Bayesian Sparsification of Neural Networks

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these slides
are here

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Agenda

- Sparsification: what and why
- Bayesian neural networks
- Sparse variational dropout
- Practical assignment: implementation of SparseVD
- Model enhancements

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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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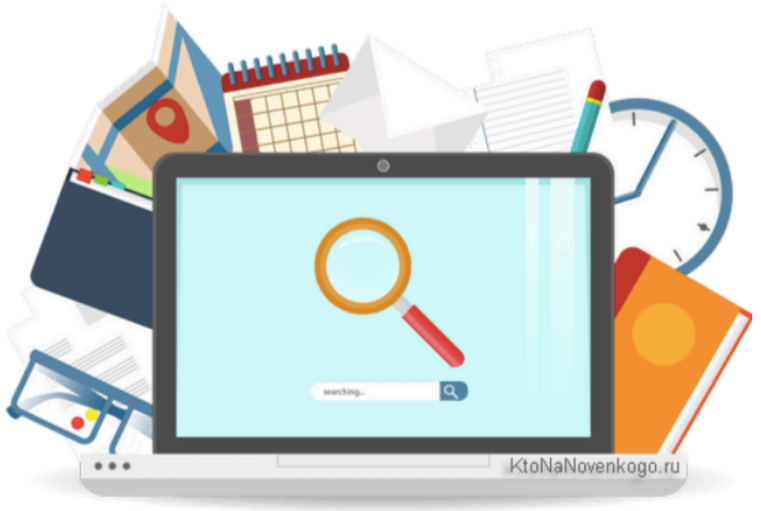

Urgent industrial problem! well solved using Bayesian deep learning!

Compression of neural networks

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Methods for neural network compression:

- Quantization
- Matrix factorizations
- Sparsification

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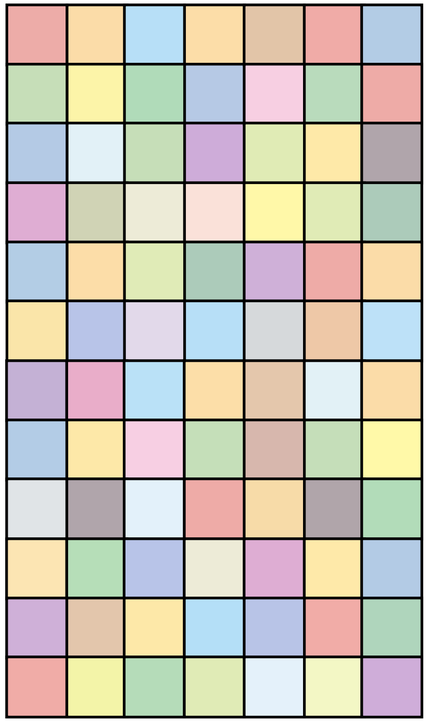
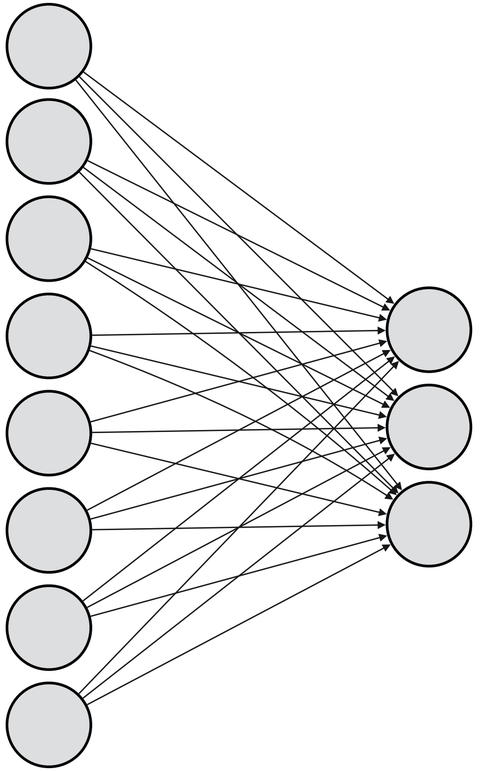
Neural network

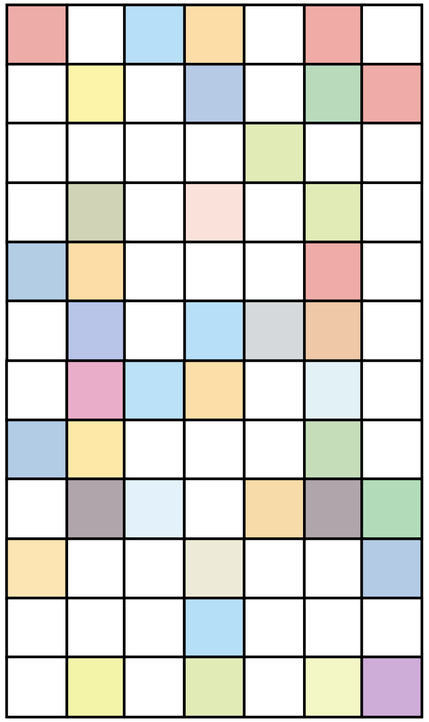


Weight matrix W

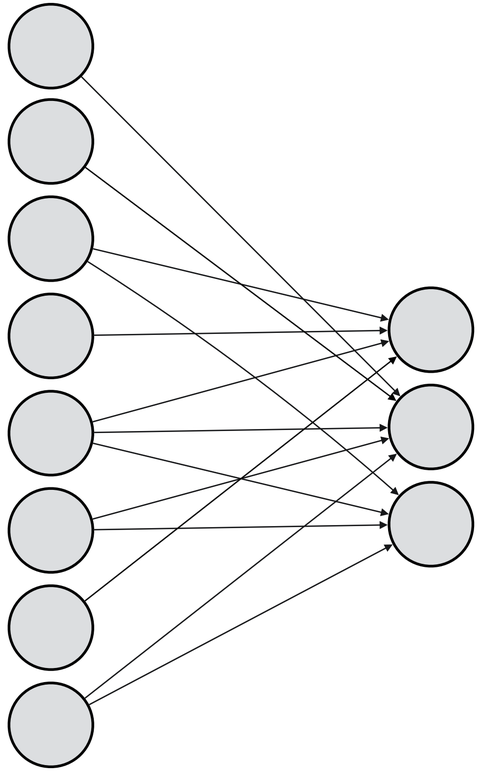


Computational graph

Sparse neural network



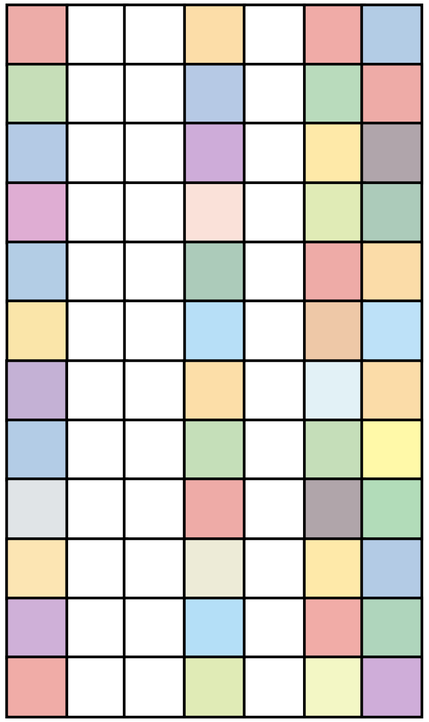
A lot of weights
set to zero



Weight matrix W

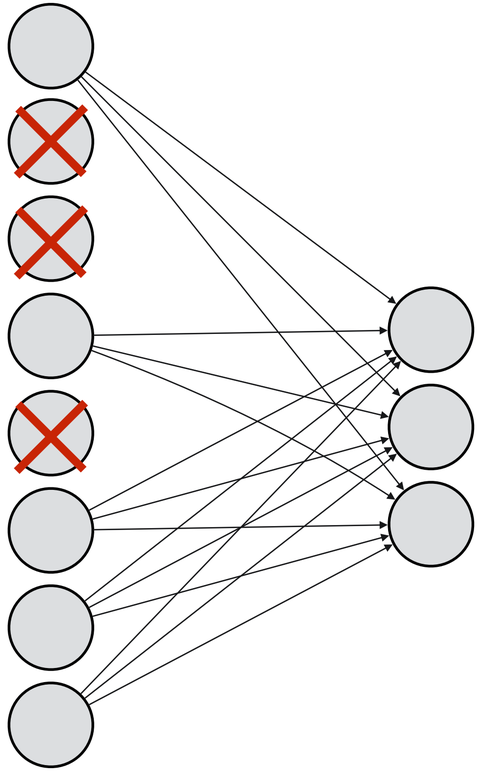
Computational graph

Structured sparsity



Weight matrix W

No outgoing edges
⇒ remove neuron



Computational graph

Sparsification of neural networks

Benefits:
- sparse matrices $\Rightarrow$ less memory consumption
- structured sparsification $\Rightarrow$ faster testing stage (prediction)
- Regularization
- A bit more interpretable model

Drawbacks:
- Sometimes leads to small quality drop

Applications:
- Mobile devices, smartphones
- Online services (where fast reply is needed)

Pruning

- Popular approach to NN sparsification
- Example training algorithm:

  - Optimize L_1-regularized loss (induces sparsity)
  - At the beginning of each epoch, set to 0 all weights satisfying $|w| < T$.

Wei Wen et al. Learning Intrinsic Sparse Structures within Long Short-Term Memory. ICLR 2018

Pruning

- Popular approach to NN sparsification
- Example training algorithm:
  - Optimize L_1-regularized loss
  - At the beginning of each epoch, set to 0 all weights satisfying $|w| < T$.
- Variants:
  - Different pruning schedule (increase T gradually / constant T)
  - Prune based on threshold T / prune percent of weights
  - Propagate gradients through zero weights or not
  - Prune from scratch / train - prune - retrain
  - …

huge number of hyperparameters

Two popular frameworks for sparsification

Pruning	**Bayesian sparsification**
A lot of method hyperparameters	(Almost) no method hyperparameters
Need to choose training schedule	Need to choose training schedule
non-Bayesian	Bayesian!

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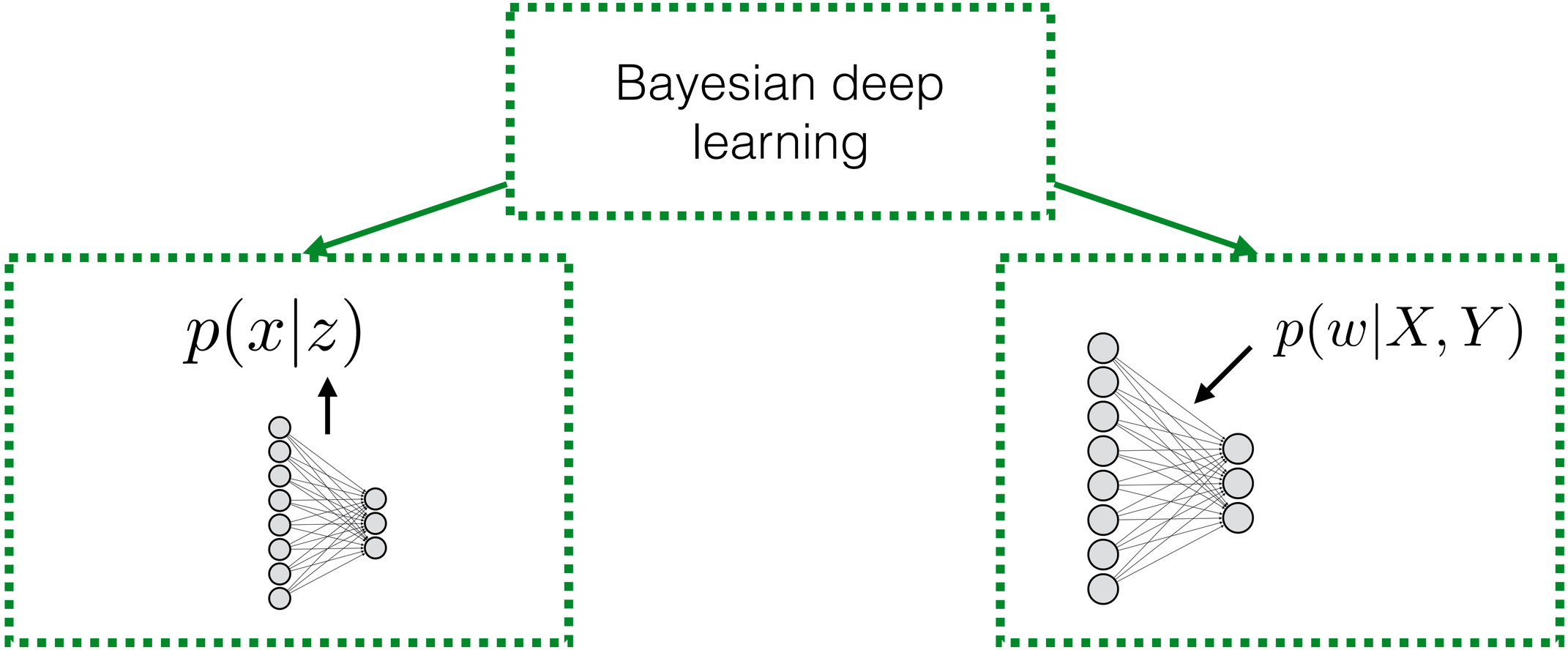
Bayesian deep learning



