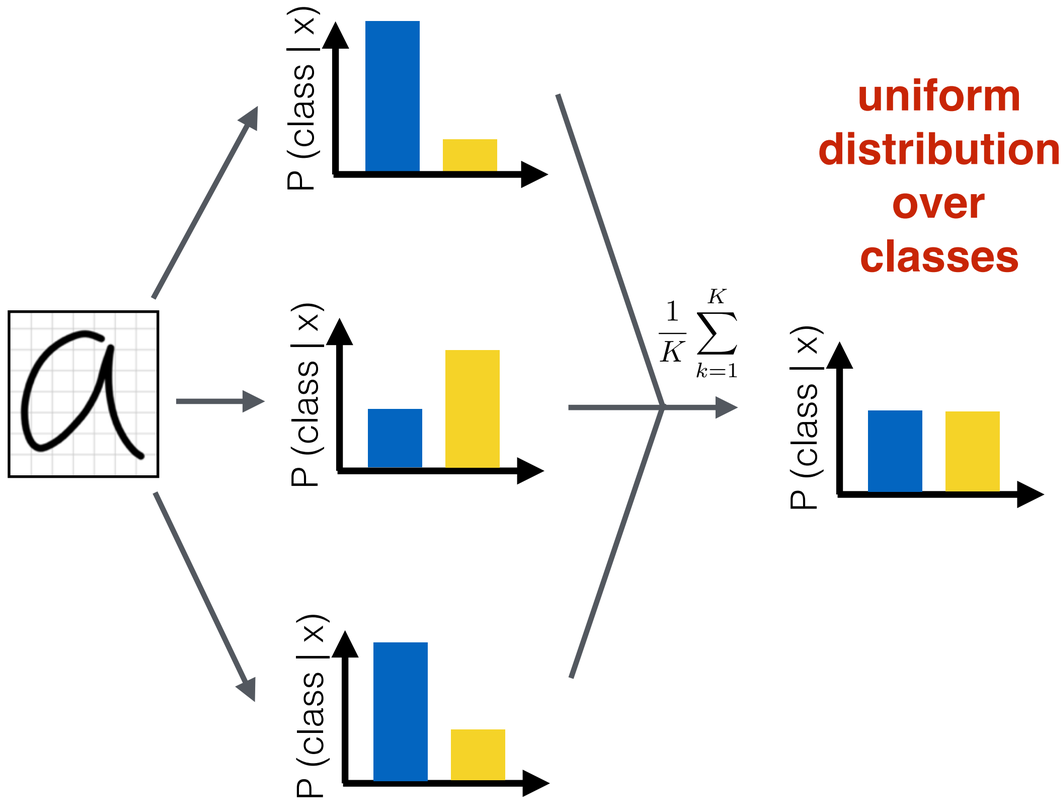
- Regularization
- Ensembling
- Uncertainty estimation
- On-line / continual learning
- Different priors lead to different properties of the network
- Automatic hyperparameter choice

Uncertainty estimation

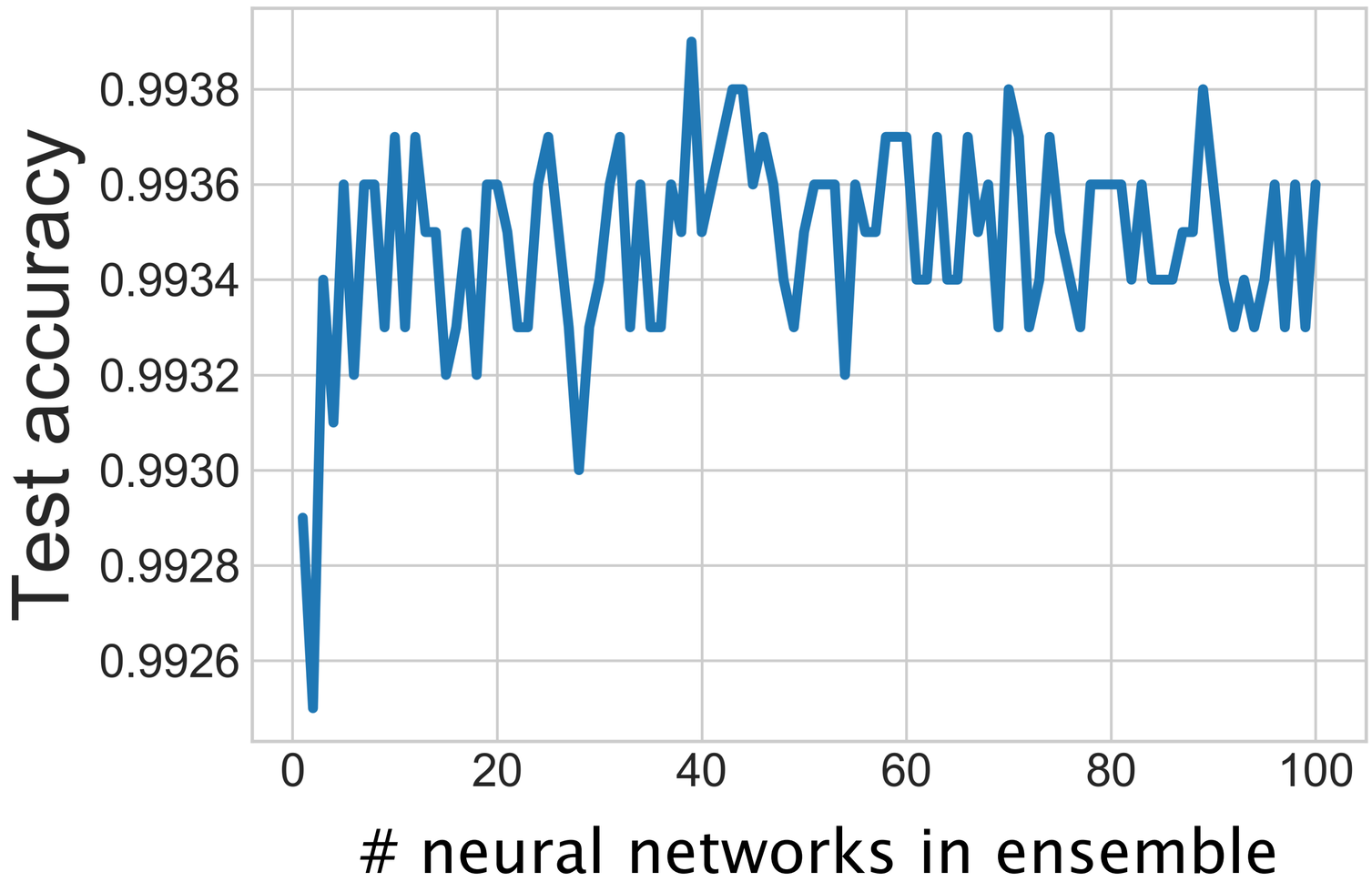


Uncertainty estimation





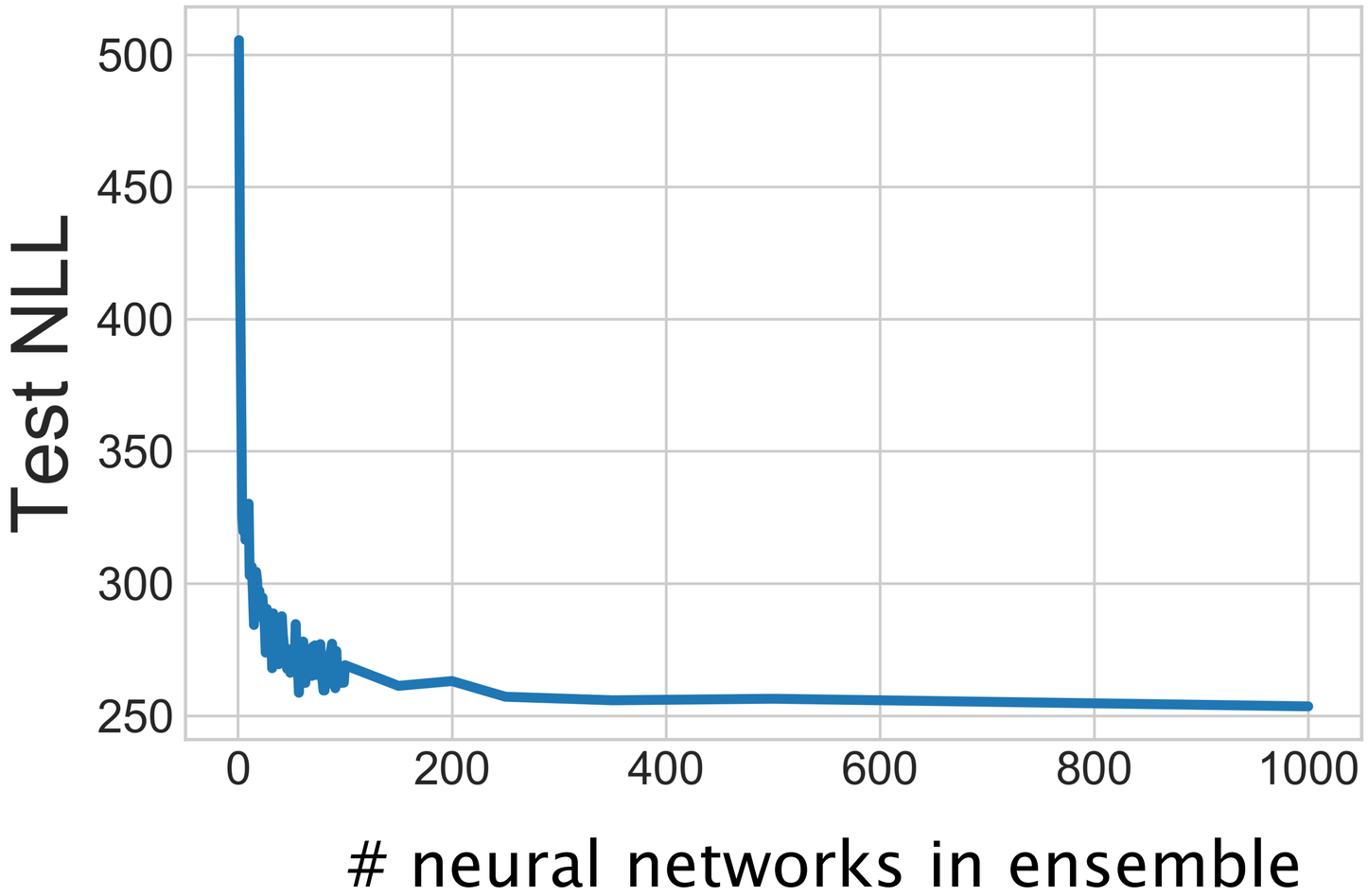
Ensembling: accuracy



Accuracy quickly saturates

Slide From Dmitry Molchanov's presentation, deepbayes.ru/2018

Ensembling: uncertainty estimation

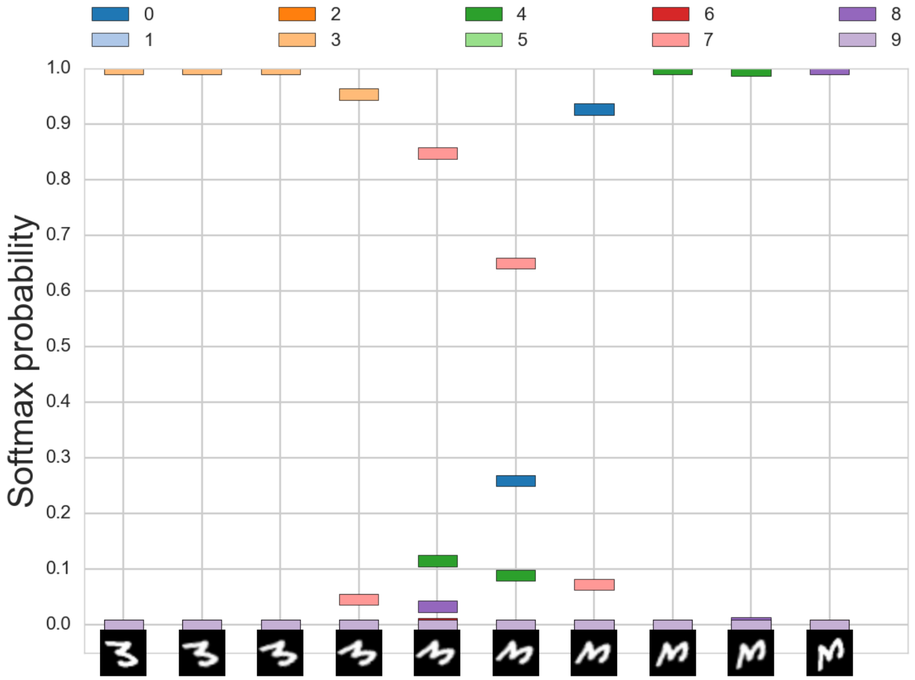


But the negative log—likelihood keeps improving! This is a measure of "**uncertainty**"

Slide From Dmitry Molchanov's presentation, deepbayes.ru/2018

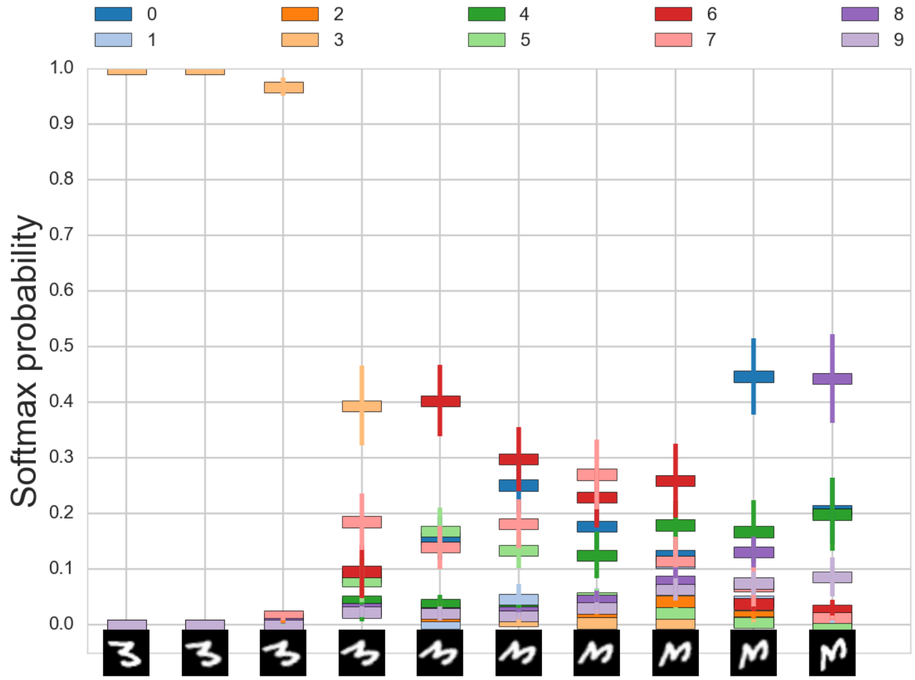
Uncertainty in classification: experiment

Deterministic NN



(a) LeNet with weight decay

Bayesian NN



(b) LeNet with multiplicative formalizing flows

Louizos, Christos, and Max Welling. Multiplicative normalizing flows for variational Bayesian neural networks. ICML 2017

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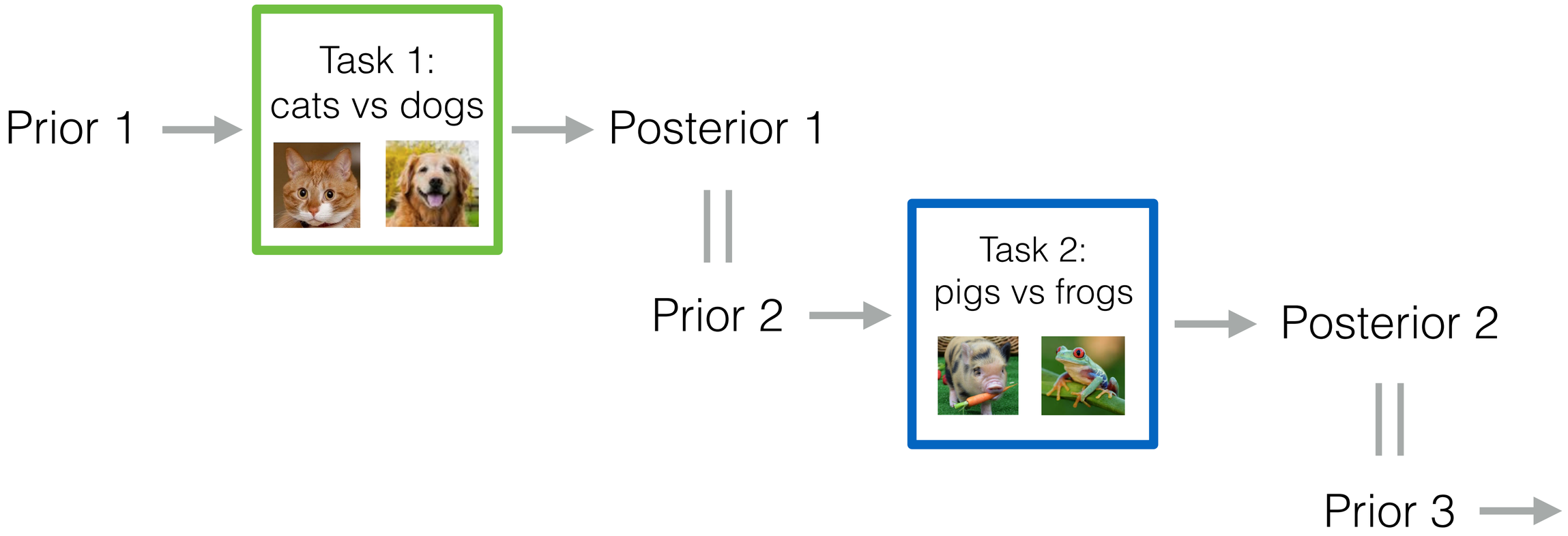
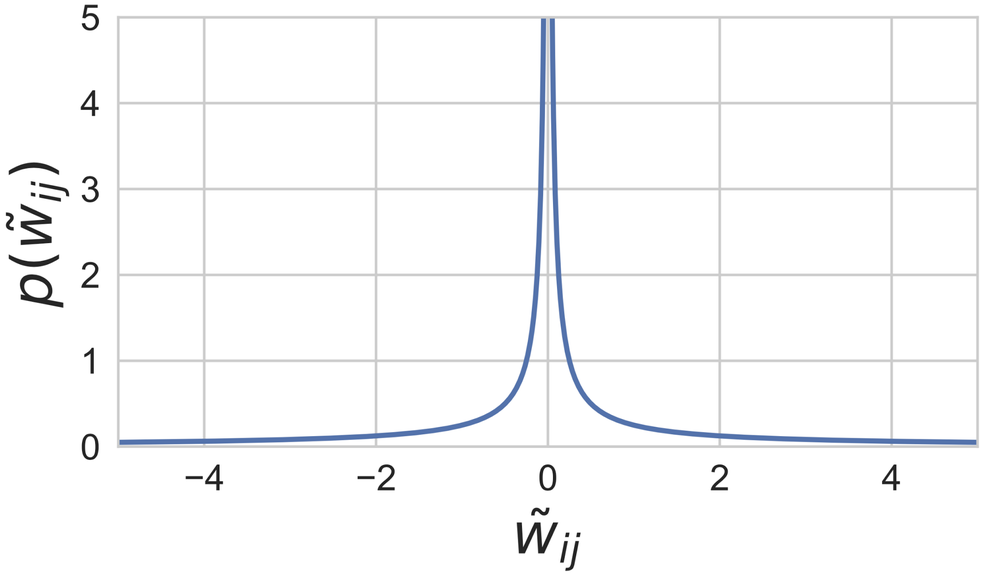
On-line / continual learning

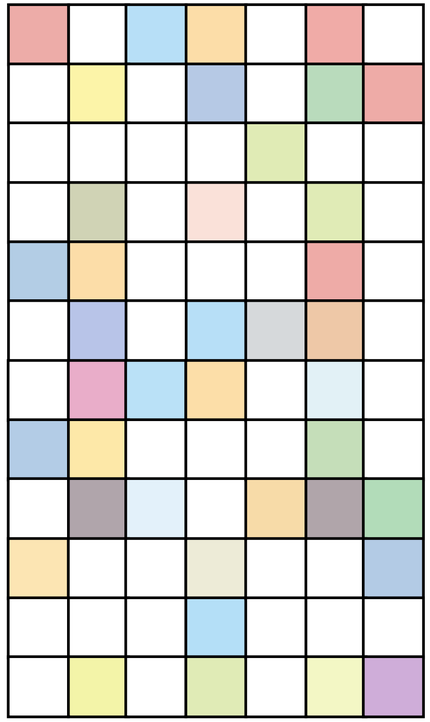


Prior can encode our desirable model properties

Prior concentrated at zero



A lot of zero weights



Weight matrix W

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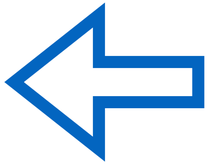
Plan

- Advantages of using Bayesian neural networks
- Training Bayesian neural networks
- Q&A + exercises

Training methods: summary

Probabilistic model: $p(Y|X,w)p(w)$ We want to compute: $p(w|X,Y)$

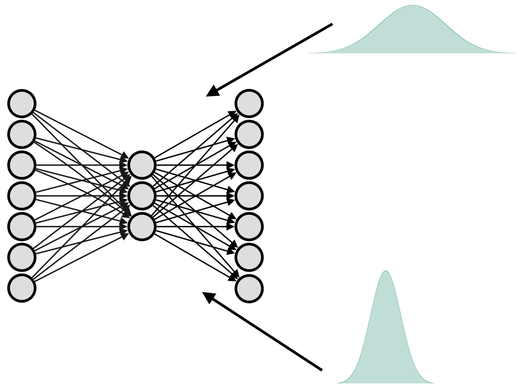
Approximation		Inference
Exact	$p(w\|X,Y)$	Full Bayesian inference
Parametric	$p(w\|X,Y) \approx q(w\|\lambda)$	Parametric Var. Inference
Delta function	$p(w\|X,Y) \approx \delta(w_{MP})$	Max. posterior inference
No prior	w_{ML}	Max. likelihood inference



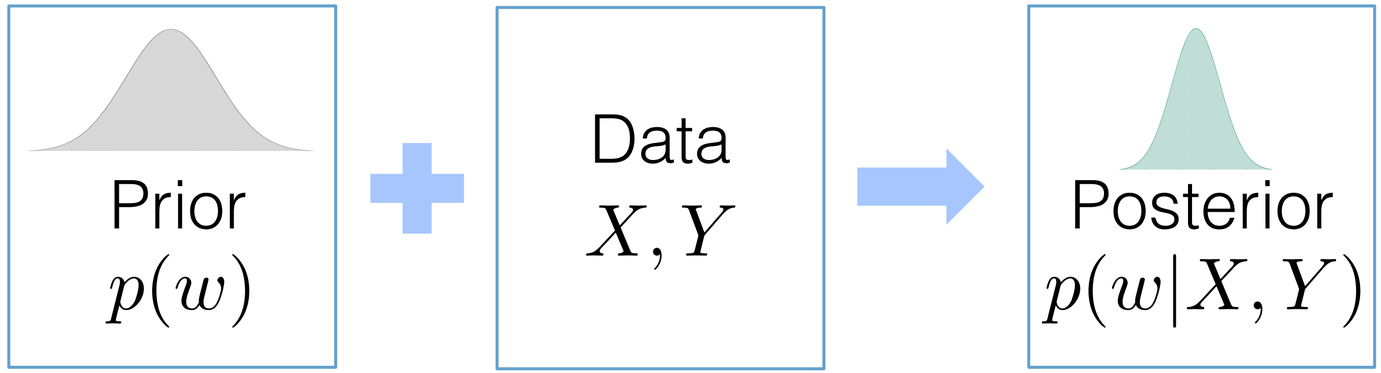
Modified slide from Ekaterina Lobacheva's presentation

Training Bayesian neural networks

Stochastic weights:



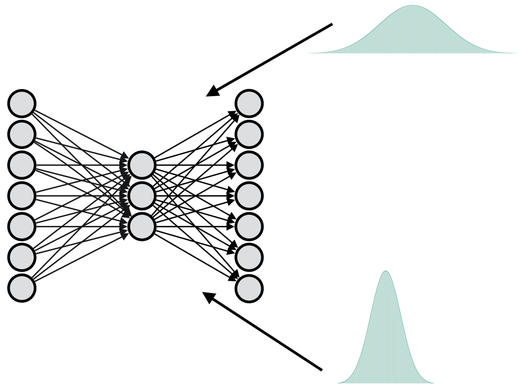
Bayesian Inference:



$$p(w|X,Y) = \frac{p(Y|X,w)p(w)}{\int p(Y|X,\tilde{w})p(\tilde{w})d\tilde{w}}$$

Training Bayesian neural networks

Stochastic weights:



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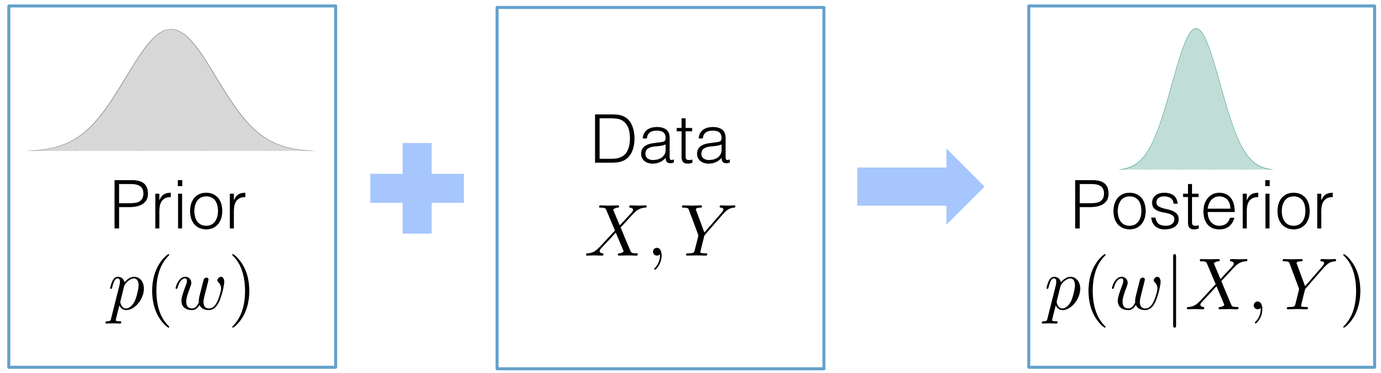
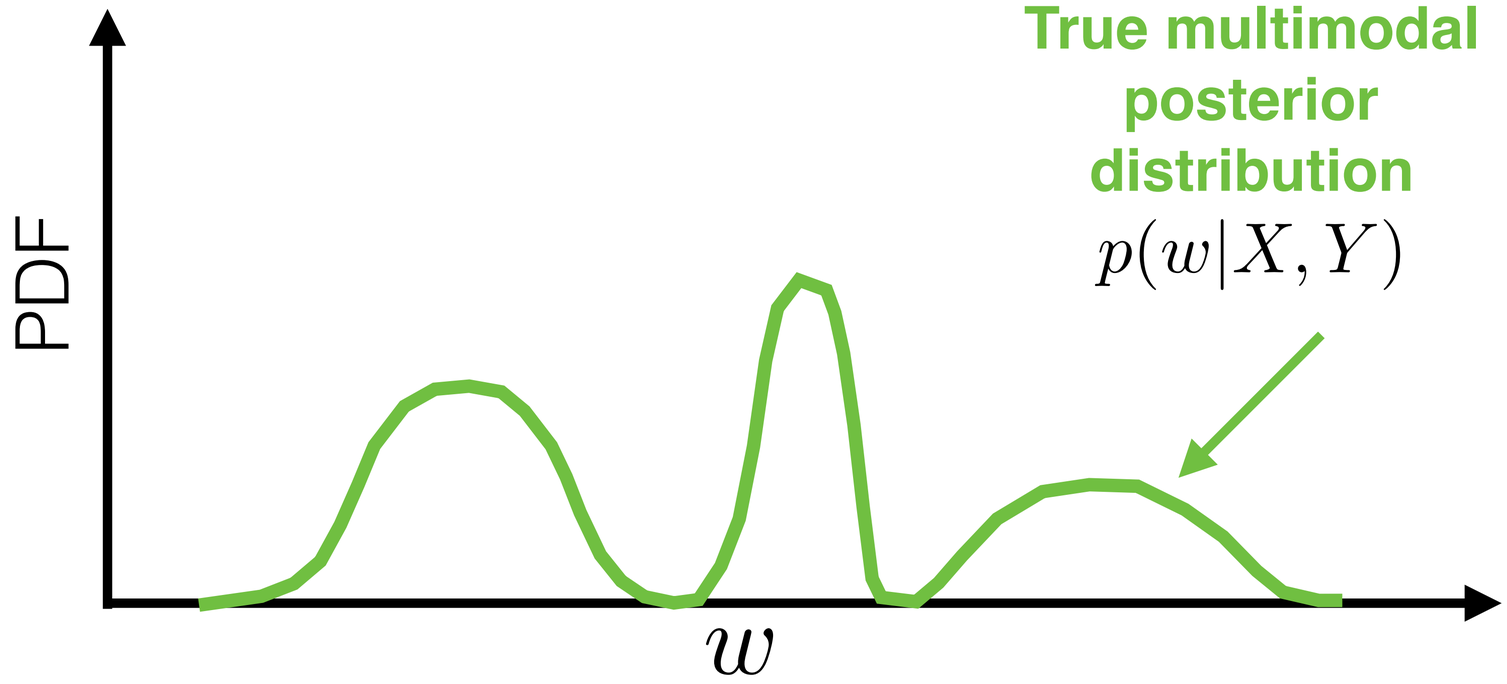


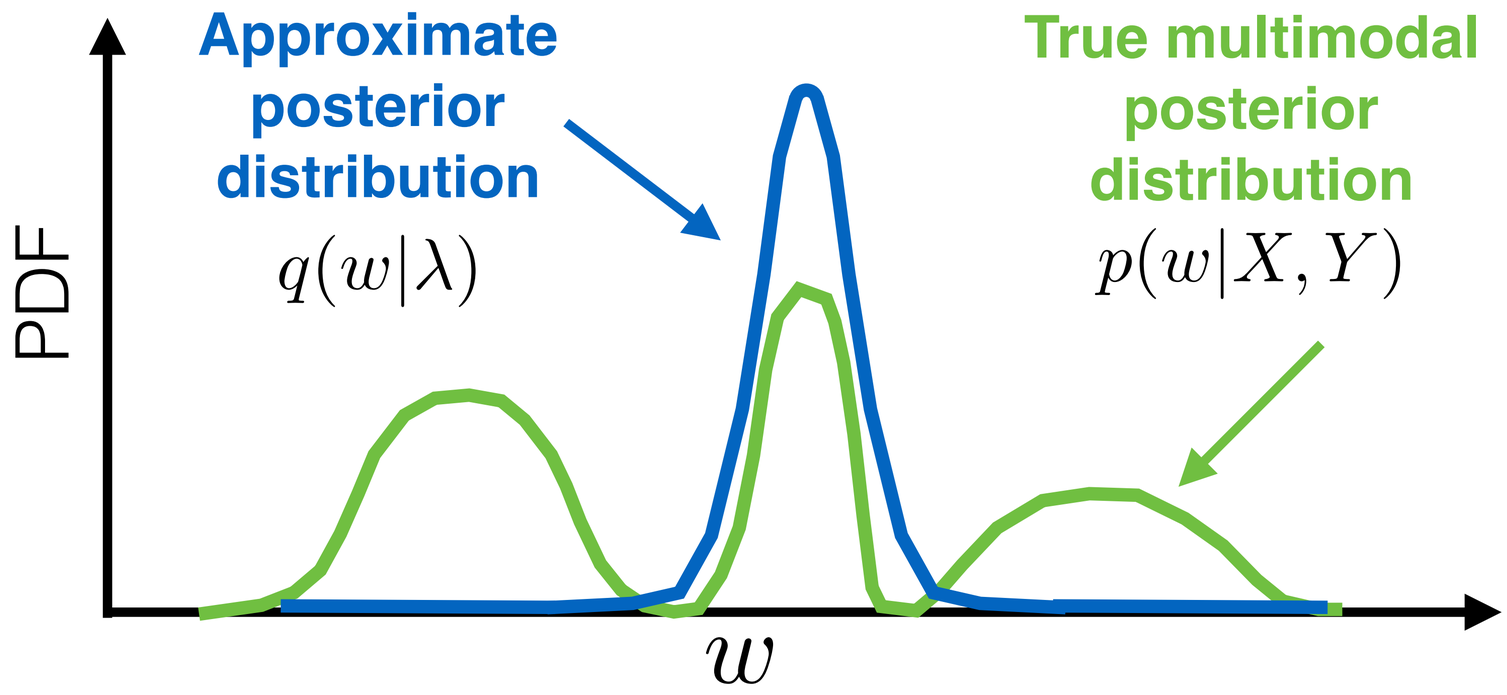
$$p(w|X,Y) = \frac{p(Y|X,w)p(w)}{\int p(Y|X,\tilde{w})p(\tilde{w})d\tilde{w}}$$

Intractable!