Deep generative models:
VAE, NF …

Bayesian neural networks
(discriminative)

Regularization by noise

- Traditional (1943+) regularization: add some penalty for model complexity
  - L_2, L_1 - regularization, max norm constraint

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

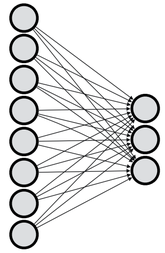
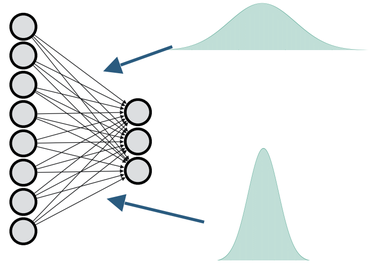
- More recent (1990+) approaches: regularization by noise
    - Data augmentation, dropout, gradient noise

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

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	Prior $p(w)$ + Data X, Y → Posterior $p(w\|X, Y)$
Prediction:	$p(y_*\|x_*, w)$	$\mathbb{E}_{p(w\|X,Y)}p(y_*\|x_*, w)$

Why go Bayesian?

A principled framework with many useful applications

- Regularization
- Ensembling
- Uncertainty estimation
- On-line / continual learning
- Automatic hyperparameter choice
- Different prior ⇒ different properties of the network

Ensembling

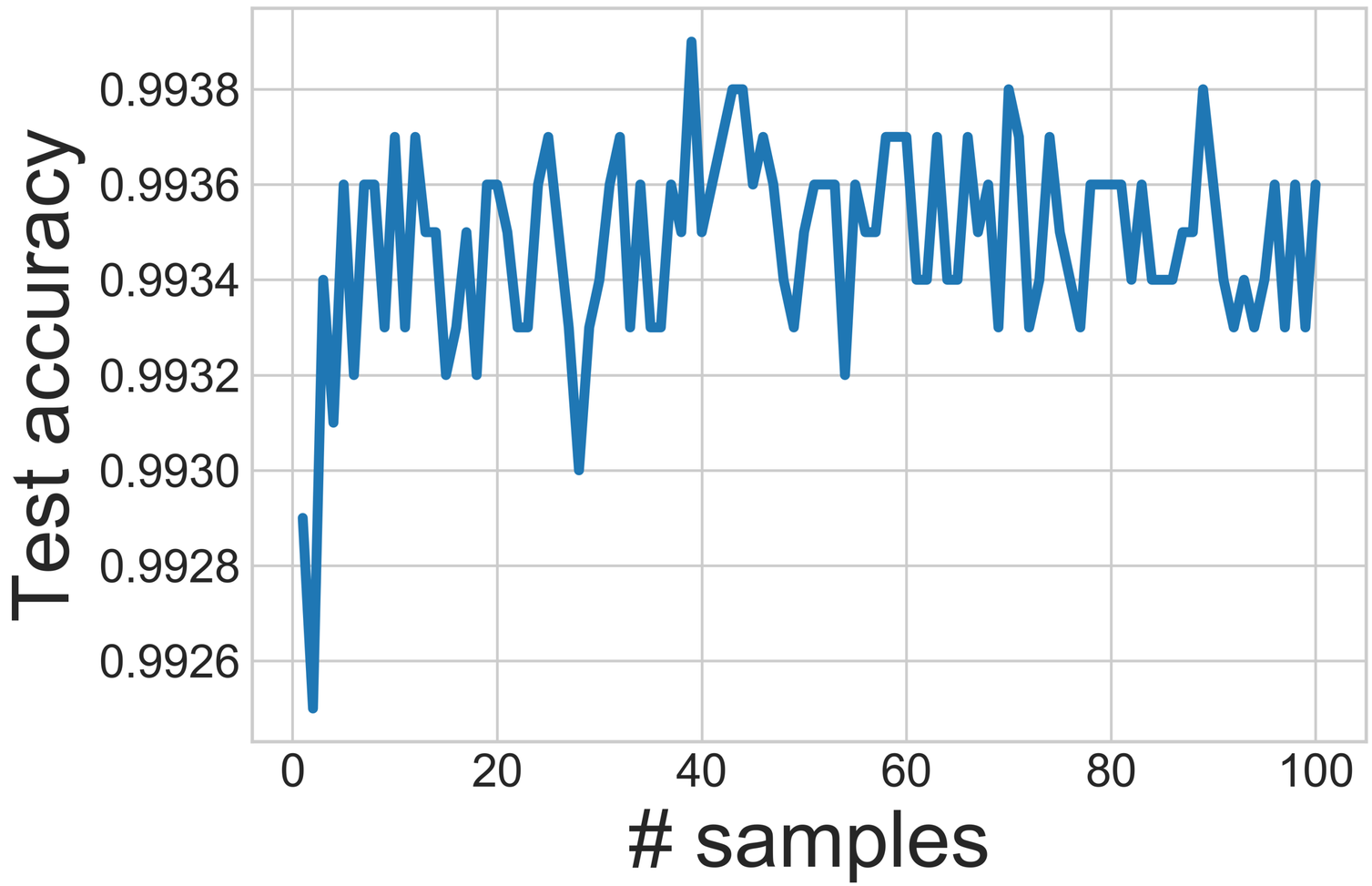
A Bayesian neural network is **an infinite ensemble** of neural networks

$$p(y_*|x_*, X, Y) = \int p(y_*|x_*, w)p(w|X, Y)dw \approx \frac{1}{K}\sum_{i=1}^{K} p(y_*|x_*, w^k)$$

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

Average SoftMax outputs across several samples

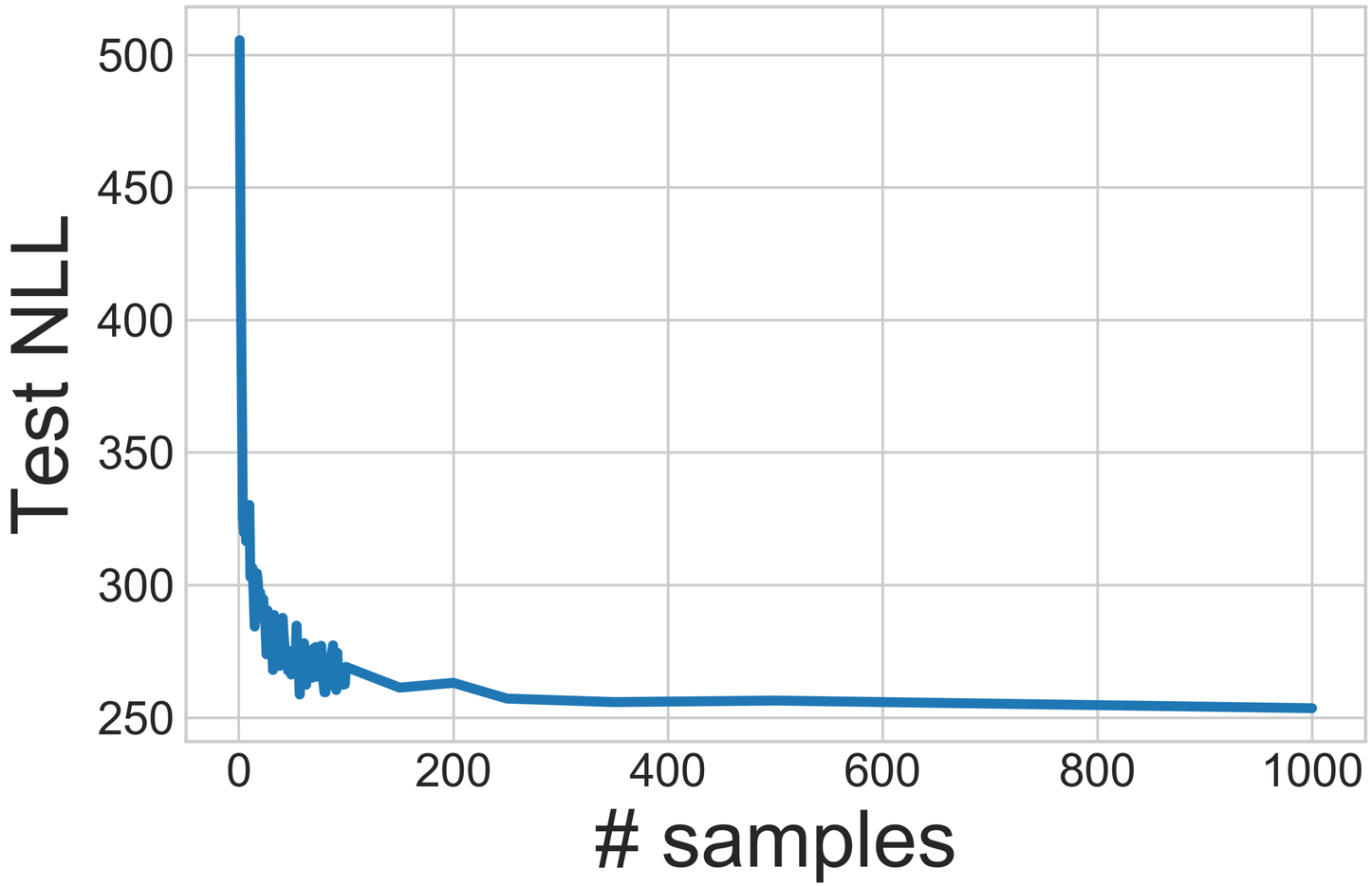
Ensembling



Accuracy quickly saturates

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

Ensembling



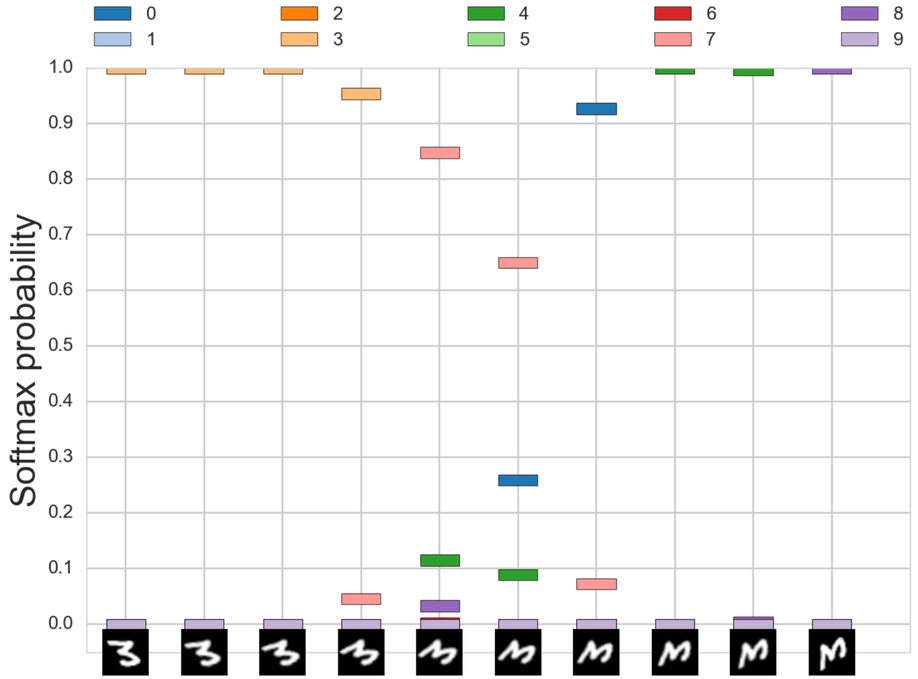
But the negative log—likelihood keeps improving! This is a measure of “uncertainty”