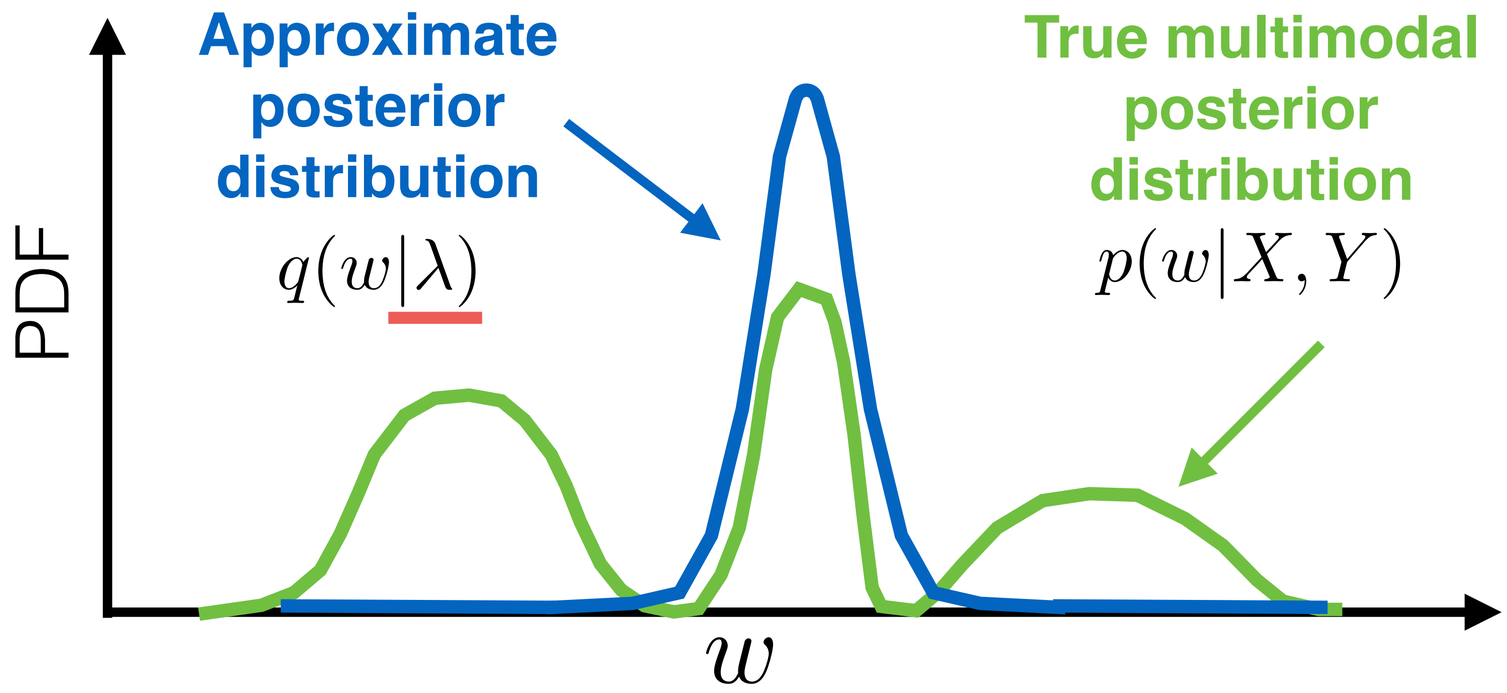
Training Bayesian neural networks



Training Bayesian neural networks

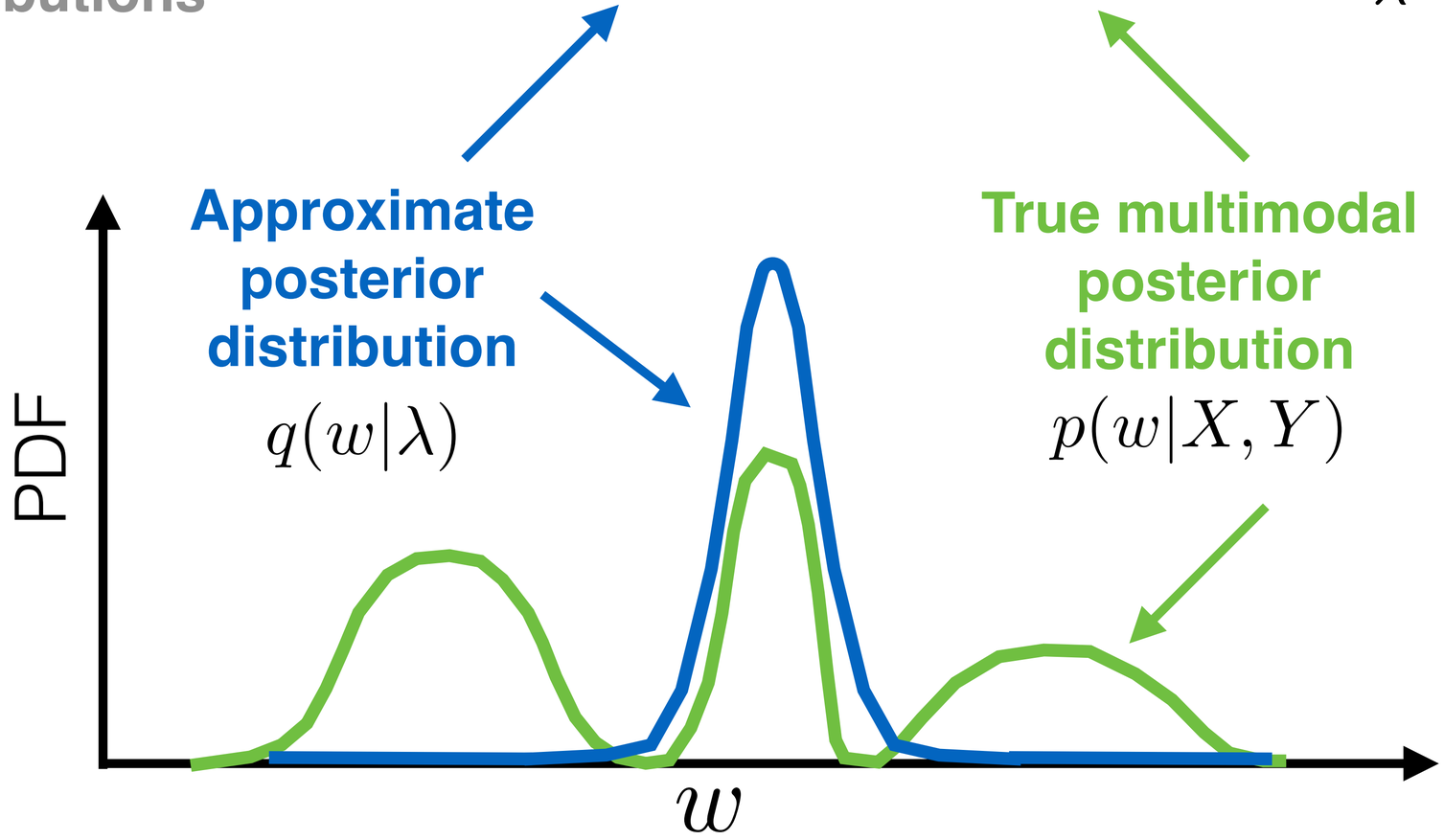


Training Bayesian neural networks



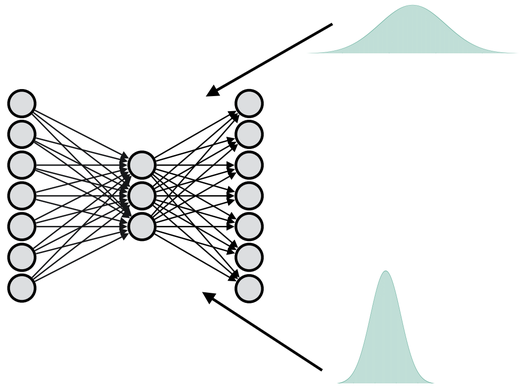
Training Bayesian neural networks

“distance” between two distributions → $KL(q(w|\lambda)||p(w|X,Y)) \rightarrow \min_{\lambda}$

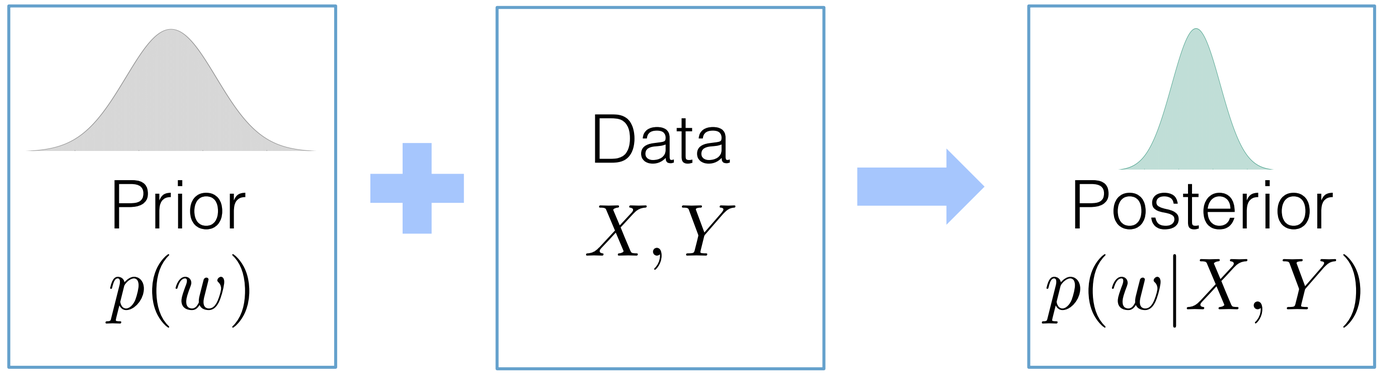


Training Bayesian neural networks

Stochastic weights:



Bayesian Inference:

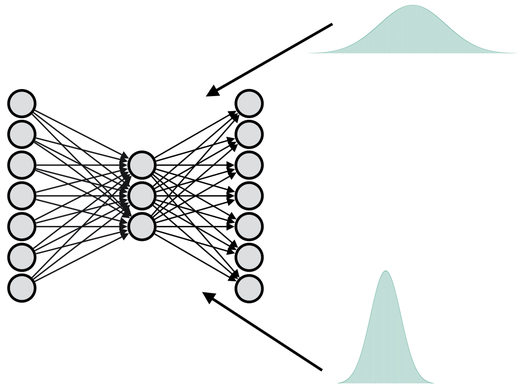


Posterior is intractable in neural networks → approximate it with $q(w|\lambda)$:

$$KL(q(w|\lambda)||p(w|X,Y)) \rightarrow \min_{\lambda}$$

Training Bayesian neural networks

Stochastic weights:



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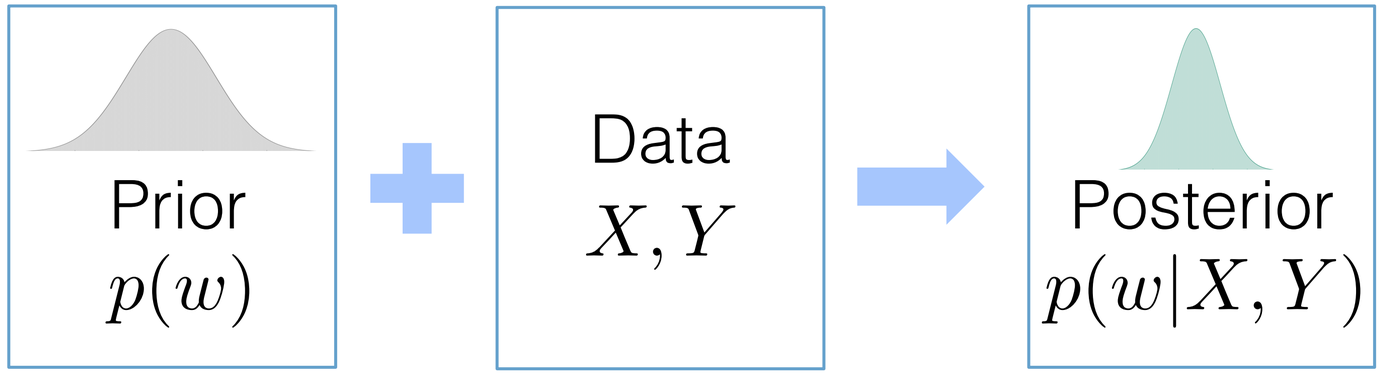

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Intractable!

Training Bayesian neural networks

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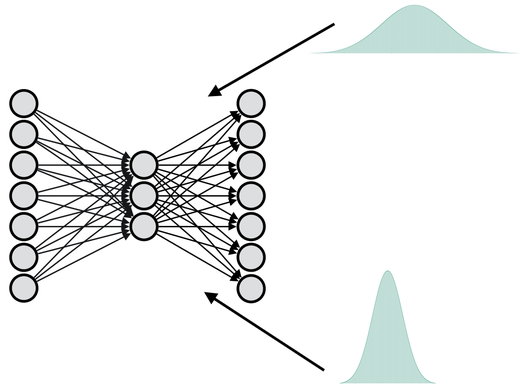

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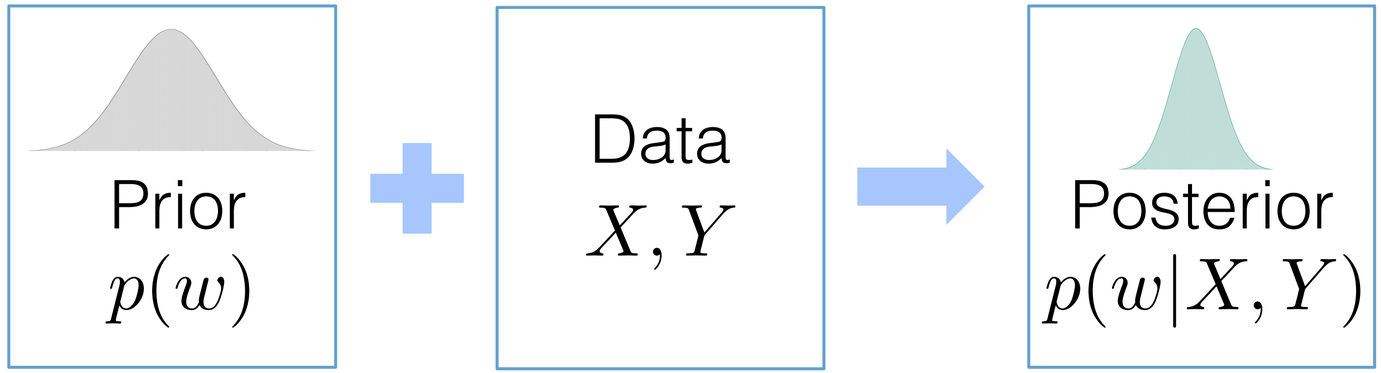

Equivalently, we can optimize ELBO to find approximate posterior $q(w|\lambda)$:

$$\sum_{i=1}^{N} \underbrace{\mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w)}_{\text{Data term}} - \underbrace{KL(q(w|\lambda)||p(w))}_{\text{Regularizer}} \to \max_{\lambda}$$

KL-divergence: note there are two of them!

$$\sum_{i=1}^{N} \underbrace{\mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w)}_{\text{Data term}} - \underbrace{KL(q(w|\lambda)||p(w))}_{\text{Regularizer}} \to \max_{\lambda}$$

constant | **we optimize** | **non-negative we wish to optimize**

$$\log p(Y|X) = \sum_{i=1}^{N} \mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w) - KL(q(w|\lambda)||p(w)) + KL(q(w|\lambda)||p(w|X, Y))$$

- approx. posterior || prior
- tractable!
- acts like a regularizer

- approx. posterior || true posterior
- intractable :(
- represents our ideal objective

Doubly stochastic variational inference

How to estimate the data term?

$$\sum_{i=1}^{N} \underbrace{\mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w)}_{\text{Data term}} - \underbrace{KL(q(w|\lambda)||p(w))}_{\text{Regularizer}} \to \max_{\lambda}$$

???