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

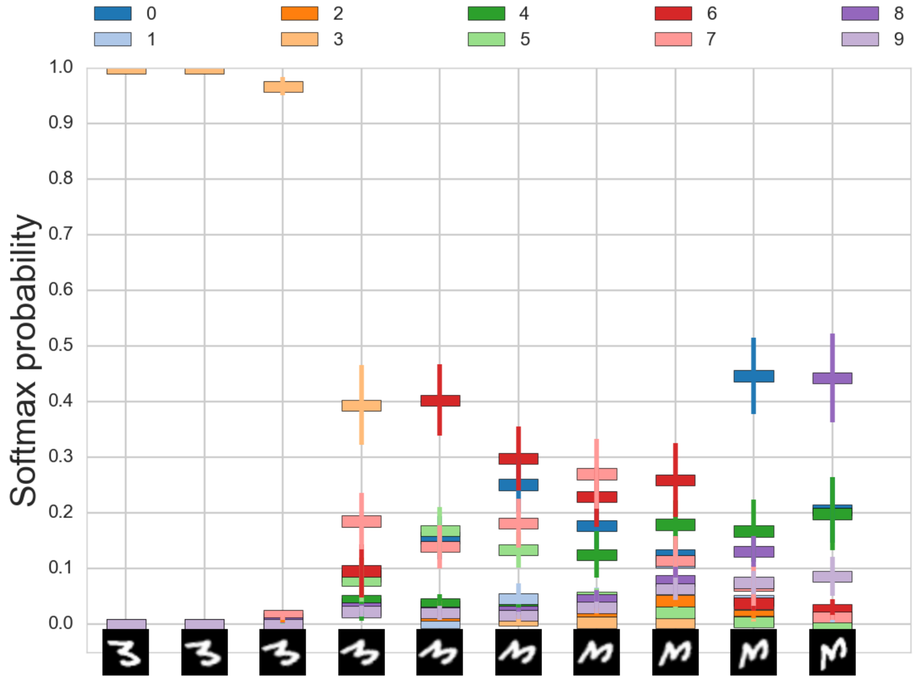
Uncertainty estimation

Deterministic NNs: a point estimate of the output, overconfident

Bayesian framework: a distribution over the outputs



(a) LeNet with weight decay



(b) LeNet with multiplicative formalizing flows

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

Model selection

- Empirical Bayes (maximum evidence)
  - Optimize w. r. t. prior parameters ⇒ Choose hyperparameters
- Discuss later

Online / incremental learning

Assume that dataset arrives gradually in independent parts:

$$\mathcal{D} = \mathcal{D}_1 \cup \mathcal{D}_2 \cup \mathcal{D}_3 \cup \cdots \cup \mathcal{D}_M$$

We can first train on the first dataset as usual:

$$p(w|\mathcal{D}_1) = \frac{p(\mathcal{D}_1|w)p(w)}{\int p(\mathcal{D}_1|\tilde{w})p(\tilde{w})d\tilde{w}}$$

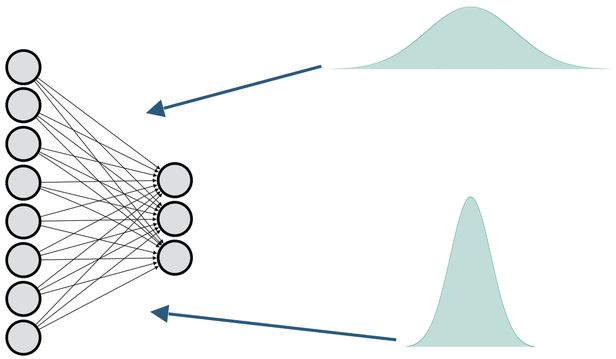
And then use the obtained posterior as the prior for the next step!

$$p(w|\mathcal{D}_2, \mathcal{D}_1) = \frac{p(\mathcal{D}_2|w)p(\mathcal{D}_1|w)p(w)}{\int p(\mathcal{D}_2|\tilde{w})p(\mathcal{D}_1|\tilde{w})p(\tilde{w})d\tilde{w}}$$

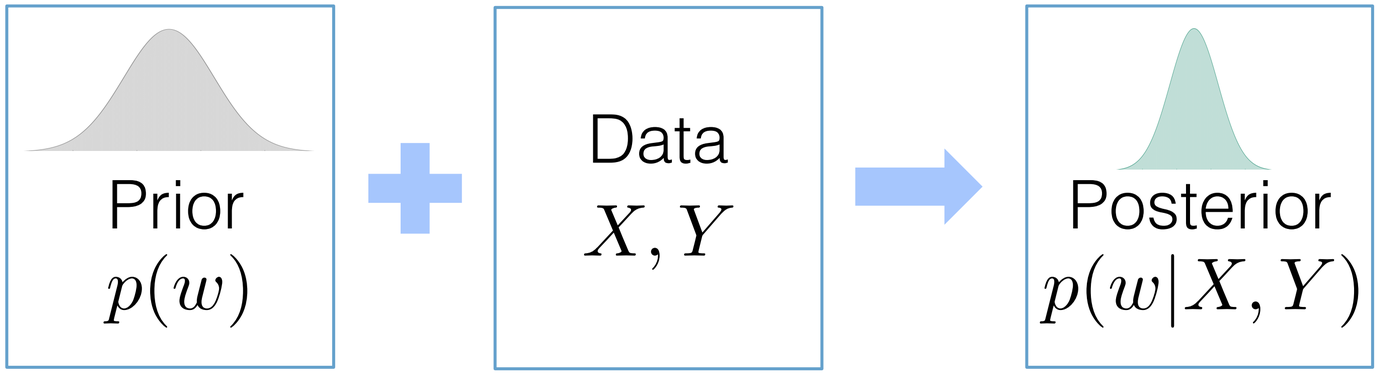
Using these sequential updates, we can find $p(w|\mathcal{D})$.

Training Bayesian neural networks

Stochastic weights:



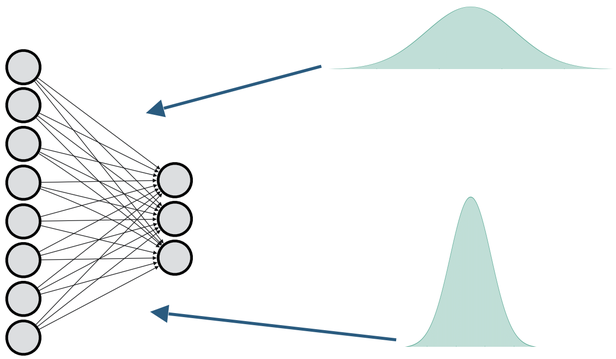
Bayesian Inference:



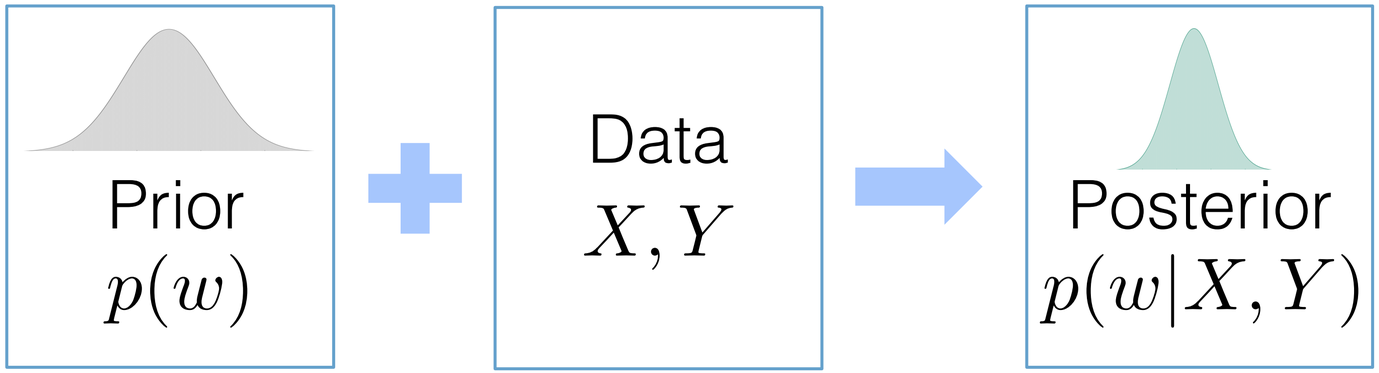
$$p(w|X,Y) = \frac{p(Y|X,w)p(w)}{\int p(Y|X,\tilde{w})p(\tilde{w})d\tilde{w}}$$

Training Bayesian neural networks

Stochastic weights:



Bayesian Inference:

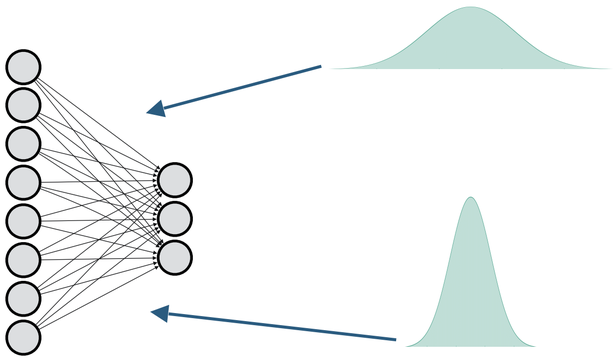


Posterior is intractable in neural networks → approximate it with $q(w|\lambda)$:

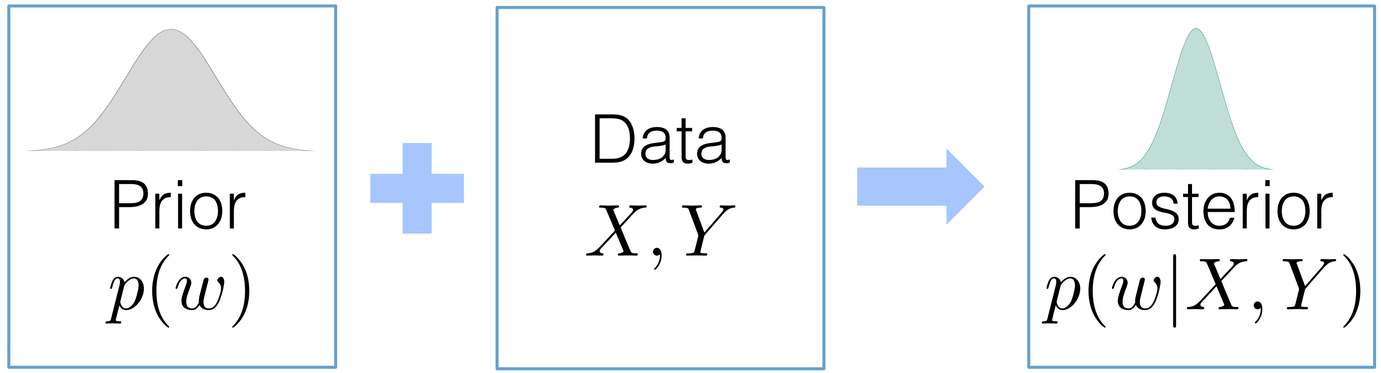
$$KL(q(w|\lambda)||p(w|X,y)) \rightarrow \min_{\lambda}$$

Training Bayesian neural networks

Stochastic weights:



Bayesian Inference:



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

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

Training Bayesian neural networks

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

Variational autoencoders are also trained using variational inference.