Doubly stochastic variational inference

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sample mini-batch of the training objects

sample weights from q

Doubly stochastic variational inference

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$$\sum_{j=1}^{m} \log p(y^{i_j}|x^{i_j}, \hat{w}_j), \qquad \hat{w}_j \sim q(w|\lambda) \qquad i_j \sim \text{Unif}(1, \ldots, N)$$

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λ? **How to differentiate?**

Doubly stochastic variational inference

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$$\frac{\partial}{\partial \lambda}?$$

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λ? **How to differentiate?**

Gradient of expectation

$$\frac{\partial}{\partial \lambda} \mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w) = \frac{\partial}{\partial \lambda} \int q(w|\lambda) \log p(y^i|x^i, w) dw =$$

$$= \int \left(\frac{\partial}{\partial \lambda} q(w|\lambda) \right) \log p(y^i|x^i, w) dw$$

Not an expectation over q anymore!

Most popular solution: **reparametrization trick**

Diederik P Kingma, Max Welling . Auto-Encoding Variational Bayes. ICLR 2013

Reparametrization trick

As an example, consider 1-dim normal approximate posterior:

$$q(w|\lambda) = \mathcal{N}(\mu, \sigma^2), \quad \lambda = \{\mu, \sigma\}$$

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Diederik P Kingma, Max Welling . Auto-Encoding Variational Bayes. ICLR 2013
Image inspired by https://jaan.io/what-is-variational-autoencoder-vae-tutorial/

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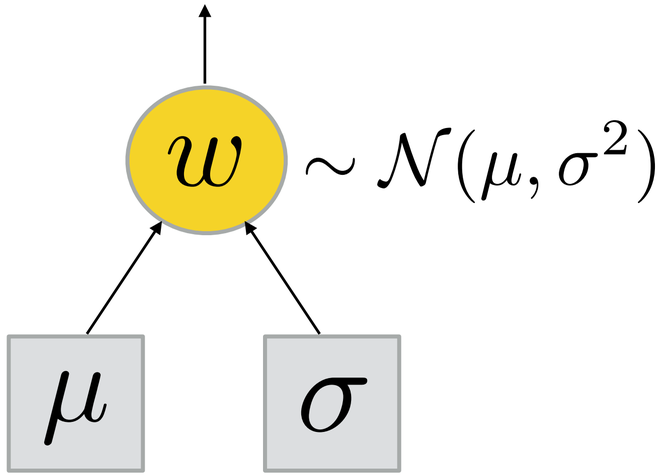

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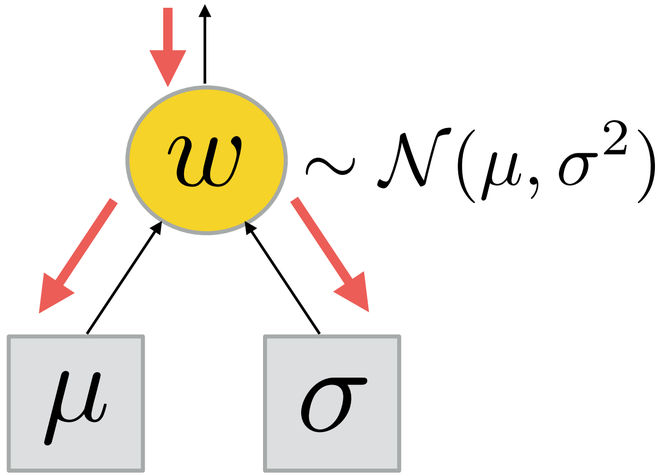

Gradients propagate through randomness

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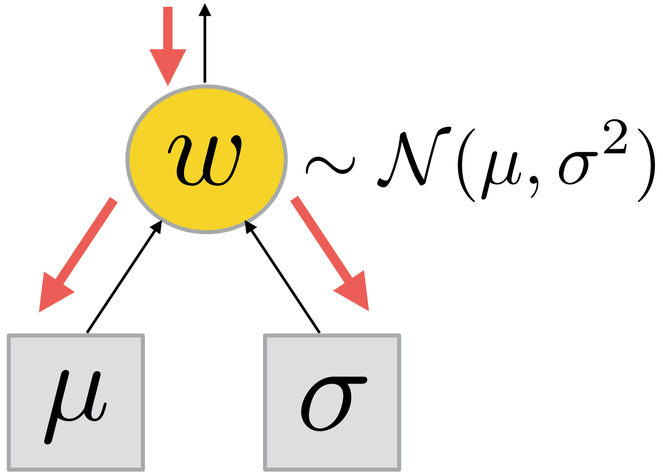

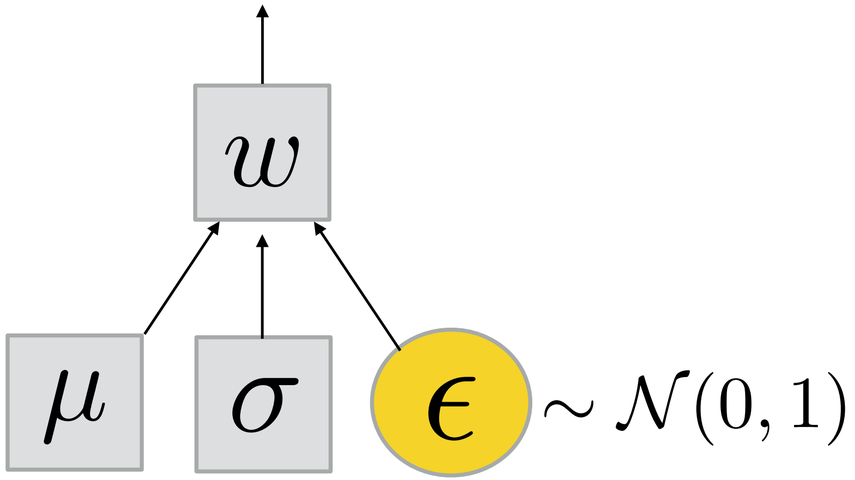

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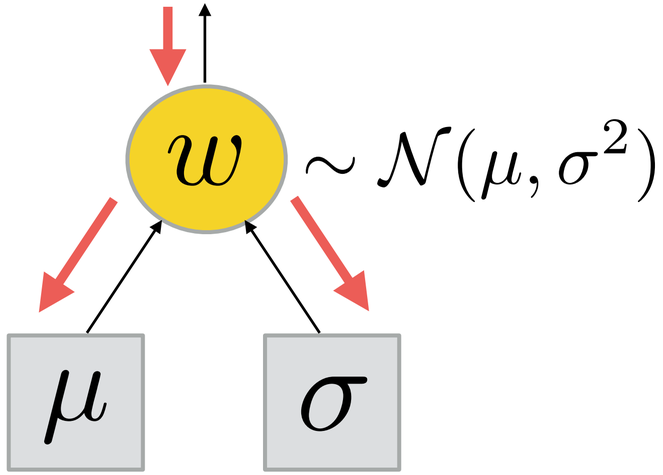

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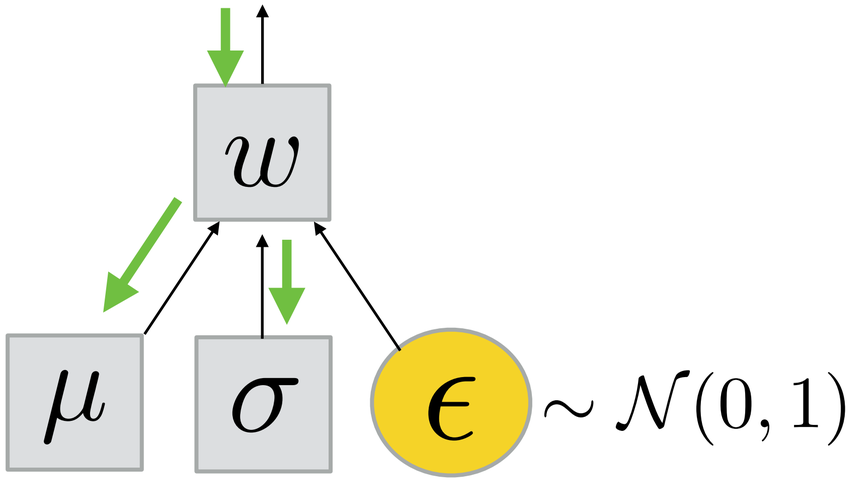

Gradients propagate only through deterministic nodes

Diederik P Kingma, Max Welling . Auto-Encoding Variational Bayes. ICLR 2013
Image inspired by https://jaan.io/what-is-variational-autoencoder-vae-tutorial/

Reparametrization trick: general form

$$w \sim \mathcal{N}(\mu, \sigma^2) \quad \Leftrightarrow \quad w = \mu + \sigma\epsilon, \quad \epsilon \sim \mathcal{N}(0, 1)$$

$$w \sim q(w|\lambda) \quad \Leftrightarrow \quad w = f(\lambda, \epsilon), \quad \epsilon \sim p(\epsilon)$$

distribution conditioned on parameters

dependency on parameters

unconditioned distribution

Diederik P Kingma, Max Welling . Auto-Encoding Variational Bayes. ICLR 2013

Reparametrization trick

$$\underbrace{w \sim q(w|\lambda)}_{\text{distribution conditioned on parameters}} \quad \Leftrightarrow \quad \underbrace{w = f(\lambda, \epsilon),}_{\text{dependency on parameters}} \quad \underbrace{\epsilon \sim p(\epsilon)}_{\text{unconditioned distribution}}$$

$$\nabla_\lambda \mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w) = \nabla_\lambda \mathbb{E}_{p(\epsilon)} \log p(y^i|x^i, w = f(\lambda, \epsilon)) =$$

$$= \mathbb{E}_{p(\epsilon)} \nabla_\lambda \log p(y^i|x^i, w = f(\lambda, \epsilon))$$

Diederik P Kingma, Max Welling . Auto-Encoding Variational Bayes. ICLR 2013

Reparametrization trick: examples

$$q(w|\lambda) \quad \longrightarrow \quad w = f(\lambda, \epsilon), \;\; p(\epsilon)$$

$q(w\|\lambda)$	$p(\epsilon)$	$f(\lambda, \epsilon)$
$\mathcal{N}\left(\mu, \sigma^2\right)$	$\mathcal{N}(0, 1)$	$w = \sigma\epsilon + \mu$
$\mathcal{G}(1, \beta)$	$\mathcal{G}(1, 1)$	$w = \beta\epsilon$
$\mathcal{E}(\lambda)$	$\mathcal{U}(0, 1)$	$w = -\frac{\log \epsilon}{\lambda}$
$\mathcal{N}(\mu, \Sigma)$	$\mathcal{N}(0, I)$	$w = A\epsilon + \mu, \;\text{where}\; AA^T = \Sigma$

Reparametrization trick: examples

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noise on weights!

Local reparametrization trick

1. Reparametrization trick ⇒ unbiased estimate of the gradients

$$w_{ij} = \mu_{ij} + \epsilon_{ij}\sigma_{ij}, \quad \epsilon_{ij} \sim \mathcal{N}(0, 1)$$

- Too expensive! ($|w|\times$ mini-batch size)
- One sample per mini-batch? High variance of stochastic gradients & correlated predictions

Local reparametrization trick

1. Reparametrization trick ⇒ unbiased estimate of the gradients

$$w_{ij} = \mu_{ij} + \epsilon_{ij}\sigma_{ij}, \quad \epsilon_{ij} \sim \mathcal{N}(0, 1)$$

2. Local reparametrization trick: **sample preactivations** instead of weights
⇒ reduced variance of the gradients & uncorrelated predictions

$$w_{ij} \sim \mathcal{N}(\mu_{ij}, \sigma_{ij}^2) \qquad \mathbb{E}X_2 = MX_1 \quad VarX_2 = \Sigma^2 {X_1}^2$$

$$X_2 = WX_1 \qquad X_2 \sim \mathcal{N}(MX_1, \Sigma^2 {X_1}^2)$$

blue means element-wise

$$X_2 = MX_1 + \sqrt{\Sigma^2 {X_1}^2} \odot \epsilon$$

Diederik P. Kingma et al. Variational dropout and the local reparameterization trick. NIPS 2015

Training: putting everything together

How to estimate the data term?

$$\sum_{i=1}^{N} \underbrace{\mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w)}_{\text{Data term}} - \underbrace{KL(q(w|\lambda)||p(w))}_{\text{Regularizer}} \to \max_{\lambda}$$

sample mini-batch of the training objects

sample weights from q using reparametrization trick

$$\sum_{j=1}^{m} \log p(y^{i_j}|x^{i_j}, w = f(\lambda, \epsilon^j)), \quad \epsilon^j \sim p(\epsilon) \quad i_j \sim \text{Unif}(1, \dots, N)$$

Training: putting everything together

Deterministic neural network:

$$w^{new} = w^{old} + \eta \frac{\partial}{\partial w} \sum_{j=1}^{m} \log p(y^{i_j} | x^{i_j}, w^{old}) \qquad i_j \sim \text{Unif}(1, \ldots, N)$$

Bayesian neural network:

$$\lambda^{new} = \lambda^{old} + \eta \frac{\partial}{\partial \lambda} \sum_{j=1}^{m} \log p(y^{i_j} | x^{i_j}, w = f(\lambda^{old}, \epsilon^j)), \qquad i_j \sim \text{Unif}(1, \ldots, N)$$

$$\epsilon^j \sim p(\epsilon)$$

m — mini-batch size η — learning rate

Questions

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- Assume $|w| = M$. If we approximate the posterior with a fully-factorized normal distribution, how many parameters do we train?

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- What can we do if we cannot compute the KL-regularizer?

$$KL(q(w|\lambda)||p(w)) = \int q(w|\lambda) \log \frac{q(w|\lambda)}{p(w)} dw$$

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- If we approximate the posterior with an arbitrary normal distribution (full covariance matrix)?

- What can we do if we cannot compute the KL-regularizer?

$$KL(q(w|\lambda)||p(w)) = \int q(w|\lambda) \log \frac{q(w|\lambda)}{p(w)} dw \approx \log \frac{q(\hat{w}|\lambda)}{p(\hat{w})}, \quad \hat{w} \sim q(w|\lambda)$$

+ reparametrization trick

From general framework to particular method

$$\sum_{i=1}^{N} \mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w) - KL(q(w|\lambda)||p(w)) \to \max_{\lambda}$$

Model specification:

- Choose particular prior

Training:

- Choose particular family for approximate posterior
- How to compute the KL-divergence?

Software

- Pyro (based on PyTorch)
- TensorFlow Probability (based on TensorFlow)
- Edward (based on TensorFlow)
- PyMC (based on Theano, pre-release with TensorFlow Probability)
- https://github.com/JavierAntoran/Bayesian-Neural-Networks — PyTorch implementations of popular Bayesian deep learning papers

Summary

- A lot of BNN advantages: regularization, ensembling, uncertainty estimation, …
- To train BNN, one should optimize ELBO using DSVI & RT
- Three steps towards a particular method

Plan

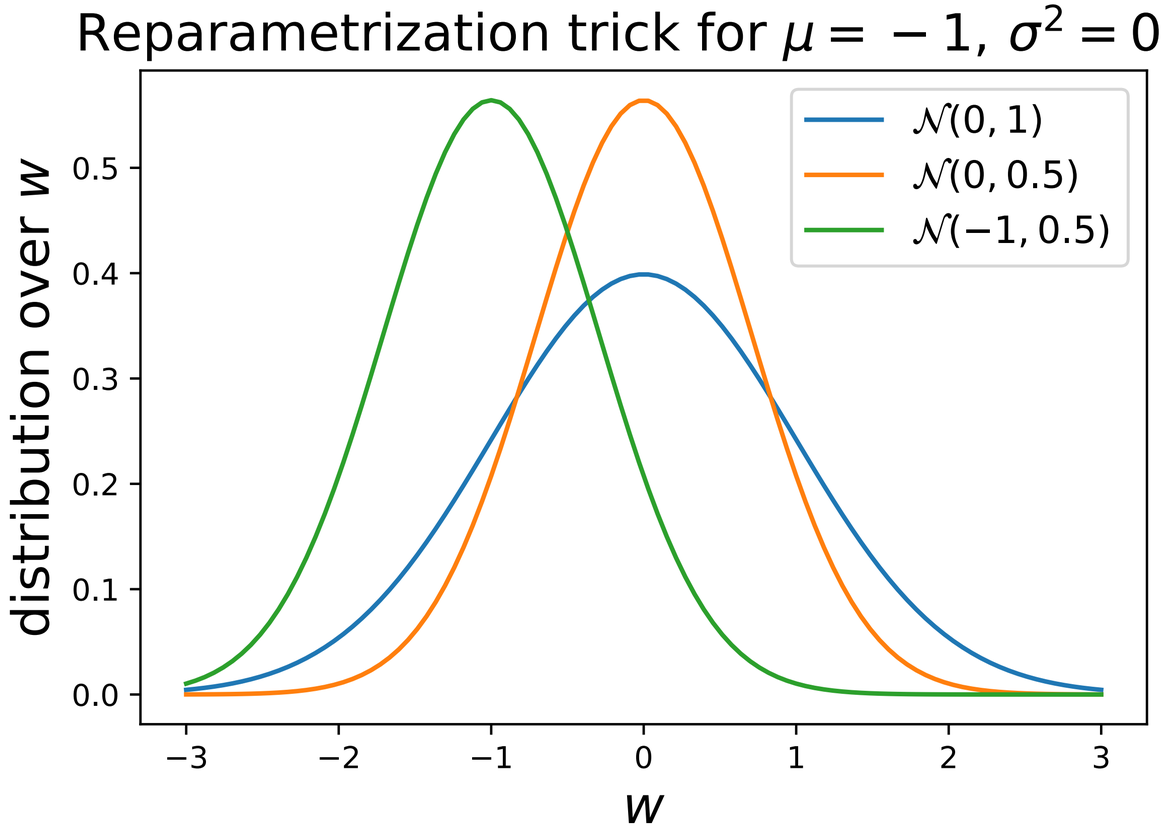
- Advantages of using Bayesian neural networks
- Training Bayesian neural networks
- Q&A + exercises

Questions

Reparametrization trick: recup

$$w \sim \mathcal{N}(\mu, \sigma^2) \quad \Leftrightarrow \quad w = \mu + \sigma\epsilon, \quad \epsilon \sim \mathcal{N}(0, 1)$$

$$w \sim q(w|\lambda) \quad \Leftrightarrow \quad w = f(\lambda, \epsilon), \quad \epsilon \sim p(\epsilon)$$

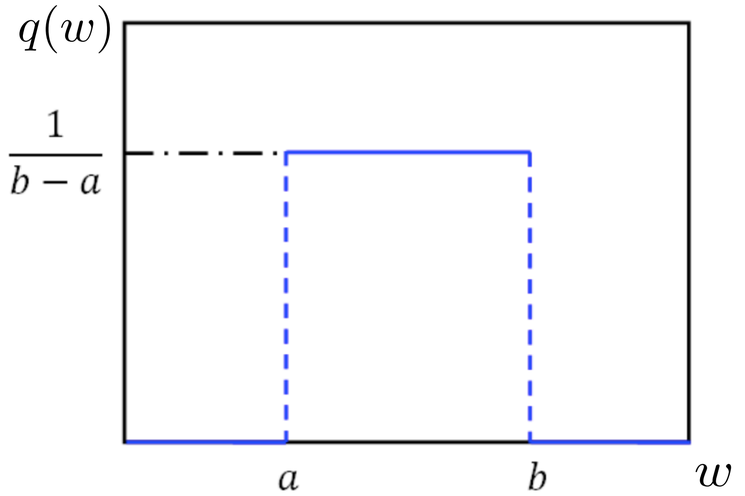


Exercises

Reparametrization trick: $w \sim q(w|\lambda) \quad \Leftrightarrow \quad w = f(\lambda, \epsilon), \qquad \epsilon \sim p(\epsilon)$

- How can we reparametrize uniform distribution?

$$q(w|a,b) = \begin{cases} \frac{1}{b-a}, \; w \in [a,b] \\ 0, \text{ otherwise} \end{cases}$$



- How can we reparametrize a mixture of normal distributions?

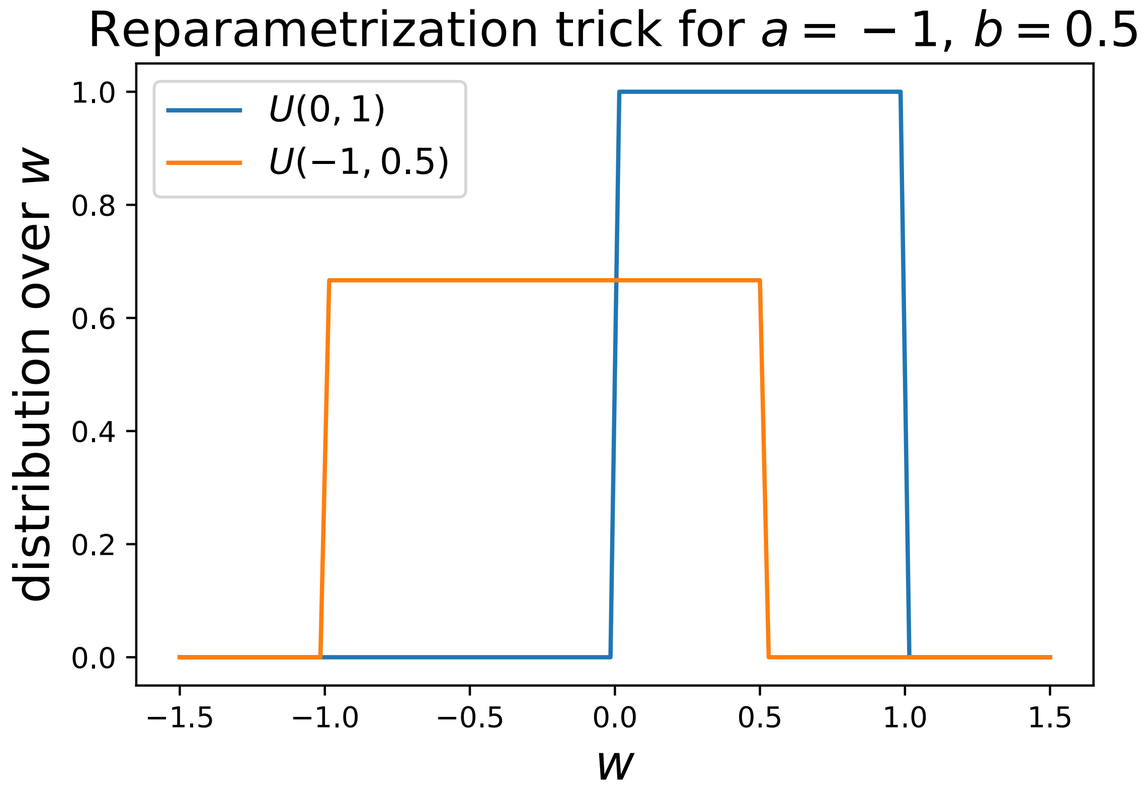
$$q(w|\mu,\sigma) = \sum_{s=1}^{S} \pi_s \mathcal{N}(w|\mu_s,\sigma_s), \quad \sum_{s=1}^{S} \pi_s = 1, \; \pi_s \geqslant 0 \qquad w \in \mathbb{R}$$

(π is fixed)

Reparametrizing uniform distribution

$$q(w|a,b) = \begin{cases} \frac{1}{b-a}, \ w \in [a,b] \\ 0, \text{ otherwise} \end{cases}$$

$$w \sim q(w|a,b) \Leftrightarrow$$
$$w = (1-t)a + tb, \ t \sim U(0,1)$$



Reparametrizing a mixture of normal distributions

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$$w \sim q(w|\mu,\sigma) \quad \Leftrightarrow \quad w = f(\mu,\sigma,\epsilon,z) = \mu_z + \epsilon\sigma_z$$
$$\epsilon \sim \mathcal{N}(\epsilon|0,1), \quad z \sim Cat(\pi_1,\ldots,\pi_S)$$

Example: binary dropout

Linear layer: $x_2 = Wx_1,\ W$ — weight matrix

With dropout: $x_2 = W(x_1 \odot m), \quad m_i \sim \mathrm{Bernoulli}(p),\ p$ — dropout rate

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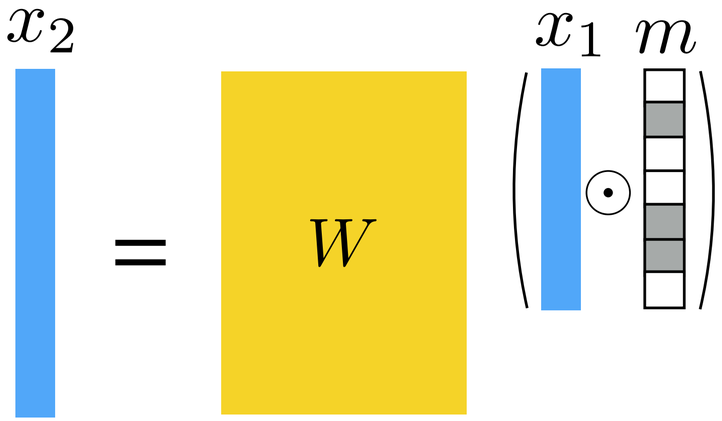

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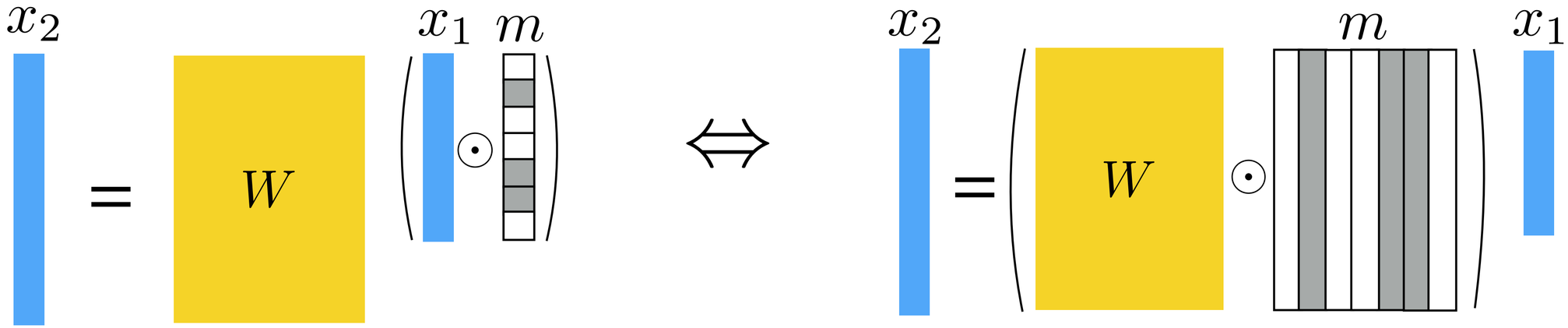

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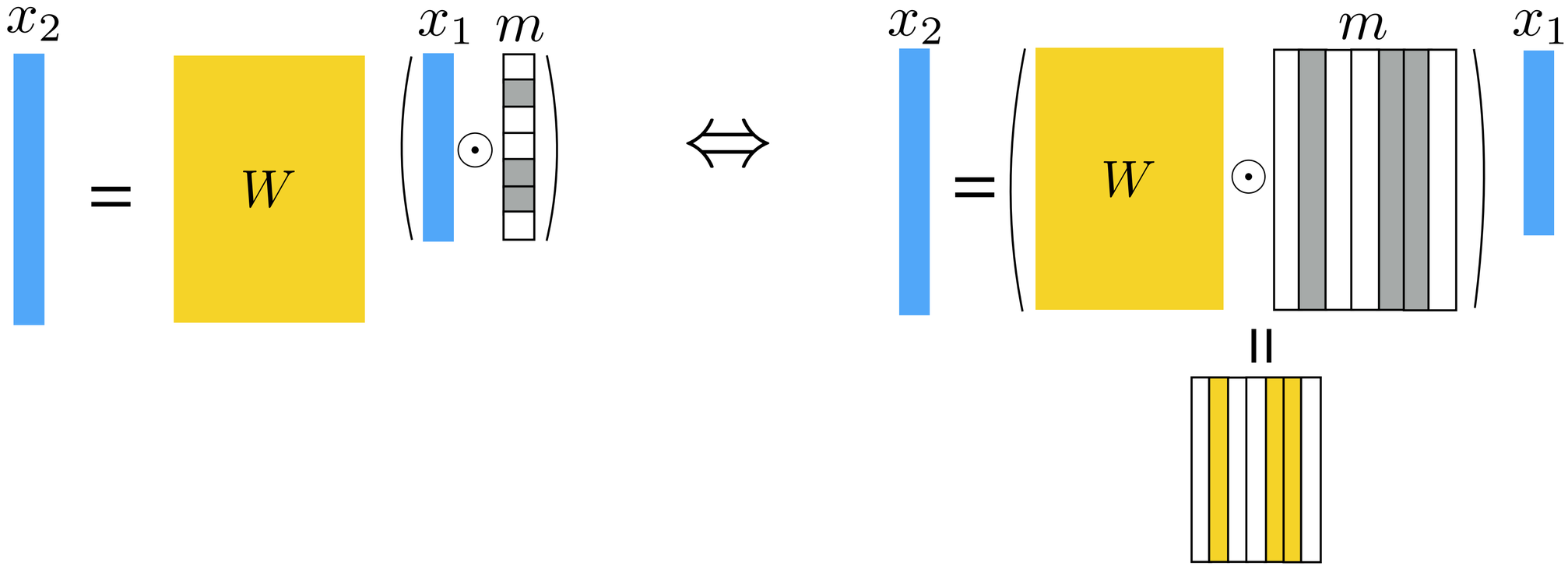