Compared to them:

- KL-term is global
- Extremely high-dimensional approximate posterior

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?
- How to estimate the expectation?

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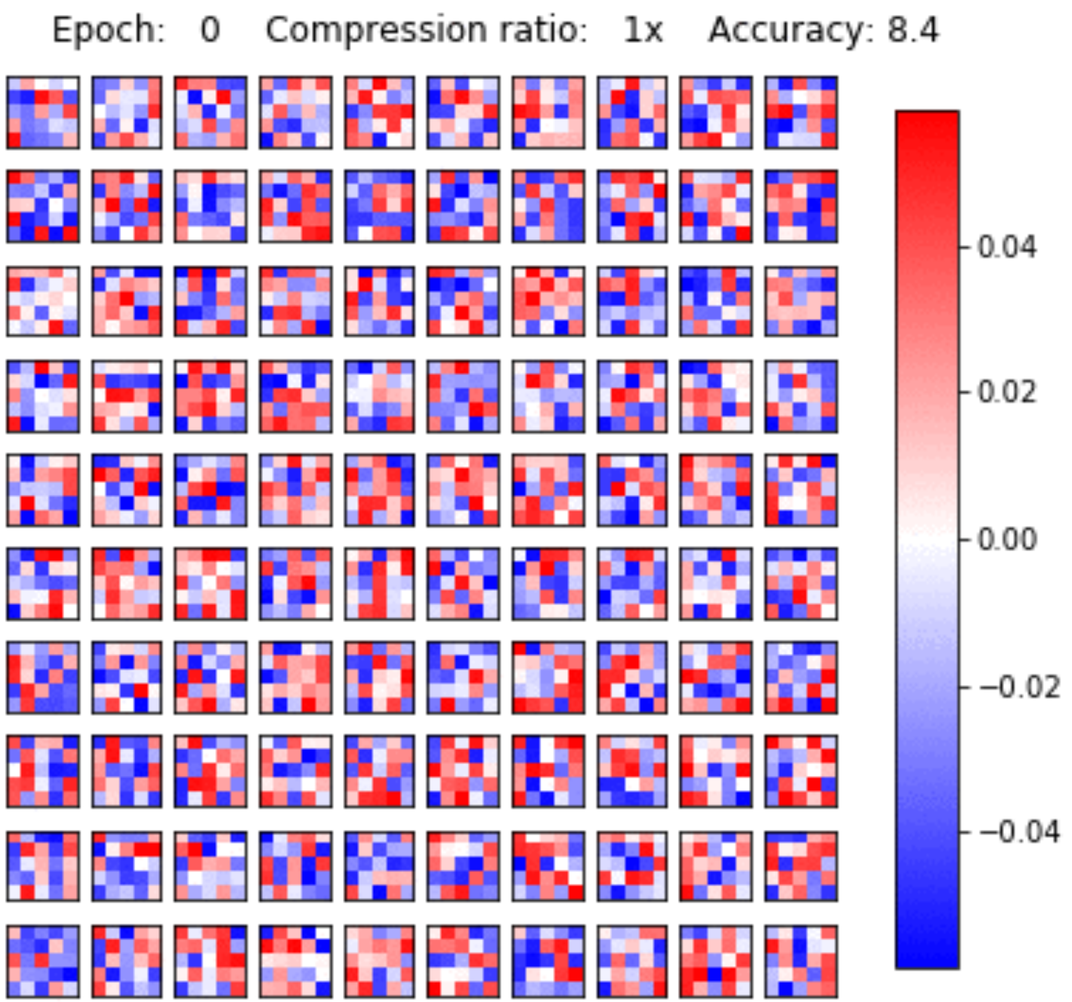
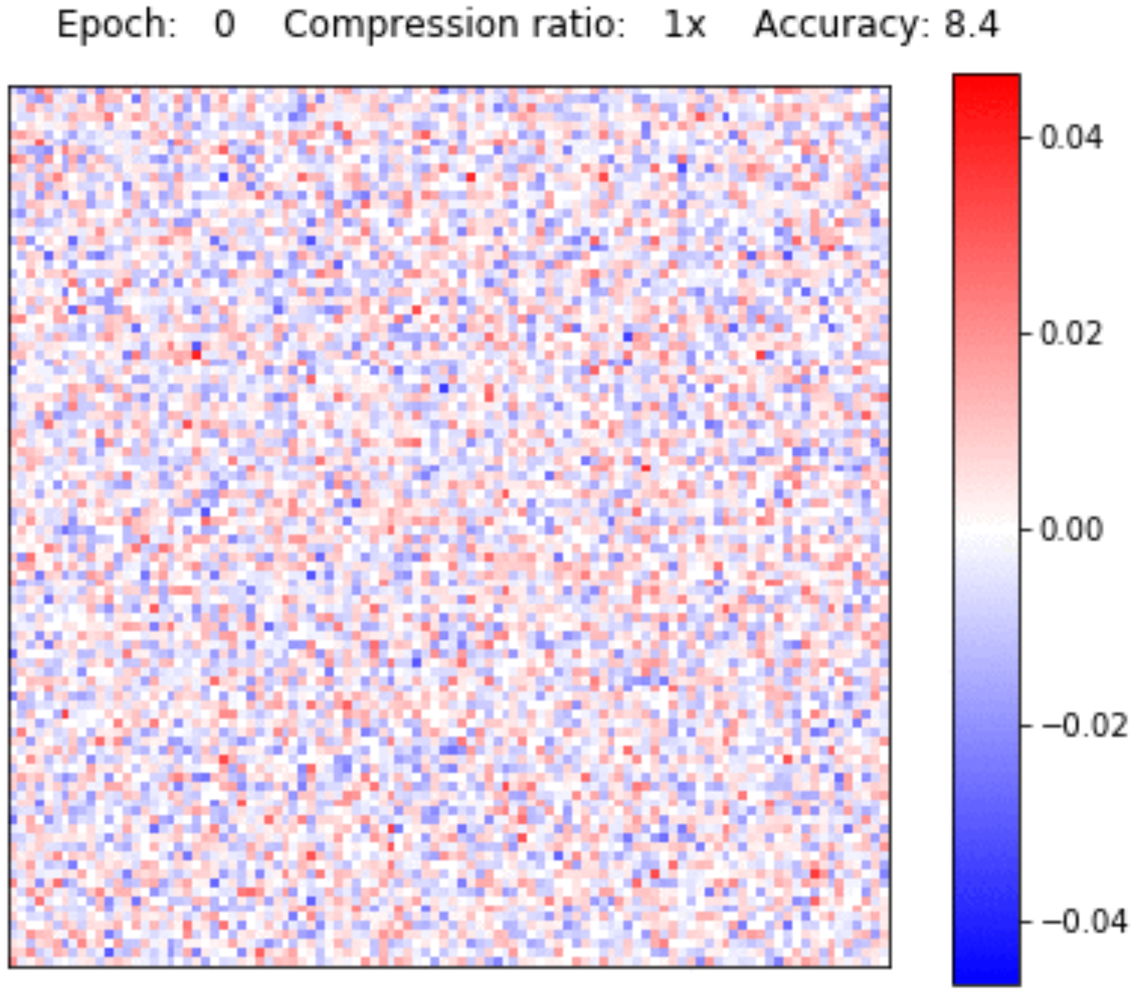
Sparse variational dropout: visualization

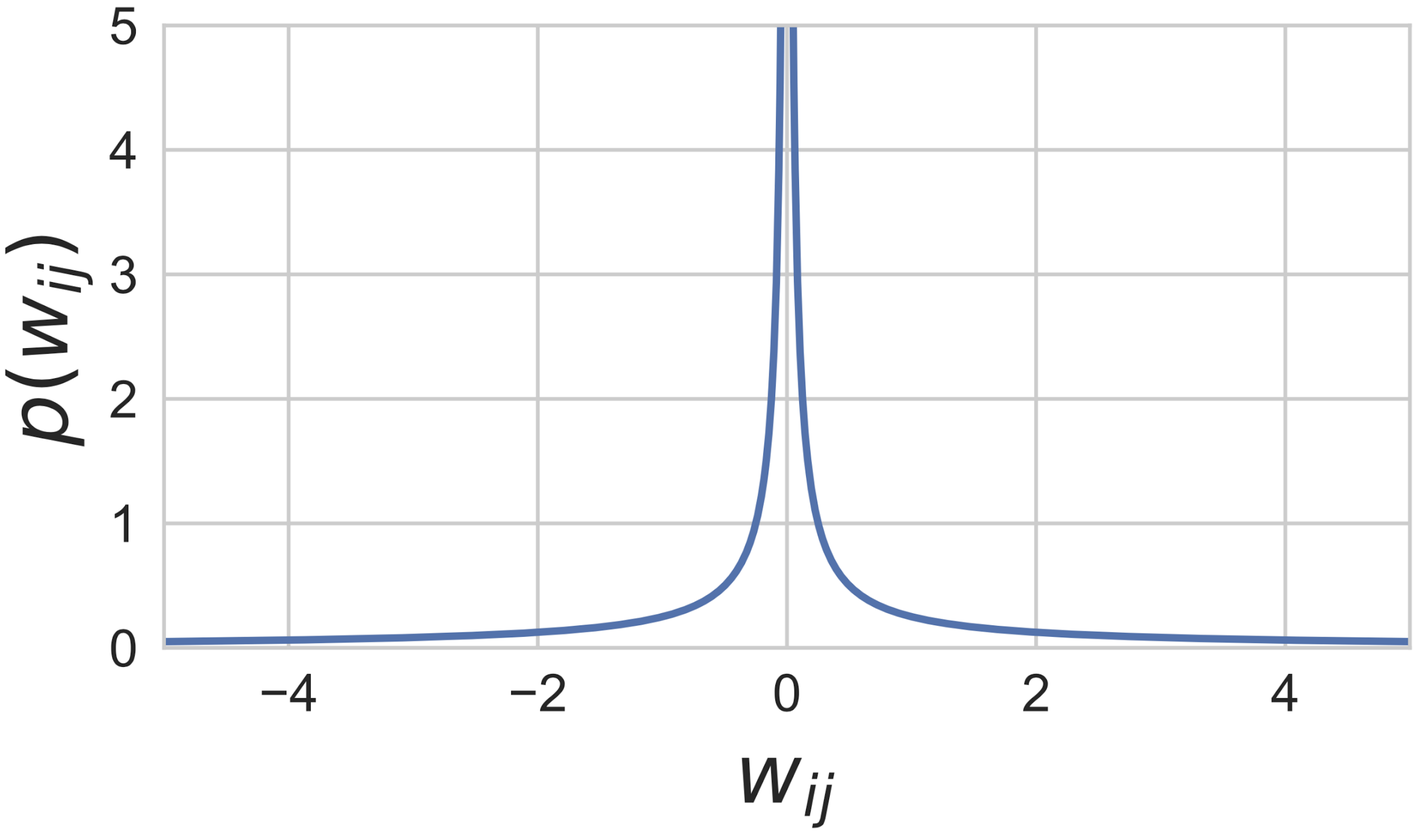


LeNet-5: convolutional layer



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

Log-uniform prior distribution

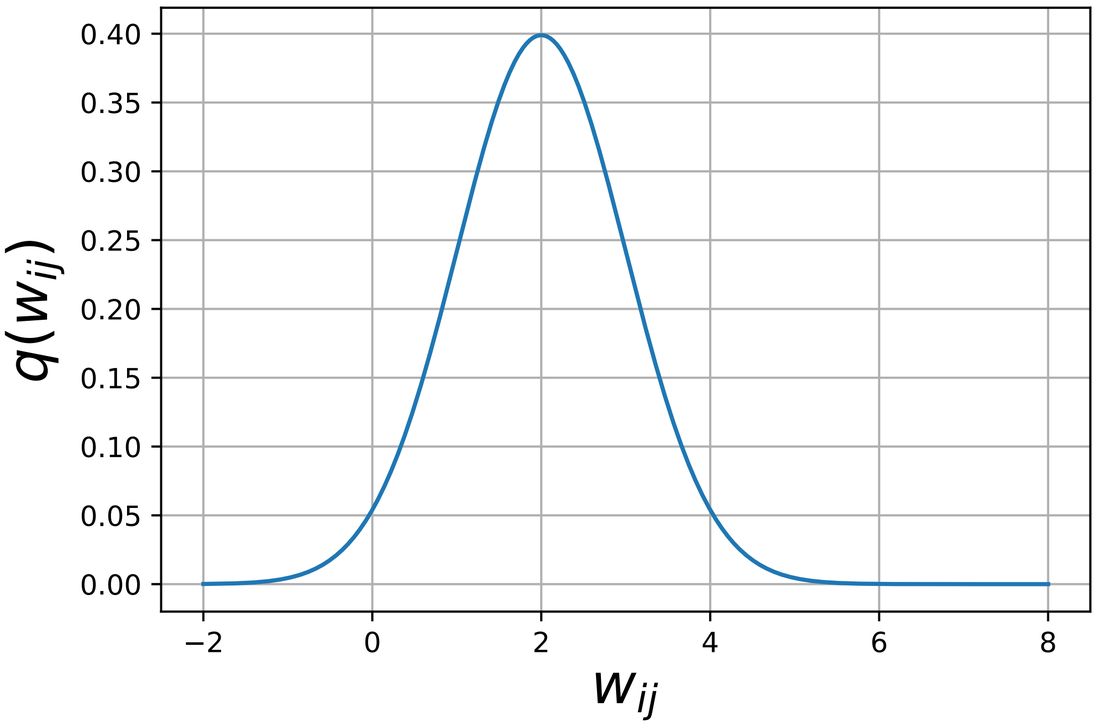


$$p(w_{ij}) \propto \frac{1}{|w_{ij}|}$$

Favors removing noisy weights
(few slides later)