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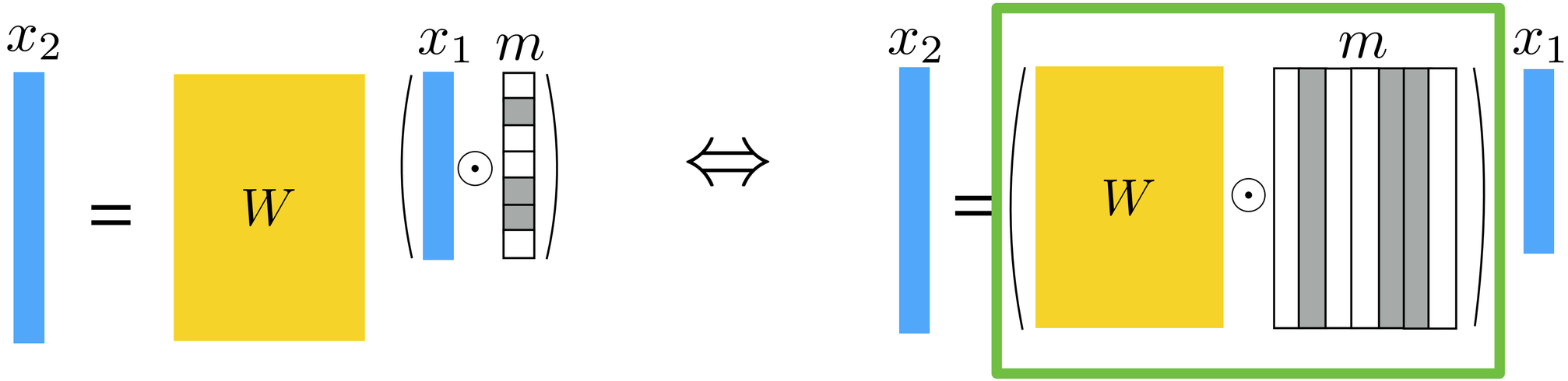
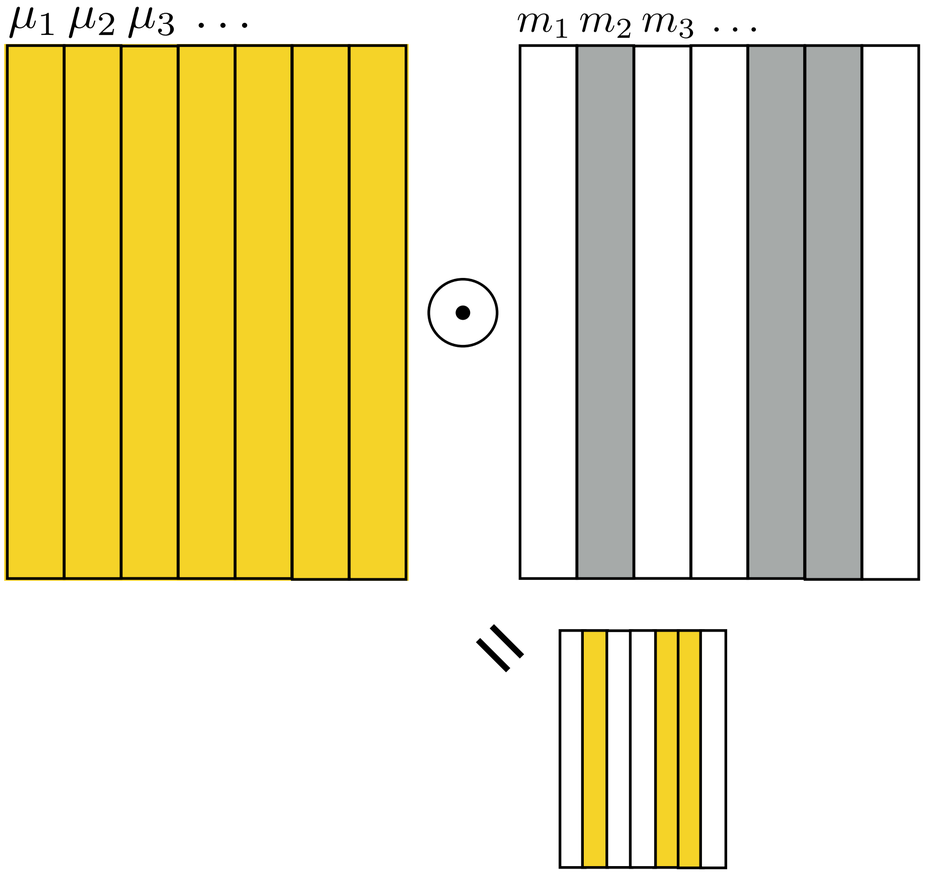


Applying dropout means sampling weights!

Example: binary dropout

Weight matrix:



reparametrization

$$w_i = f(\mu_i, m_i) = \mu_i \cdot m_i$$

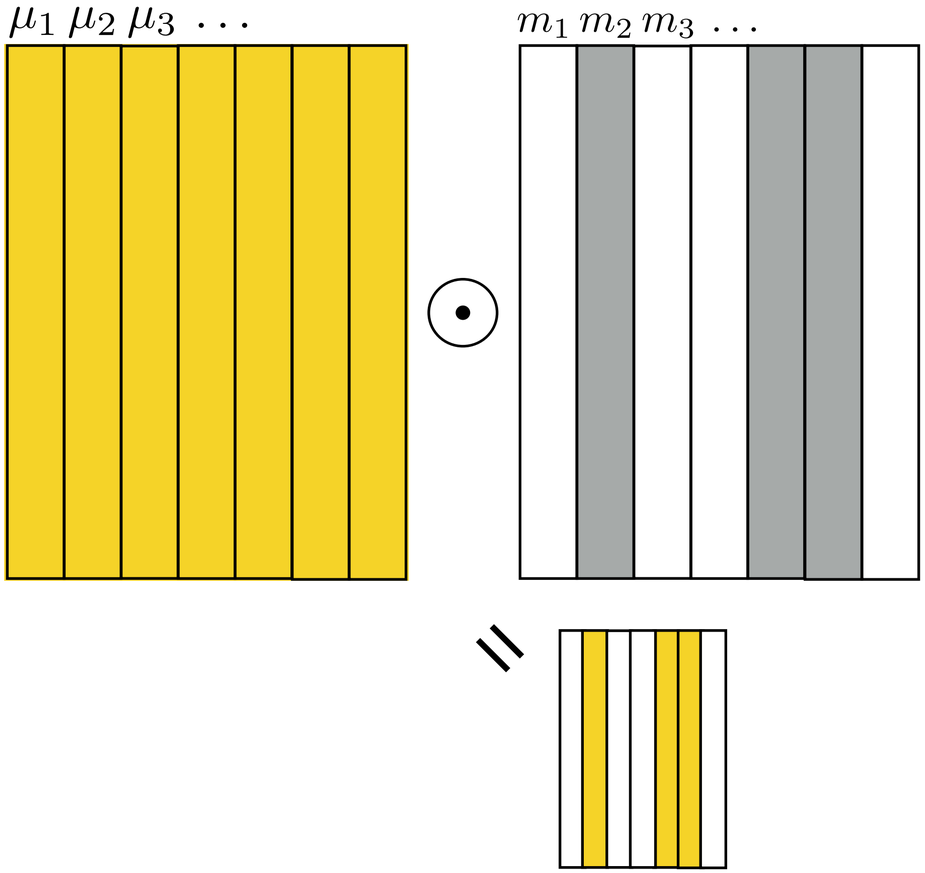
$$m_i \sim \text{Bernoulli}(p) \longleftarrow \text{0 or 1!}$$

p is a fixed hyperparameter!

Gal, Yarin and Ghahramani, Zoubin.
Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. ICML 2016

Example: binary dropout

Weight matrix:



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$$q(w_i|\mu_i) = p\,\delta(0) + (1-p)\,\delta(\mu_i)$$

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Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. ICML 2016

Example: binary dropout

Prior: ?

Approximate posterior: $q(W|\mu) = \prod_i q(w_i|\mu_i)$

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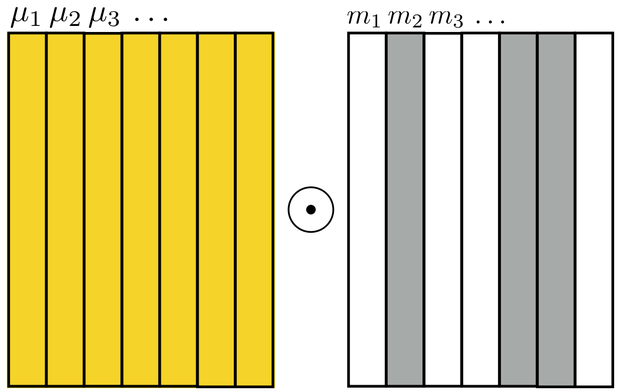
Weight matrix:



Approximate KL-divergence: ?

Gal, Yarin and Ghahramani, Zoubin.
Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. ICML 2016

Example: binary dropout

Prior: $p(W) = \prod_{i,j} p(w_{ij}), \quad p(w_{ij}) = \mathcal{N}(0, 1)$

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Approximate KL-divergence: $KL(q(W|\mu)||p(W)) \approx \alpha||\mu||_2^2$

L2-regularization

Gal, Yarin and Ghahramani, Zoubin.
Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. ICML 2016

Example: binary dropout, putting all together

$$\sum_{i=1}^{N} \underbrace{\mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w)}_{\text{Data term}} - \underbrace{KL(q(w|\lambda)||p(w))}_{\text{Regularizer}} \to \max_{\lambda}$$

$$\sum_{i=1}^{N} \mathbb{E}_{p(m)} \log p(y^i|x^i, w = \mu \cdot \text{diag}(m)) - ||\mu||_2^2 \to \max_{\mu}$$

sampling dropout masks

usual feed-forward pass & loss

applying dropout

applying L_2 regularization

Usual NN training with binary dropout

Gal, Yarin and Ghahramani, Zoubin.
Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. ICML 2016

Example: binary dropout, Bayesian benefits

Key messages of this example:

- Using binary dropout means being Bayesian!
- There are other dropout profits beyond regularization:
  - ensembling
  - uncertainty estimation

Gal, Yarin and Ghahramani, Zoubin.
Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. ICML 2016

Plan

- Advantages of using Bayesian neural networks
- Training Bayesian neural networks
- First example: binary dropout
- Second example: Bayesian sparsification

Compression of neural networks

- Deep neural networks achieve state-of-the-art performance in a variety of domains
- Model quality scales with model and dataset size
- State-of-the-art models usually incorporate **tens of millions of parameters**
- But **resources** (memory, processing time) **may be limited**

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- Model quality scales with model and dataset size
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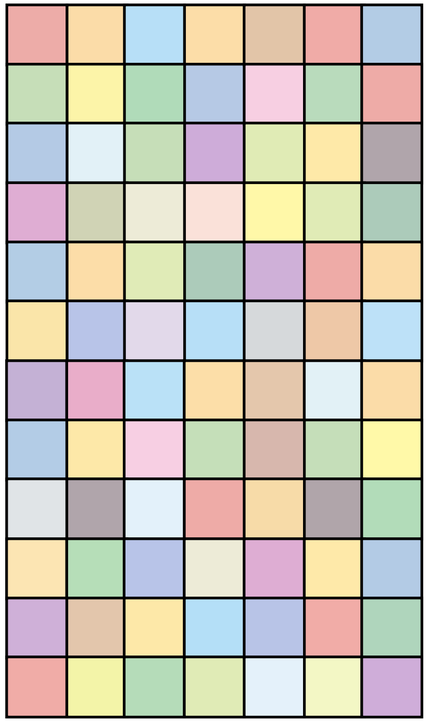
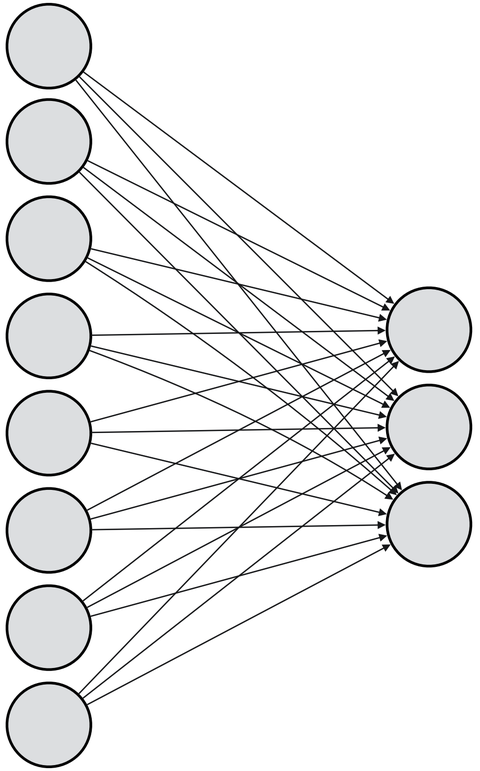
- But **resources** (memory, processing time) **may be limited**

- One of the solutions — sparsification

Neural network

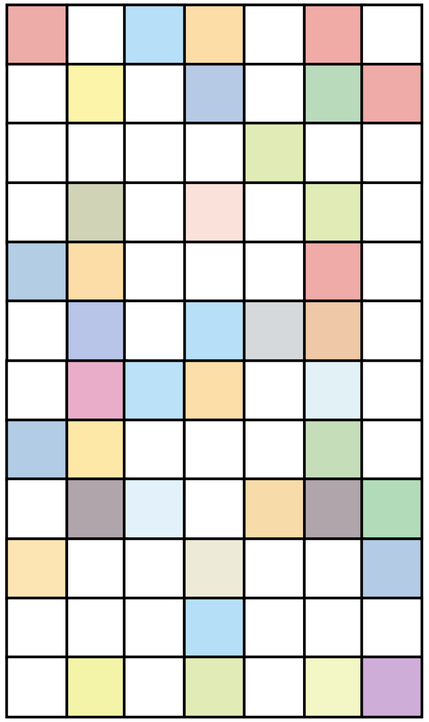


Weight matrix W

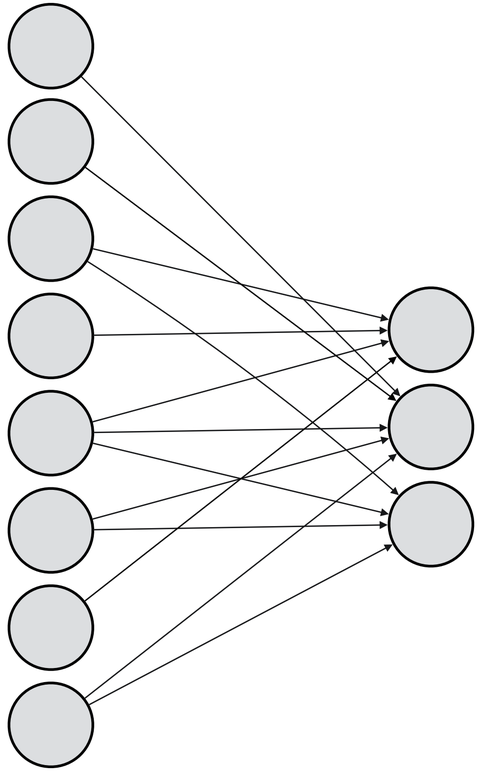


Computational graph

Sparse neural network



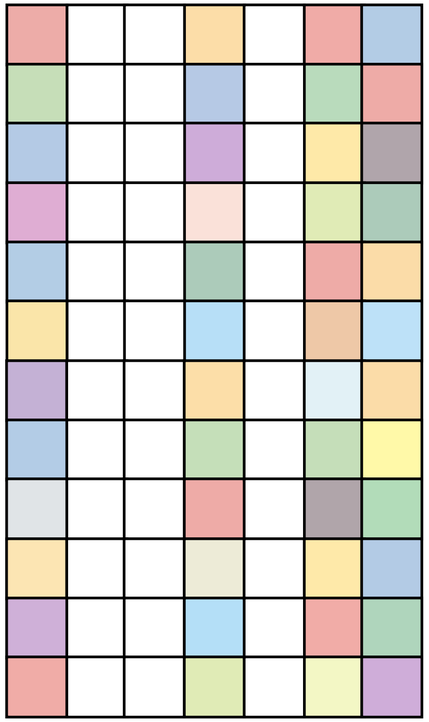
A lot of weights
set to zero



Weight matrix W

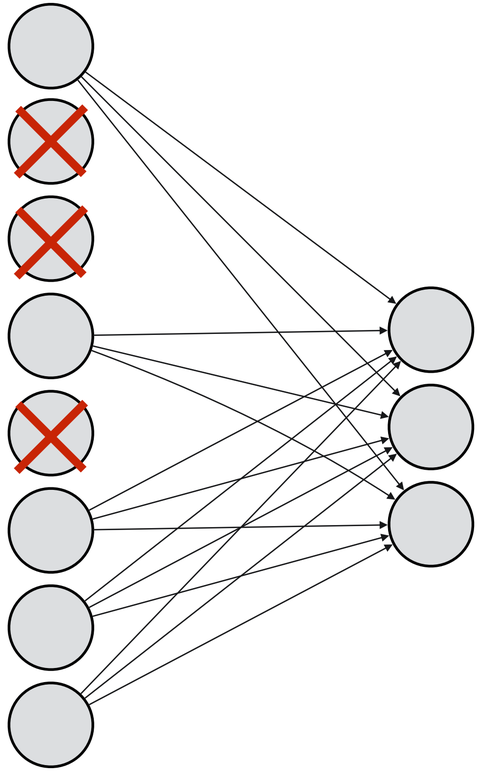
Computational graph

Structured sparsity



Weight matrix W

No outgoing edges
⇒ remove neuron



Computational graph

From general framework to particular method

$$\sum_{i=1}^{N} \mathbb{E}_{q(w|\lambda)} \log p(y^i|x^i, w) - KL(q(w|\lambda)||p(w)) \to \max_{\lambda}$$

Model specification:

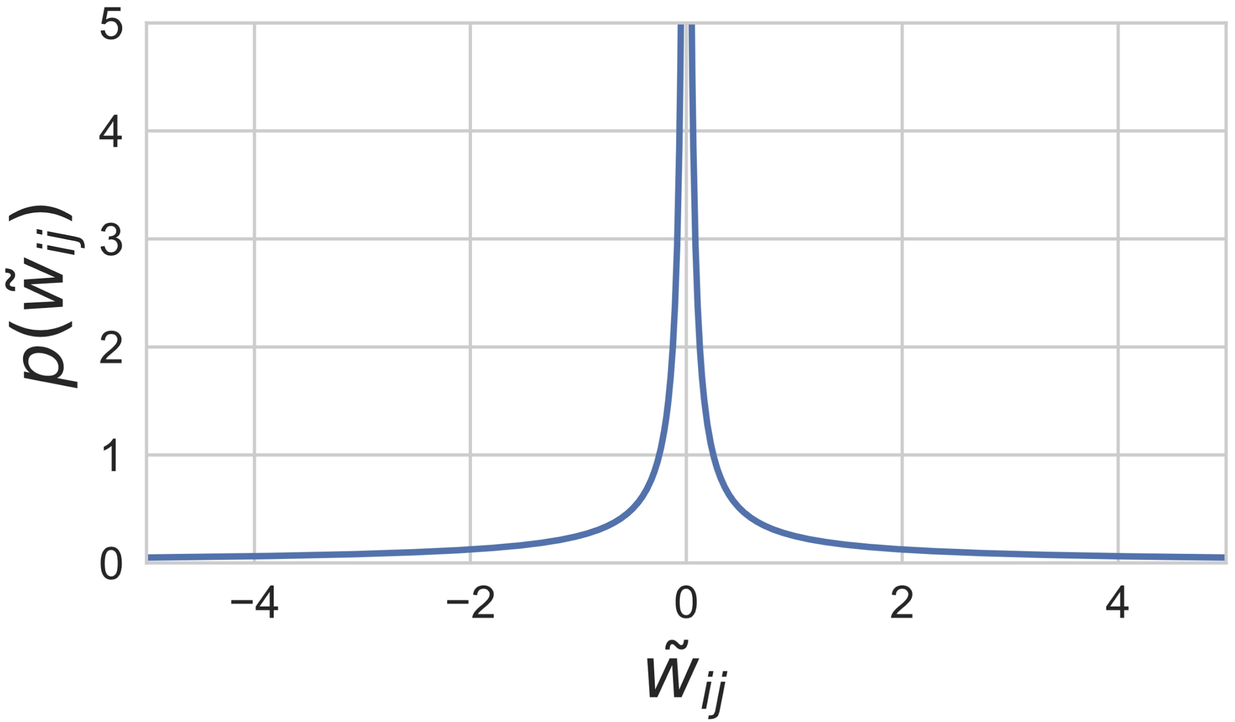
- Choose particular prior

Training:

- Choose particular family for approximate posterior
- How to compute the KL-divergence?

Example: sparse variational dropout

Prior: $p(w_{ij}) \propto \frac{1}{|w_{ij}|}$



Favors removing noisy weights!

Diederik P. Kingma et al. Variational dropout and the local reparameterization trick. NIPS 2015

Molchanov, Dmitry et al. Variational dropout sparsifies deep neural networks. ICML 2017

Example: sparse variational dropout

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Approximate posterior: ?

Approximate KL-divergence: ?

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Approximate posterior: $q(w_{ij}|\mu_{ij}, \sigma_{ij}) = \mathcal{N}(\mu_{ij}, \sigma_{ij}^2)$

Approximate KL-divergence: $-KL(q(w_{ij}|\mu_{ij}, \sigma_{ij}) \,\|\, p(w_{ij})) \approx f_{KL}(\alpha_{ij})$

$$\alpha_{ij} = \frac{\sigma_{ij}^2}{\mu_{ij}^2}$$

Favors large $\alpha_{ij} \Rightarrow$ removing noisy weights

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Approximating KL-divergence

Remember: training Bayesian neural networks — optimizing ELBO:

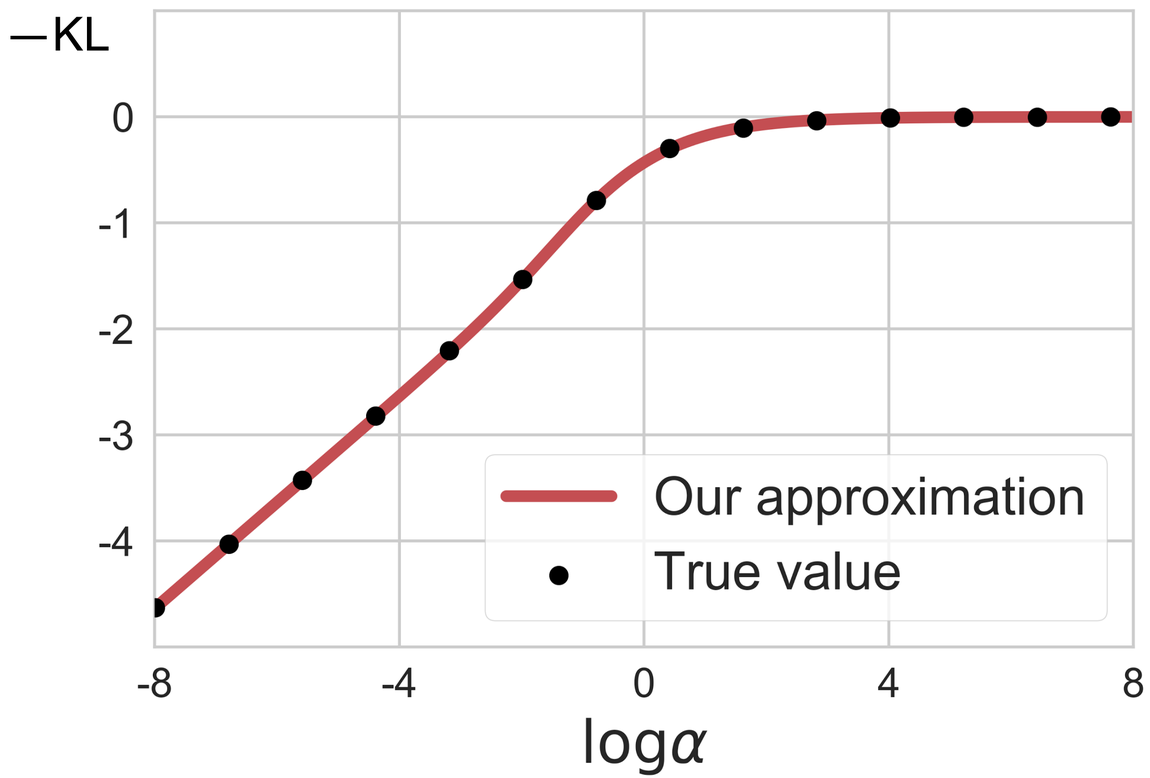
$$\sum_{i=1}^{N} \underbrace{\mathbb{E}_{q(w|\mu,\sigma)} \log p(y^i|x^i, w)}_{\text{Data term}} - \underbrace{KL(q(w|\mu,\sigma)||p(w))}_{\text{Regularizer}} \rightarrow \max_{\mu,\, \log\sigma}$$

Data term
Sample weights from q

Regularizer
Analytical approximation

Diederik P. Kingma et al. Variational dropout and the local reparameterization trick. NIPS 2015
Molchanov, Dmitry et al. Variational dropout sparsifies deep neural networks. ICML 2017

Approximating KL-divergence
(fully factorized)



$$-KL(q(w_{ij}|\mu_{ij},\sigma_{ij})\,\|\,p(w_{ij})) \approx$$

$$\approx k_1\sigma(k_2 + k_3\log\alpha_{ij})) - 0.5\log(1+\alpha_{ij}^{-1}) + \mathrm{C}$$

$$k_1 = 0.63576 \qquad k_2 = 1.87320 \qquad k_3 = 1.48695$$

$$\alpha_{ij} = \frac{\sigma_{ij}^2}{\mu_{ij}^2}$$

- KL depends only on α_{ij}
- Favors large α_{ij} ⇒

  removing noisy weights

Diederik P. Kingma et al. Variational dropout and the local reparameterization trick. NIPS 2015

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Ok, sparsify weights. What about biases?

$$\sum_{i=1}^{N} \mathbb{E}_{q(w|\mu,\sigma)} \log p(y^i|x^i, w) - KL(q(w|\mu,\sigma)||p(w)) \to \max_{\mu,\, \log\sigma}$$

Treat biases as deterministic parameters and find a point estimate:

$$\sum_{i=1}^{N} \mathbb{E}_{q(w|\mu,\sigma)} \log p(y^i|x^i, w, b) - KL(q(w|\mu,\sigma)||p(w)) \to \max_{\mu,\, \log\sigma, b}$$

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Final algorithm

Training on a mini-batch X with labels Y:

1. Sample weights: $\hat{w}_{ij} = \mu_{ij} + \hat{\epsilon}_{ij}\sigma_{ij}, \quad \hat{\epsilon}_{ij} \sim \mathcal{N}(0, 1)$
2. Forward pass: $Y_{\text{pred}} = NN(X, \hat{w}, b)$
3. Backward pass + SGD step: compute stochastic gradients of ELBO:

$$\nabla_{\mu, \log \sigma, b} \left(N \cdot \text{Loss}\big(Y, Y_{\text{pred}}\big) + \text{SparseReg}(\sigma/\mu) \right)$$

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Pruning after training:

If $\mu_{ij}^2/\sigma_{ij}^2 < \text{threshold}$:

$\mu_{ij} = 0, \ \sigma_{ij} = 0$

signal-to-noise ratio

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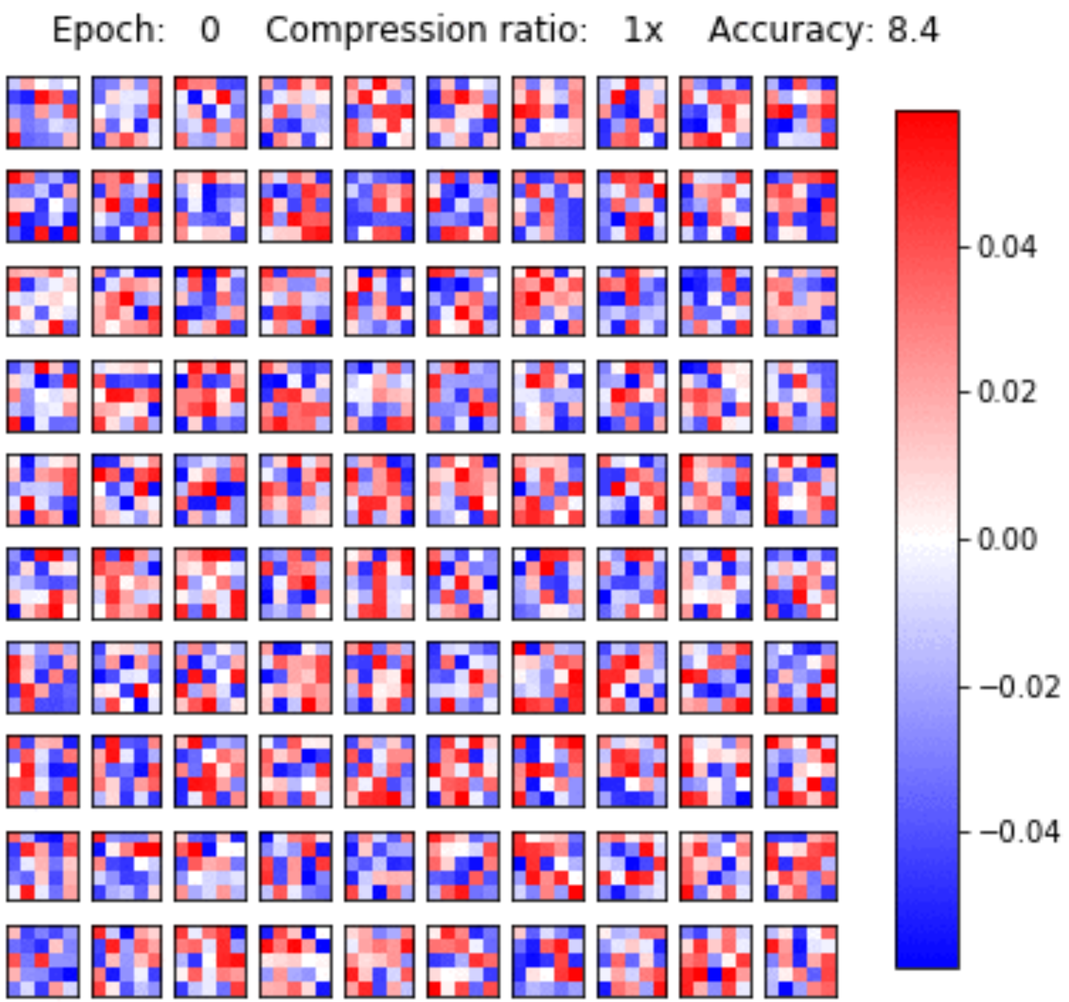
Prediction for a mini-batch X :