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

Normal approximate posterior distribution
(fully factorized)



$$q(w_{ij}|\mu_{ij}, \sigma_{ij}) = \mathcal{N}\left(\mu_{ij}, \sigma_{ij}^2\right)$$

Reparametrization trick:

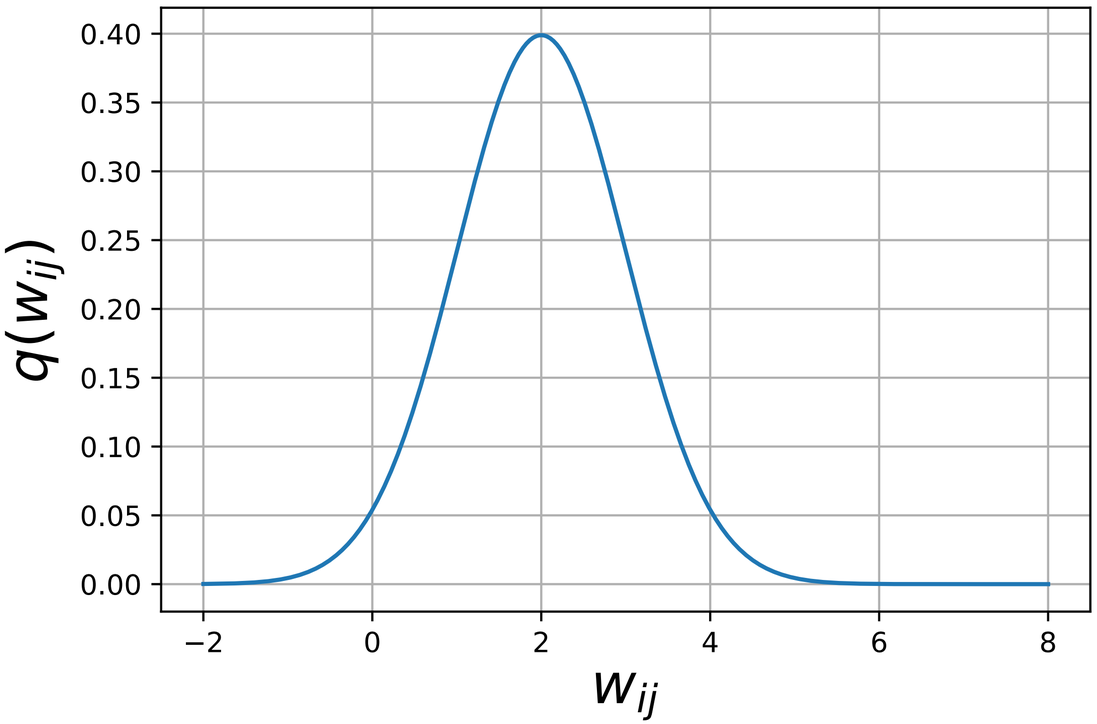
$$\hat{w}_{ij} = \mu_{ij} + \hat{\epsilon}_{ij}\sigma_{ij}, \quad \hat{\epsilon}_{ij} \sim \mathcal{N}(0, 1)$$

weight mean

zero-centered noise with learnable variance

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

Another possible parametrization (actually bad for sparsification)



Same approx. posterior distribution but different parametrization:

$$q(w_{ij}|\mu_{ij}, \alpha_{ij}) = \mathcal{N}\left(\mu_{ij}, \alpha_{ij}\mu_{ij}^2\right)$$

Reparametrization trick:

$$\hat{w}_{ij} = \mu_{ij}(1 + \sqrt{\alpha_{ij}}\hat{\epsilon}_{ij}), \quad \hat{\epsilon}_{ij} \sim \mathcal{N}(0, 1)$$

one-centered **multiplicative** noise with learnable variance

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

Compare two parametrizations

$$\frac{\partial \mathcal{L}}{\partial \mu_{ij}} = \frac{\partial \mathcal{L}}{\partial \hat{w}_{ij}} \boxed{\frac{\partial \hat{w}_{ij}}{\partial \mu_{ij}}}$$

With multiplicative noise:

$$\hat{w}_{ij} = \mu_{ij}(1 + \sqrt{\alpha_{ij}}\hat{\epsilon}_{ij})$$

$$\frac{\partial \mathcal{L}}{\partial \mu_{ij}} = \frac{\partial \mathcal{L}}{\partial \hat{w}_{ij}} \boxed{(1 + \sqrt{\alpha_{ij}}\hat{\epsilon}_{ij})}$$

Very noisy!

With additive noise:

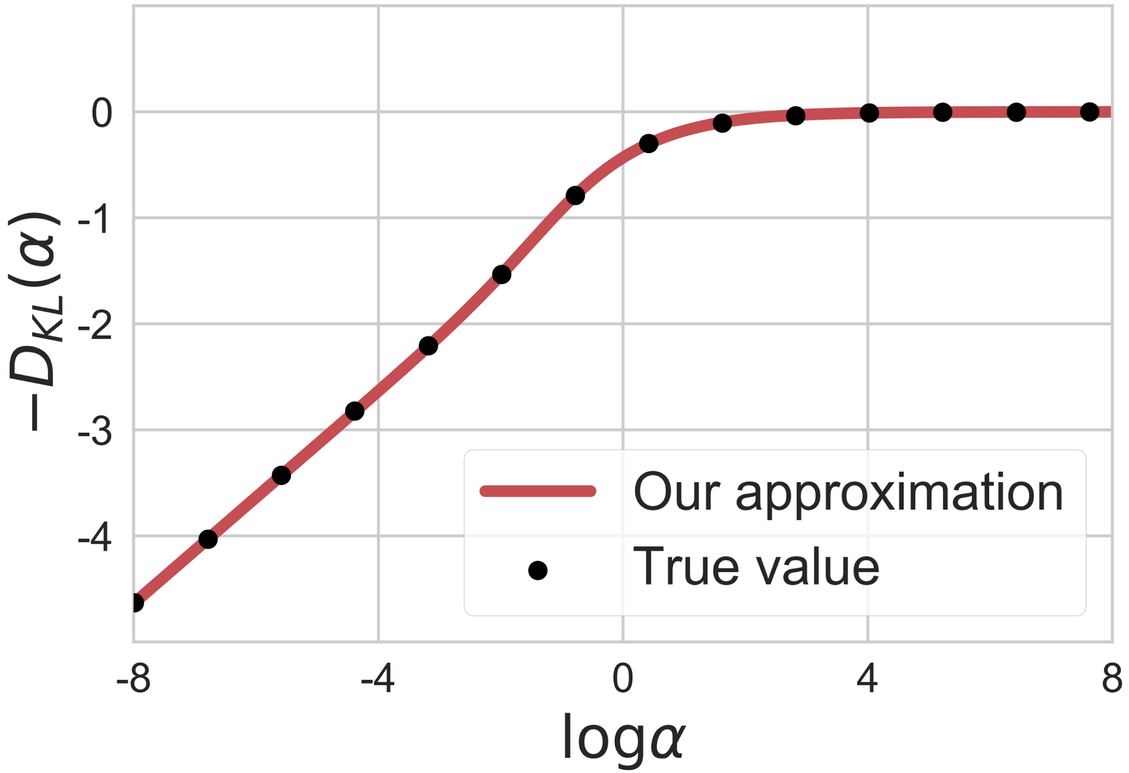
$$\hat{w}_{ij} = \mu_{ij} + \hat{\epsilon}_{ij}\sigma_{ij}$$

$$\frac{\partial \mathcal{L}}{\partial \mu_{ij}} = \frac{\partial \mathcal{L}}{\partial \hat{w}_{ij}} \cdot \boxed{1}$$

No noise!

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} $\Rightarrow$

  removing noisy weights

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

Doubly stochastic variational inference

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

???

Analytical approximation

Doubly stochastic variational inference

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

Data term
???

Regularizer
Analytical approximation

sample mini-batch
of the training objects

sample weights from q

Estimating expectation in ELBO

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

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Data term
Sample weights from q

Regularizer
Analytical approximation

1. Reparametrization trick ⇒ unbiased estimate of the gradients

$$\hat{w}_{ij} = \mu_{ij} + \hat{\epsilon}_{ij}\sigma_{ij}, \quad \hat{\epsilon}_{ij} \sim \mathcal{N}(0, 1)$$

Estimating expectation in ELBO

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

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   - Too expensive! ($|w|\times$ mini-batch size)

Estimating expectation in ELBO

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Data term
Sample weights from q

Regularizer
Analytical approximation

1. Reparametrization trick ⇒ unbiased estimate of the gradients

$$\hat{w}_{ij} = \mu_{ij} + \hat{\epsilon}_{ij}\sigma_{ij}, \quad \hat{\epsilon}_{ij} \sim \mathcal{N}(0, 1)$$

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

Estimating expectation in ELBO

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

Data term
Sample weights from q

Regularizer
Analytical approximation

1. Reparametrization trick ⇒ unbiased estimate of the gradients

$$\hat{w}_{ij} = \mu_{ij} + \hat{\epsilon}_{ij}\sigma_{ij}, \quad \hat{\epsilon}_{ij} \sim \mathcal{N}(0, 1)$$

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

$$w_{ij} \sim \mathcal{N}(\mu_{ij}, \sigma_{ij}^2)$$
$$B = AW$$

$$\mathbb{E}B = A\mu \quad VarB = A^2\sigma^2$$
$$B \sim \mathcal{N}(A\mu, A^2\sigma^2)$$
$$B = A\mu + \sqrt{A^2\sigma^2} \odot \epsilon$$

blue means element-wise

The local reparametrization trick

Consider a linear layer with weight matrix W, input A and output B:

$$w_{ij} \sim \mathcal{N}(\mu_{ij}, \sigma_{ij}^2)$$
$$B = AW$$

Predictions have **high** correlation because there is one weight sample **per mini-batch**

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

The local reparametrization trick

Consider a linear layer with weight matrix W, input A and output B:

$$w_{ij} \sim \mathcal{N}(\mu_{ij}, \sigma_{ij}^2)$$
$$B = AW$$

Predictions have **high** correlation because there is one weight sample **per mini-batch**

$$\mathbb{E}B = A\mu \quad VarB = A^2\sigma^2$$
$$B \sim \mathcal{N}(A\mu, A^2\sigma^2)$$
$$B = A\mu + \sqrt{A^2\sigma^2} \odot \epsilon$$

blue means element-wise

Predictions have **zero** correlation because there is one weight sample **per object**

Less correlation ⇒ lower variance of the stochastic gradients **for a mini-batch**

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

The local reparametrization trick

The LRT also reduces the variance of the stochastic gradient w.r.t $\sigma_{i,j}$ for **an object.**

Sketch of the proof:

ELBO

$$\mathrm{Var}_{q_\phi,\mathcal{D}}\left[\frac{\partial L_{\mathcal{D}}^{\mathrm{SGVB}}}{\partial \sigma_{i,j}^2}\right] = \mathrm{Var}_{b_{m,j}}\left[\mathbb{E}_{q_\phi,\mathcal{D}}\left[\frac{\partial L_{\mathcal{D}}^{\mathrm{SGVB}}}{\partial \sigma_{i,j}^2}|b_{m,j}\right]\right] + \mathbb{E}_{b_{m,j}}\left[\mathrm{Var}_{q_\phi,\mathcal{D}}\left[\frac{\partial L_{\mathcal{D}}^{\mathrm{SGVB}}}{\partial \sigma_{i,j}^2}|b_{m,j}\right]\right]$$

same for both parametrizations

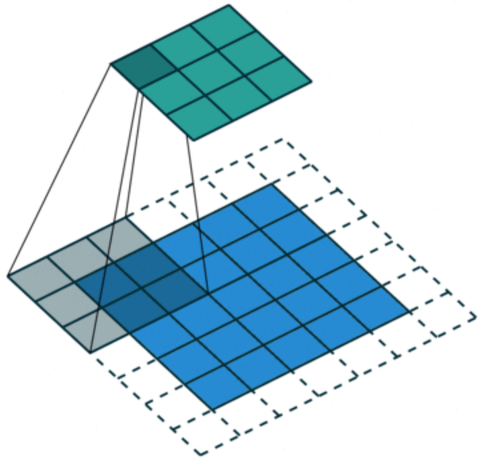
for LRT: vanishes because $b_{m,j} = \ldots + \ldots \cdot \zeta_{m,j}$ and $\zeta_{m,j}$ is uniquely determined given $b_{m,j}$

for RT: doesn't vanish (and positive)

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

LRT for convolutions

- B no longer factorizes in convolutional layers
  - Same weights sample should be used for different spatial positions

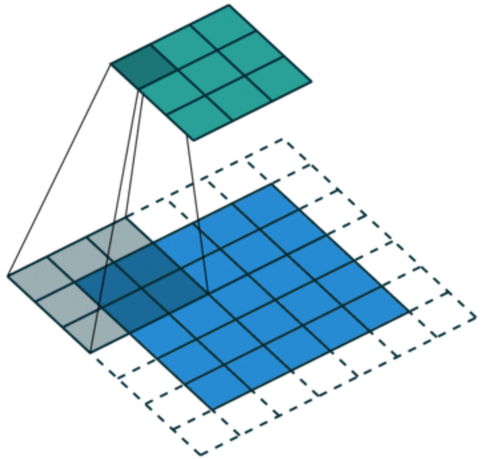


Diederik P. Kingma et al. Variational dropout and the local reparameterization trick. NIPS 2015

LRT for convolutions

- B no longer factorizes in convolutional layers
  - Same weights sample should be used for different spatial positions
- Exact local reparametrization is too complex
  - Preactivations are normal but correlated

    $\Rightarrow$ we need to estimate the full covariance matrix for each preactivation



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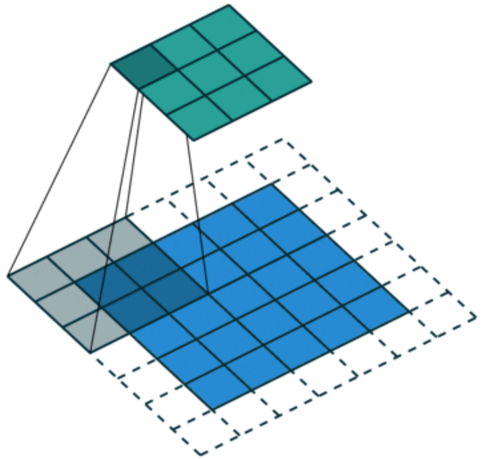


- Mean-field approximation performs much better that sampling weights:

$$B = A \star \mu + \sqrt{A^2 \star \sigma^2} \odot \epsilon$$

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

From general framework to particular method

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

Model specification:

- Choose particular prior ✓ log-uniform distribution

Training:

- Choose particular family for approximate posterior ✓ normal distribution
- How to compute KL-divergence? ✓ analytical approximation
- How to estimate the expectation? ✓ RT & LRT

From general framework to particular method

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

What about biases? batch-norm parameters?

From general framework to particular method

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

What about biases? batch-norm parameters?

Treat them as deterministic parameters and find point estimate:

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

Eventually, it assumes a flat prior and a delta-peak posterior.

Final algorithm (without LRT)

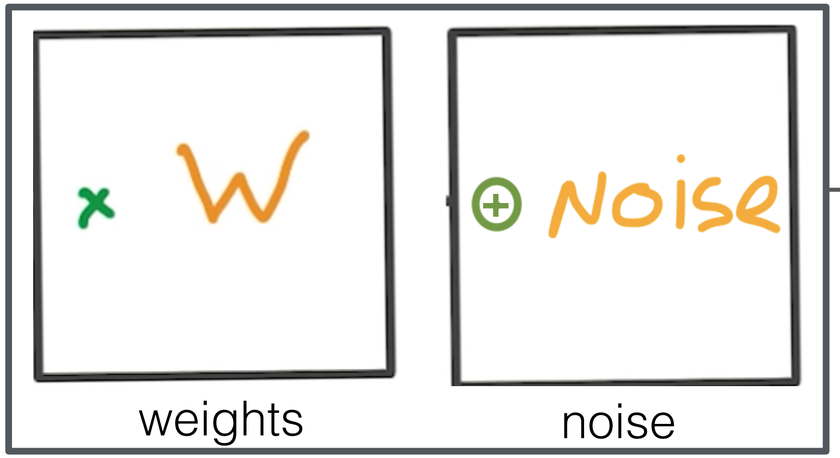
Training on a mini-batch X with labels Y:

1. Sample weights: $\hat{w} = \mu + \sigma \odot \epsilon,\ \epsilon \sim \mathcal{N}(0, I)$
2. Forward pass: $Y_{\text{pred}} = NN(X, \hat{w}, b)$
3. Backward pass: compute stochastic gradients of ELBO:

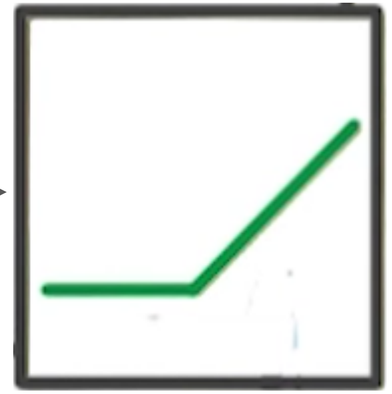
$$\nabla_{\mu, \log \sigma, b} \left(N \cdot \text{Loss}\left(Y, Y_{\text{pred}}\right) + \text{SparseReg}(\sigma/\mu) \right)$$

Forward pass with stochastic weights

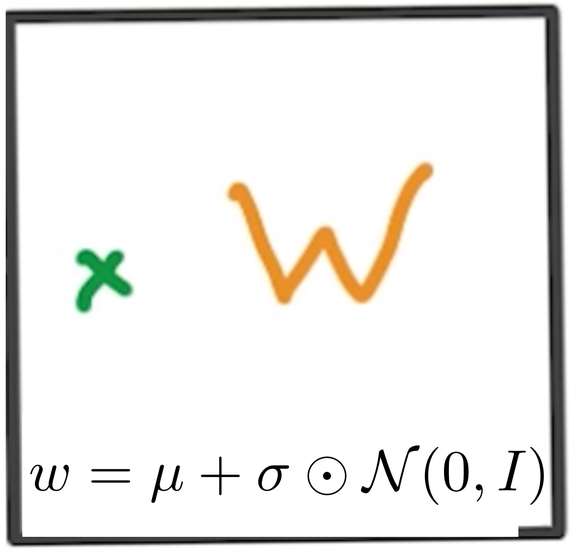
input



activations



nonlinearity



it does not change the mean value

additive noise

$w \sim \mathcal{N}(\mu, \sigma^2)$

Slide from KirIII Neklyudov's presentation, deepbayes.ru/2018

Final algorithm (without LRT)

Training on a mini-batch X with labels Y:

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Final algorithm (with LRT)

Training on a mini-batch X with labels Y:

1. Sample noise $\epsilon \sim \mathcal{N}(0, I)$
2. Forward pass with LRT: $Y_{\text{pred}} = NN(X, \mu, \sigma, \epsilon, b)$
3. Backward pass: compute stochastic gradients of ELBO:

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Pruning after training:

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

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

signal-to-noise ratio

Final algorithm (with LRT)

Training on a mini-batch X with labels Y:

1. Sample noise $\epsilon \sim \mathcal{N}(0, I)$
2. Forward pass with LRT: $Y_{\text{pred}} = NN(X, \mu, \sigma, \epsilon, b)$
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Pruning after training:

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

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

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

Automatic relevance determination

(other prior but very similar method)

- Empirical Bayes
  - optimize w. r. t. prior parameters ⇒ automatically choose hyperparameters

Kharitonov, V. et al. Variational dropout via Empirical Bayes. NeurIPS Workshop on Bayesian Deep Learning, 2018.

Automatic relevance determination

(other prior but very similar method)

- Empirical Bayes
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- Normal prior with **learnable** variance for **each weight**:

$$p(w_{ij}|\tau_{ij}) = \mathcal{N}(0, \tau_{ij}^{-1})$$

Kharitonov, V. et al. Variational dropout via Empirical Bayes. NeurIPS Workshop on Bayesian Deep Learning, 2018.

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- KL-divergence:

$$KL\big(q(w_{ij}|\mu_{ij}, \sigma_{ij})||p(w_{ij}|\tau_{ij})\big) = -\log\sigma_{ij} - \frac{1}{2}\log\tau_{ij} + \frac{1}{2}\tau_{ij}(\mu_{ij}^2 + \sigma_{ij}^2)$$

normal

normal

Kharitonov, V. et al. Variational dropout via Empirical Bayes. NeurIPS Workshop on Bayesian Deep Learning, 2018.

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- Analytical optimization w. r. t. prior parameters τ_{ij} :

$$\tau_{ij}^* = (\mu_{ij}^2 + \sigma_{ij}^2)^{-1}$$

$$\overset{\tau_{ij}^*}{\circledminus} -\frac{1}{2}\log(\mu_{ij}^2 + \sigma_{ij}^2)^{-1} = -\frac{1}{2}\log\left(1 + \frac{\mu_{ij}^2}{\sigma_{ij}^2}\right)$$

Kharitonov, V. et al. Variational dropout via Empirical Bayes. NeurIPS Workshop on Bayesian Deep Learning, 2018.