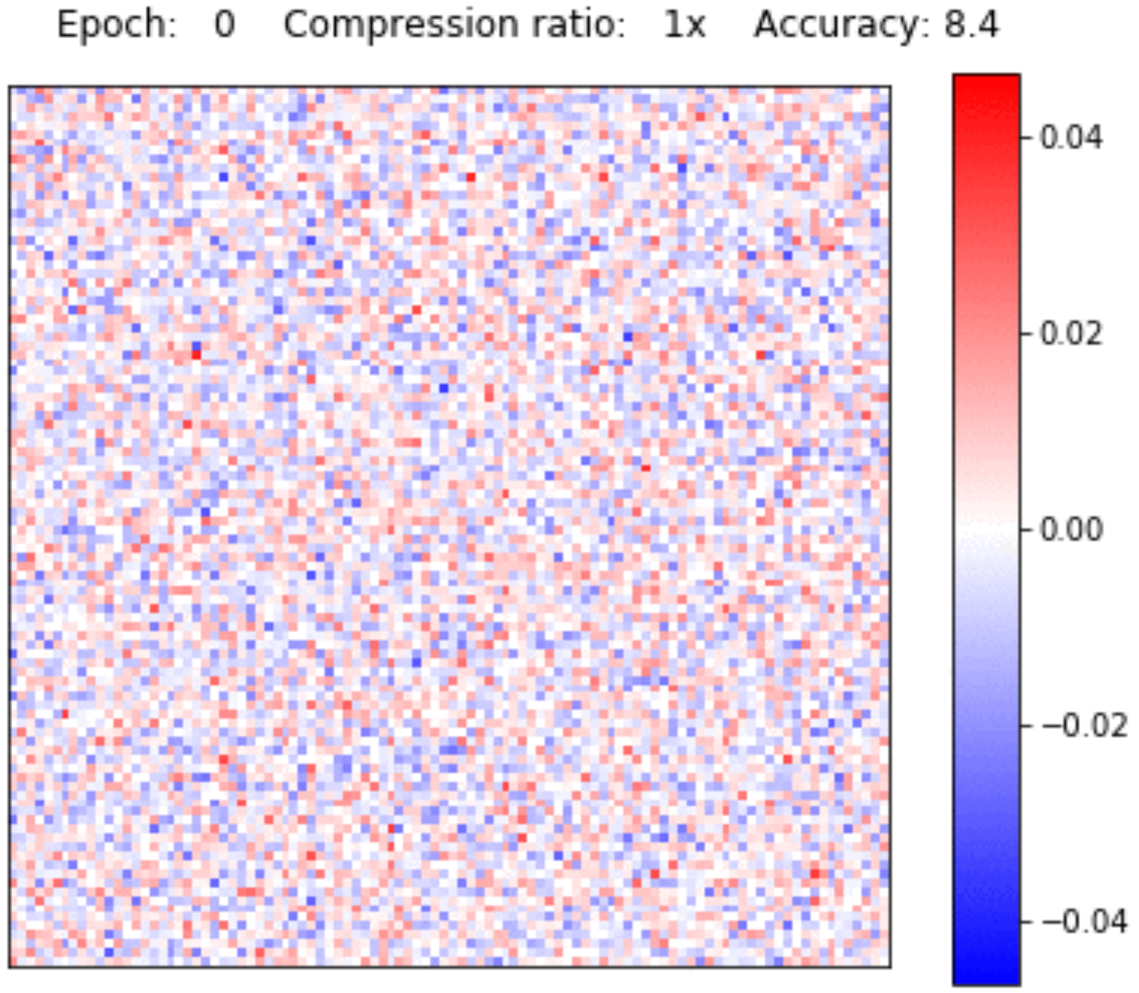
Return $Y_{\text{pred}} = NN(X, \mu, b)$

do not ensemble because we want the most compact and fast network

Sparse variational dropout: visualization



LeNet-5: convolutional layer



LeNet-5: fully-connected layer
(100 x 100 patch)

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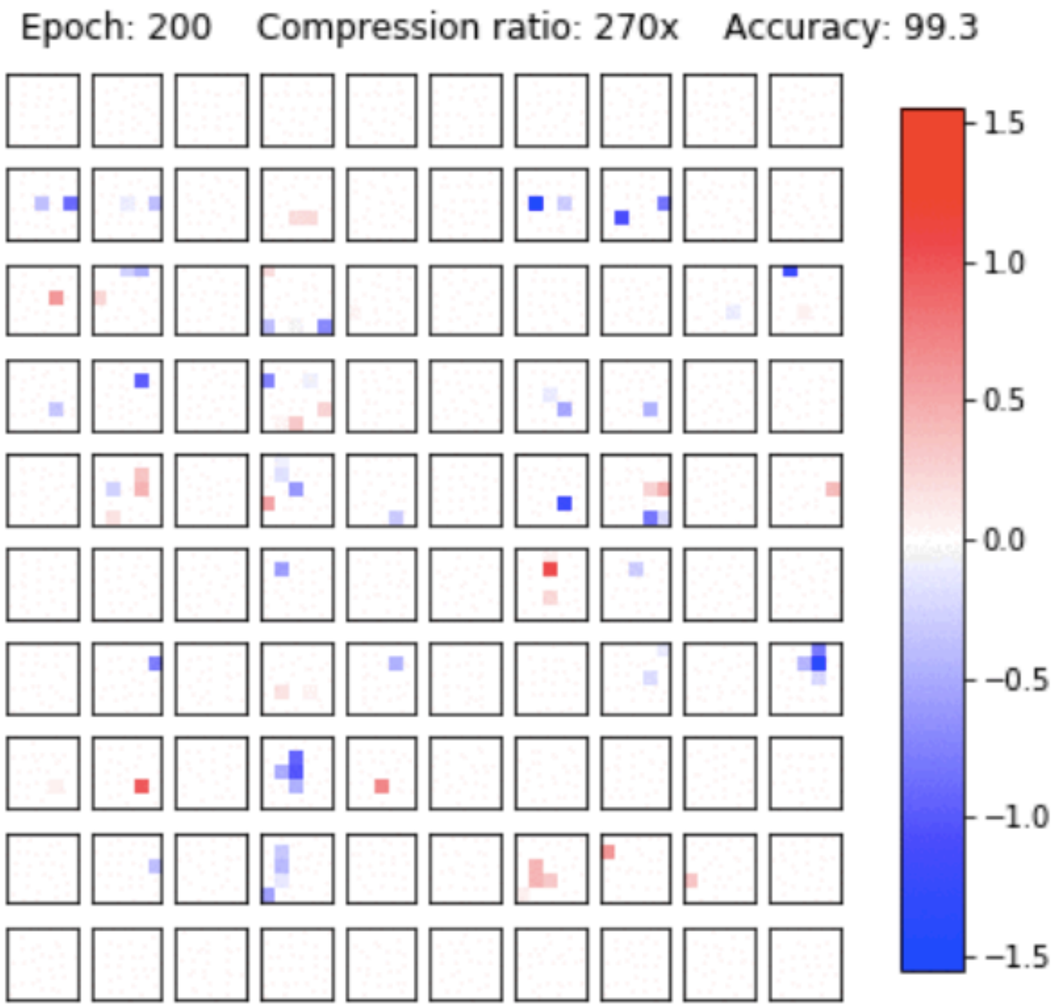
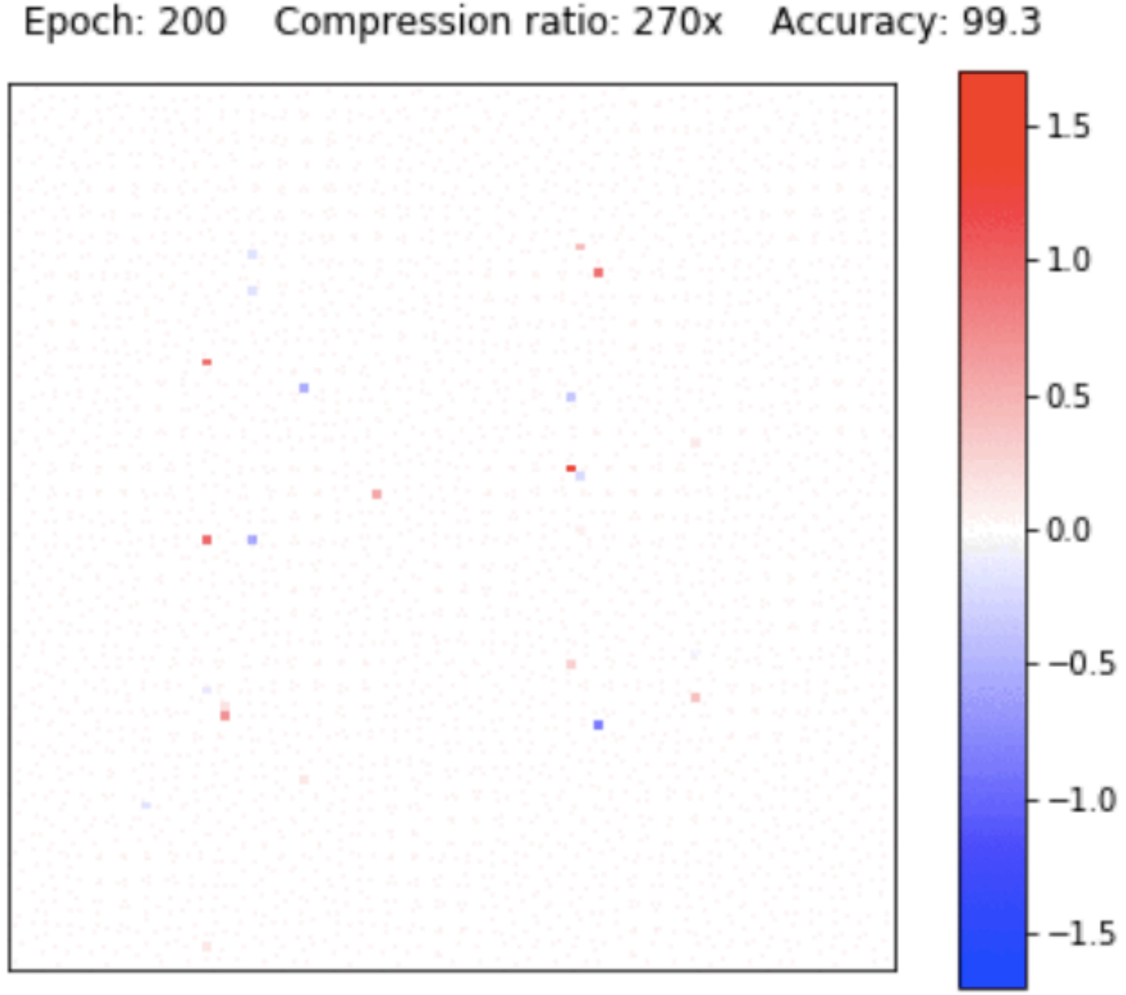


LeNet-5: convolutional layer

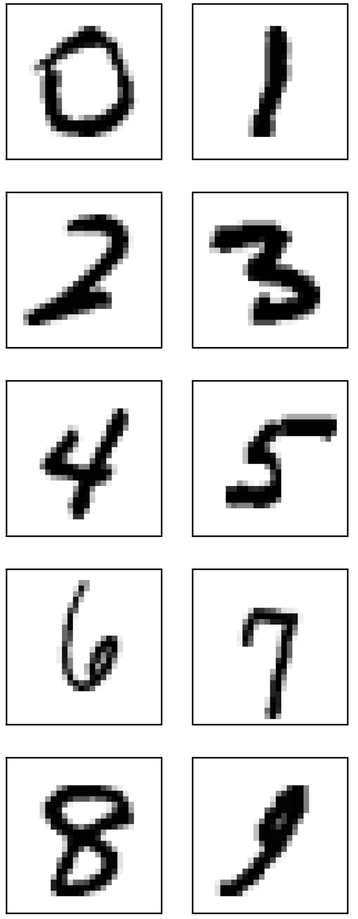


LeNet-5: fully-connected layer
(100 x 100 patch)

Lenet-5-Caffe and Lenet-300-100 on MNIST

Fully Connected network: LeNet-300-100 **Convolutional network**: Lenet-5-Caffe

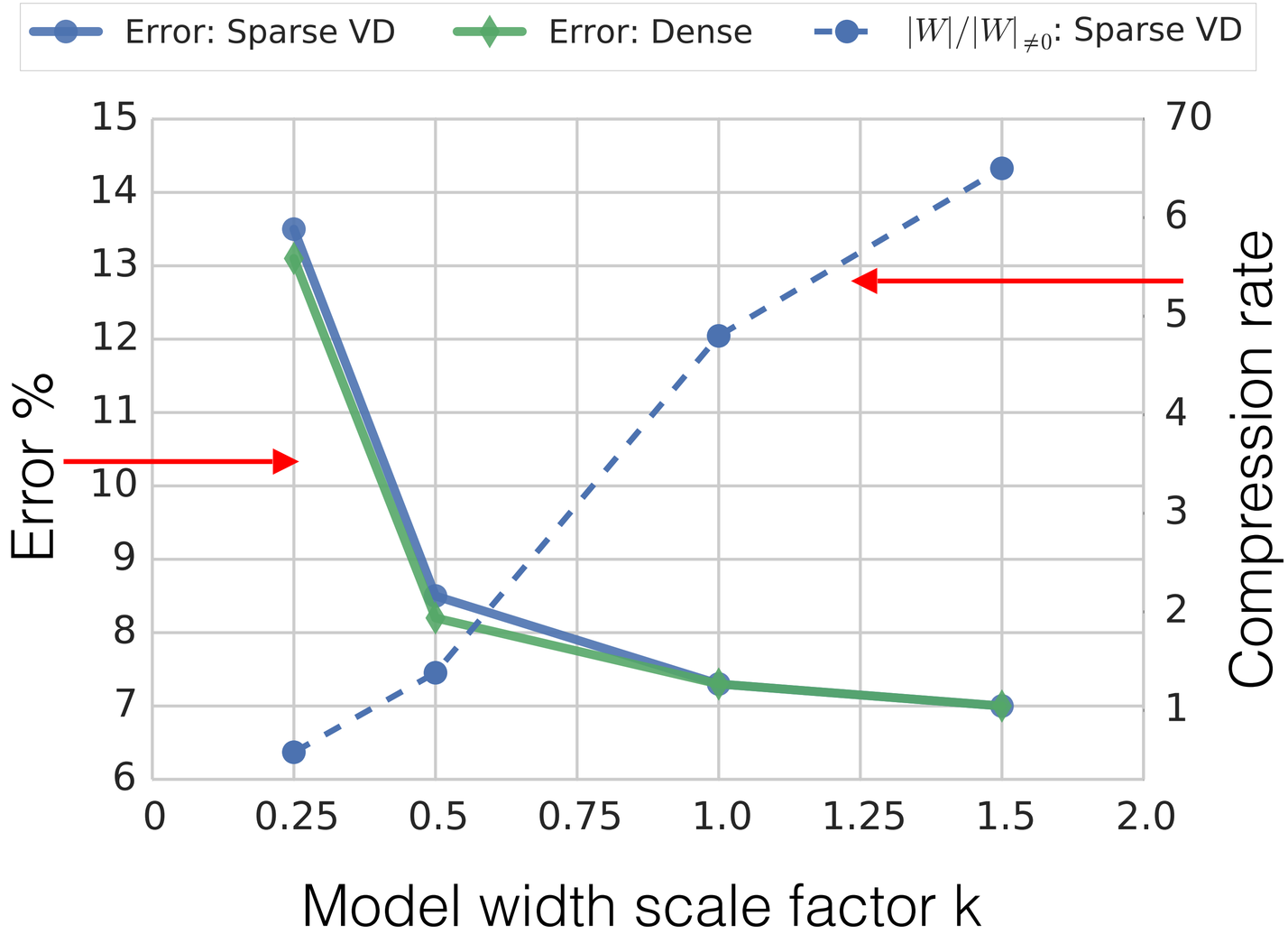
Network	Method	Error %	Sparsity per Layer %	$\frac{\lvert\mathbf{W}\rvert}{\lvert\mathbf{W}_{\neq 0}\rvert}$
LeNet-300-100	Original	1.64		1
	Pruning	1.59	$92.0 - 91.0 - 74.0$	12
	DNS	1.99	$98.2 - 98.2 - 94.5$	56
	SWS	1.94		23
(ours)	Sparse VD	1.92	$98.9 - 97.2 - 62.0$	**68**
LeNet-5-Caffe	Original	0.80		1
	Pruning	0.77	$34 - 88 - 92.0 - 81$	12
	DNS	0.91	$86 - 97 - 99.3 - 96$	111
	SWS	0.97		200
(ours)	Sparse VD	0.75	$67 - 98 - 99.8 - 95$	**280**



Molchanov, Dmitry et al. Variational dropout sparsifies deep neural networks. ICML 2017

VGG-like on CIFAR-10

Number of filters / neurons is linearly scaled by k (the width of the network)



Random Labeling

Dataset	Architecture	Train Acc.	Test Acc.	Sparsity
MNIST	FC + BD	100%	10%	—
MNIST	FC + Sparse VD	10%	10%	100%
CIFAR-10	VGG + BD	100%	10%	—
CIFAR-10	VGG + Sparse VD	10%	10%	100%

No dependency between data and labels ⇒ Sparse VD yields an empty model where conventional models easily overfit.

Zhang, Chiyuan, et al. "Understanding deep learning requires rethinking generalization."

Sparse variational dropout: key messages

- Prior distribution can encode our desirable model properties (e. g. sparse weights)
- Other Bayesian compression techniques:
  - group sparsification (removing neurons / filters)
  - quantization (low-precision weights)

Summary

- A lot of BNN advantages: regularization, ensembling, uncertainty estimation, …
- To train BNN, one should optimize ELBO using DSVI & RT
- Three steps towards a particular method
- Using binary dropout means being Bayesian
- Prior distribution can encode our desirable model properties