Comparing two models

	SparseVD	**ARD**
Prior	$p(w_{ij}) \propto \frac{1}{\lvert w_{ij} \rvert}$	$p(w_{ij}\lvert\tau_{ij}) = \mathcal{N}(0, \tau_{ij}^{-1})$
Prior parameters	None	τ_{ij}
KL-divergence	$k_1\sigma(k_2 + k_3 \log \alpha_{ij}))- -0.5\log(1+\alpha_{ij}^{-1}) + \mathrm{C}$	$-0.5\log(1+\alpha_{ij}^{-1})$

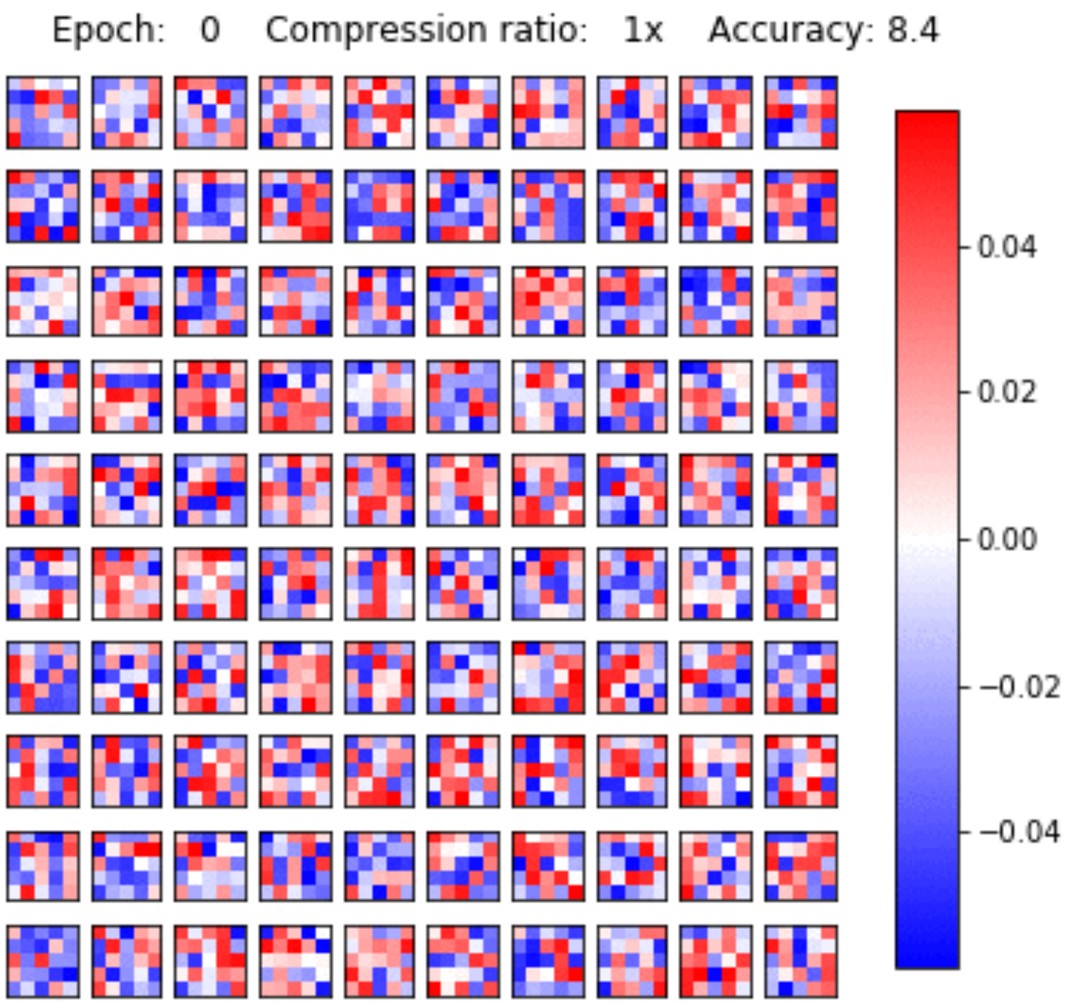
bounded

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

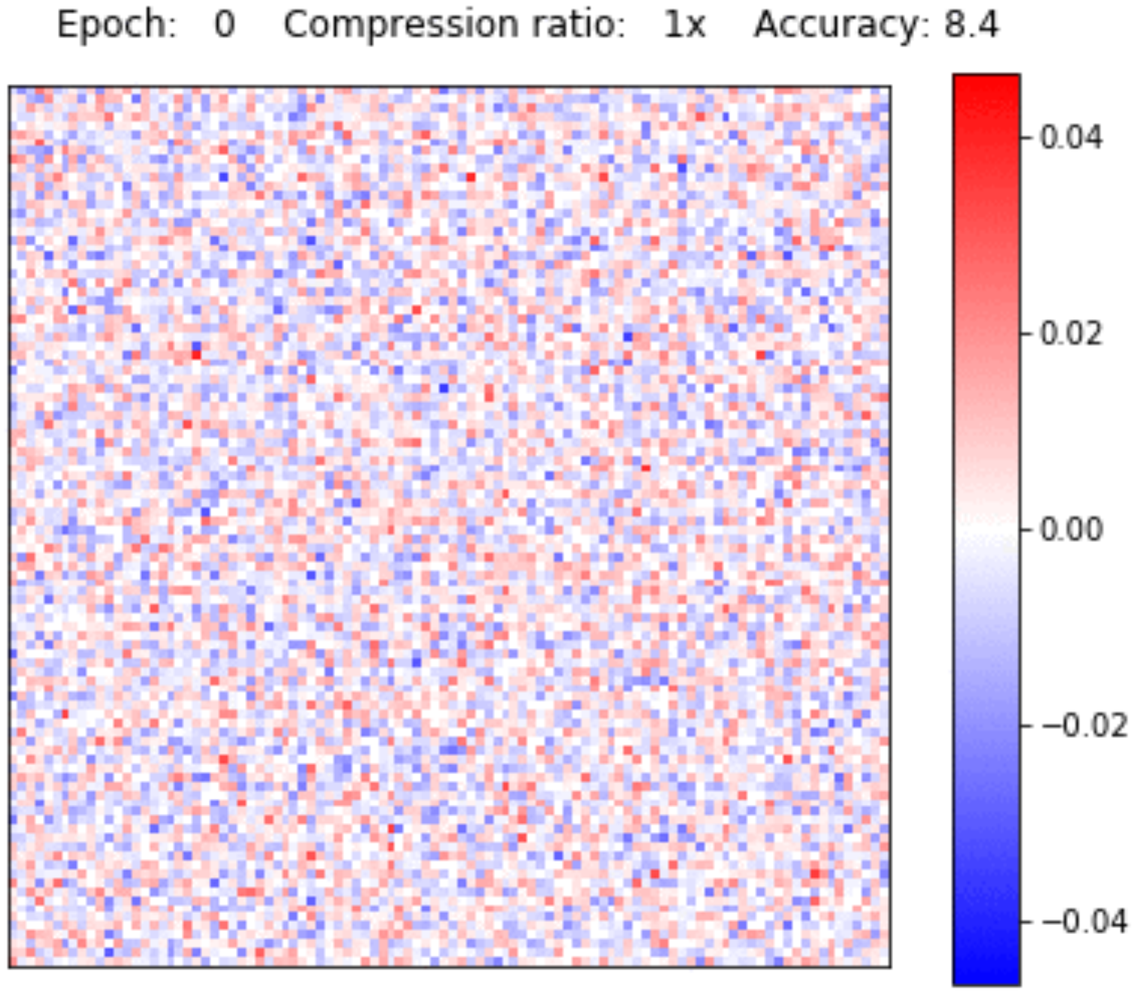
Training procedure is the same (approx. posterior, RT, LRT etc.)

Kharitonov, V. et al. Variational dropout via Empirical Bayes. NeurIPS Workshop on Bayesian Deep Learning, 2018.

Sparse variational dropout: visualization



LeNet-5: convolutional layer

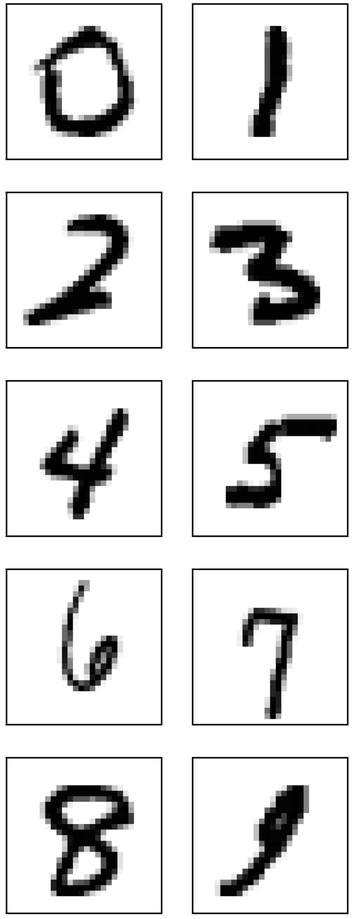


LeNet-5: fully-connected layer
(100 x 100 patch)

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

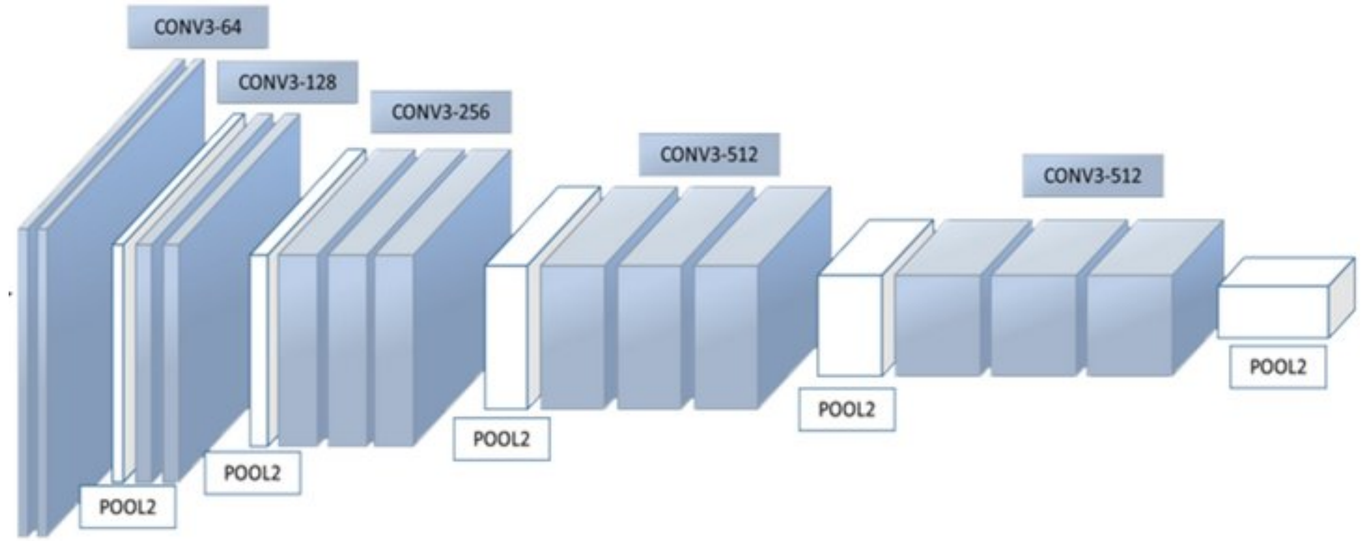
Fully Connected network: LeNet-300-100 **Convolutional network**: Lenet-5-Caffe

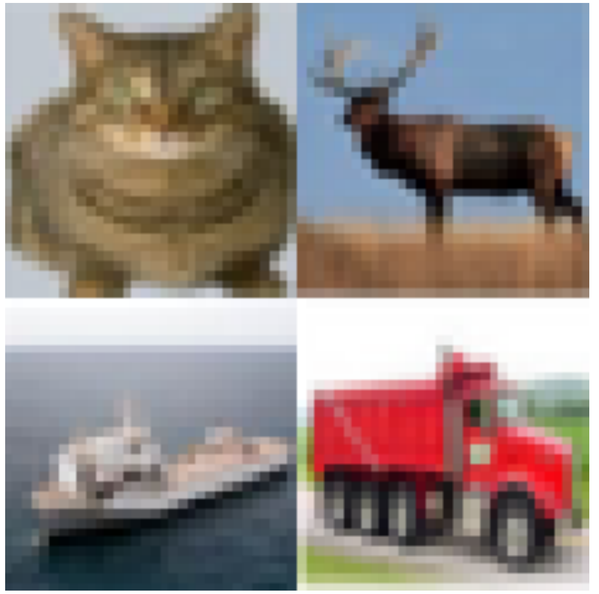
Network	Method	Error %	Sparsity per Layer %	$\frac{\lvert\mathbf{W}\rvert}{\lvert\mathbf{W}_{\neq 0}\rvert}$
	Original	1.64		1
	Pruning	1.59	$92.0 - 91.0 - 74.0$	12
LeNet-300-100	DNS	1.99	$98.2 - 98.2 - 94.5$	56
	SWS	1.94		23
(ours)	Sparse VD	1.92	$98.9 - 97.2 - 62.0$	**68**
	Original	0.80		1
	Pruning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



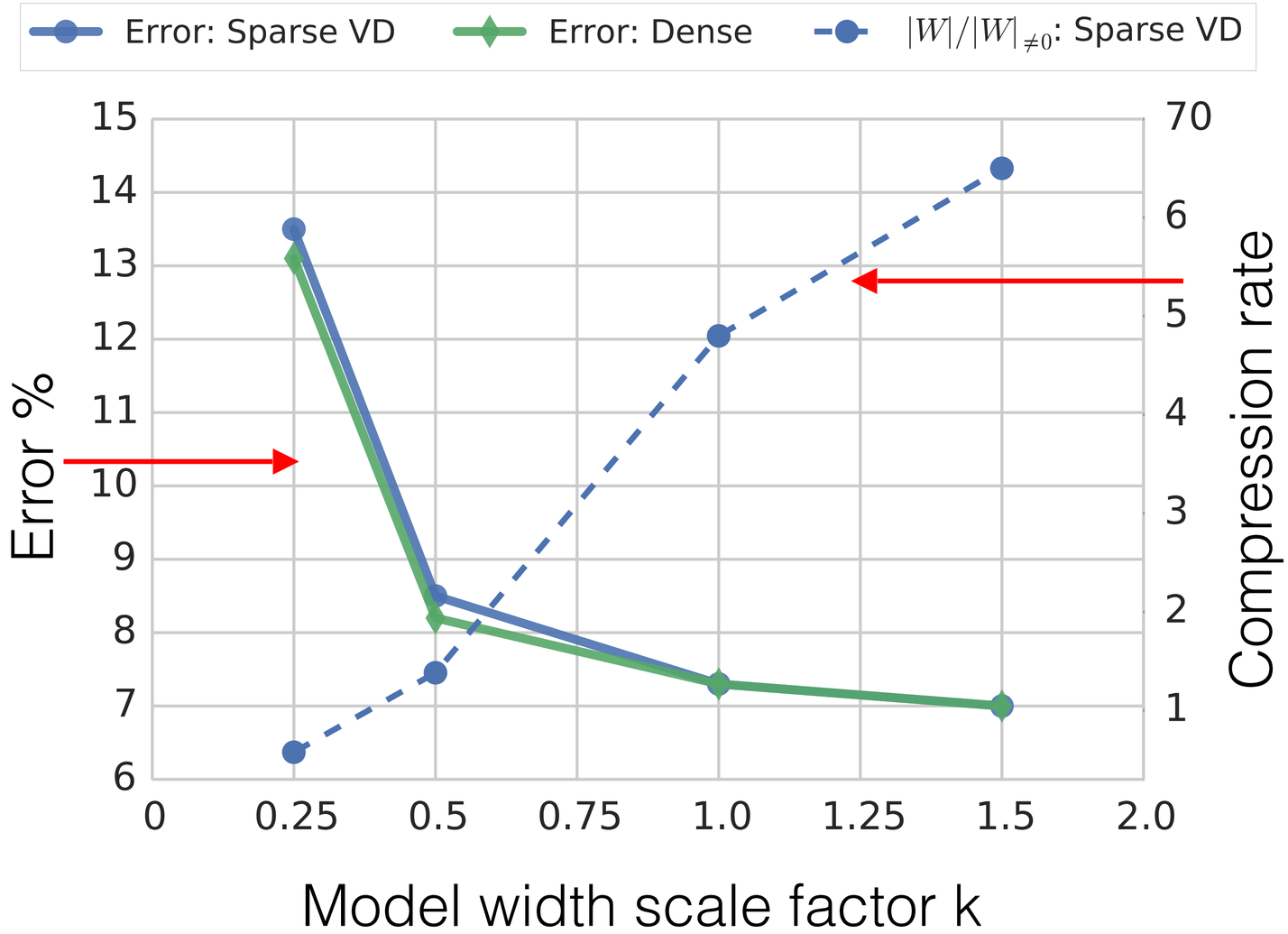


- 13 Convolutional layers and 2 Fully-Connected layers
- Pre-Activation Batch Norm and Binary Dropout after each layer

Official Torch Blog: Zagoruyko, http://torch.ch/blog/2015/07/30/cifar.html

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."

Agenda

- Sparsification: what and why
- Bayesian neural networks
- Sparse variational dropout
- Practical assignment: implementation of SparseVD
- Model enhancements

Practical assignment

1. Take a look at an example:

   FC for a MNIST in PyTorch (or skip it :)
2. Implement two classes for SparseVD and incorporate them into model training
3. Train SparseVD and visualize weights

Agenda

- Sparsification: what and why
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- Model enhancements

What’s next?

- SparseVD for RNNs
- Structured Bayesian sparsification
- How does it all works on large datasets and networks

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SparseVD for recurrent neural networks

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

Model specification:

- Choose particular prior ✓ log-uniform distribution

Training:

- Choose particular family for approximate posterior ✓ normal distribution
- How to compute KL-divergence? ✓ analytical approximation
- How to estimate the expectation? ?

Important RNN specifics

Input is a sequence: $x = x_1 \dots x_T$:

$$-\sum_{i=1}^{N} \int q(w|\theta, \sigma) \log p(y^i \overbrace{|x_0^i, \dots, x_T^i}^{\text{sequence}}, w, B) dw +$$

$$+ \sum_{w_{ij} \in \omega} KL(q(w_{ij}|\theta_{ij}, \sigma_{ij})||p(w_{ij})) \to \min_{\theta, \sigma, B}$$

1. Use one sample w for all t for 1 sequence

Gal, Yarin and Ghahramani, Zoubin. A Theoretically Grounded Application of Dropout in Recurrent Neural Networks. NIPS 2016

Important RNN specifics

Input is a sequence: $x = x_1 \dots x_T$:

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$$+ \sum_{w_{ij} \in \omega} KL(q(w_{ij}|\theta_{ij},\sigma_{ij})||p(w_{ij})) \to \min_{\theta,\sigma,B}$$

1. Use one sample w for all t for 1 sequence
2. LRT is not applicable ⇒ sample one w for a whole mini-batch

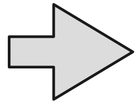
Chirkova, Nadezhda et al. Bayesian compression for natural language processing. EMNLP 2018

Why LRT is not applicable in RNNs?

$$h_{t+1} = g(W^x x_{t+1} + W^h h_t + b^h)$$

For W^h:

h_t is a random variable depending on W^h



$W^h h_t$ is not normal

For W^x:

Sampling same noise on weights for all t

$\neq$

Sampling same noise on preactivation for all t

Chirkova, Nadezhda et al. Bayesian compression for natural language processing. EMNLP 2018

Experiments: text classification

Datasets: IMDb (25K texts, 2 classes), AGNews (120K texts, 4 classes)

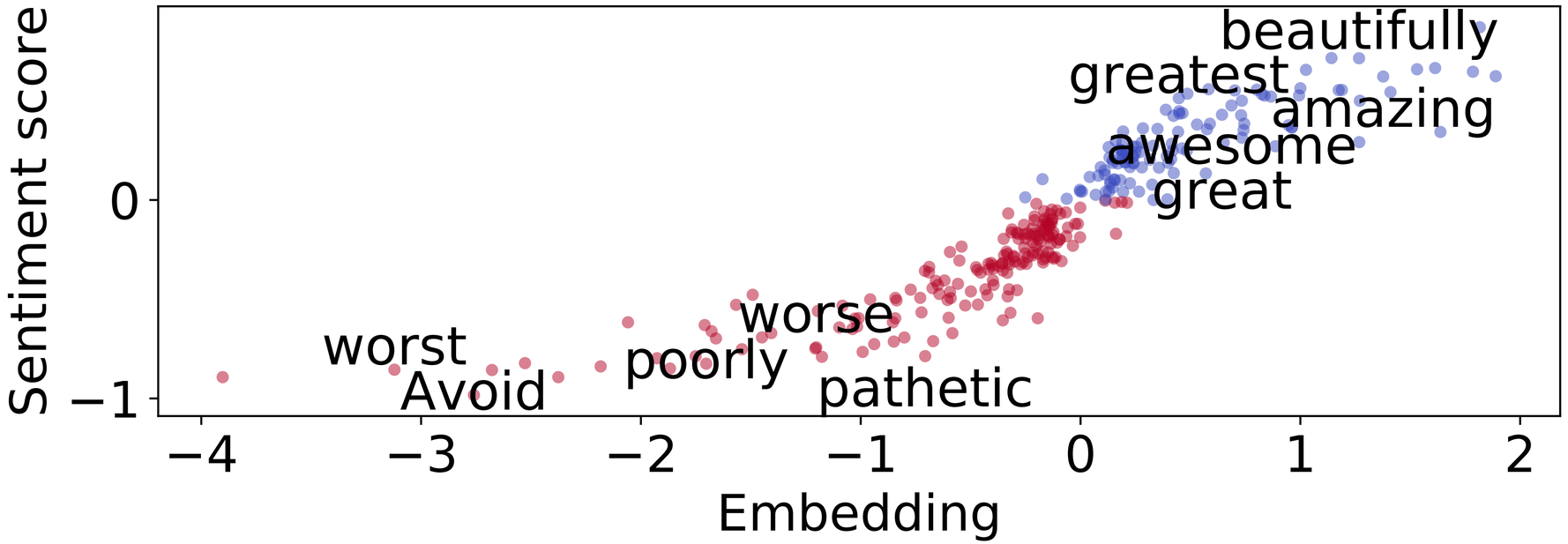
Architecture: Embedding → LSTM → FC on h_T

Task	Method	Accuracy %	Compression	Vocabulary
IMDb	Original	84.1	1x	20000
	SparseVD	**85.1**	1135x	4611
	SparseVD-Voc	83.6	**12985x**	**292**
AGNews	Original	**90.6**	1x	20000
	SparseVD	88.8	322x	5727
	SparseVD-Voc	89.2	**469x**	**2444**

Chirkova, Nadezhda et al. Bayesian compression for natural language processing. EMNLP 2018

Experiments: text classification

IMDb: the only remaining embedding component for remaining words



sentiment score = (#pos. — #neg.) / # all texts with word

Chirkova, Nadezhda et al. Bayesian compression for natural language processing. EMNLP 2018

Experiments: text generation

PTB Corpus: char-level (6M chars), word-level (0.9M words)

Architecture: LSTM → FC

Task	Method	Valid	Test	Compression	Vocabulary
Char PTB (Bits-per-char)	Original	1.498	1.454	1x	50
	SparseVD	1.472	1.429	**7.6x**	50
	SparseVD-Voc	**1.4584**	**1.4165**	5.8x	**48**
Word PTB (Perplexity)	Original	135.6	129.5	1x	10000
	SparseVD	**115.0**	**109.0**	**14.0x**	9985
	SparseVD-Voc	126.3	120.6	11.1x	**4353**

Chirkova, Nadezhda et al. Bayesian compression for natural language processing. EMNLP 2018

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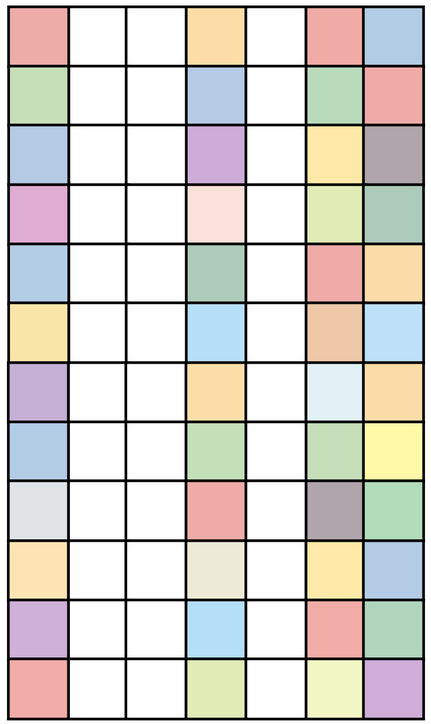
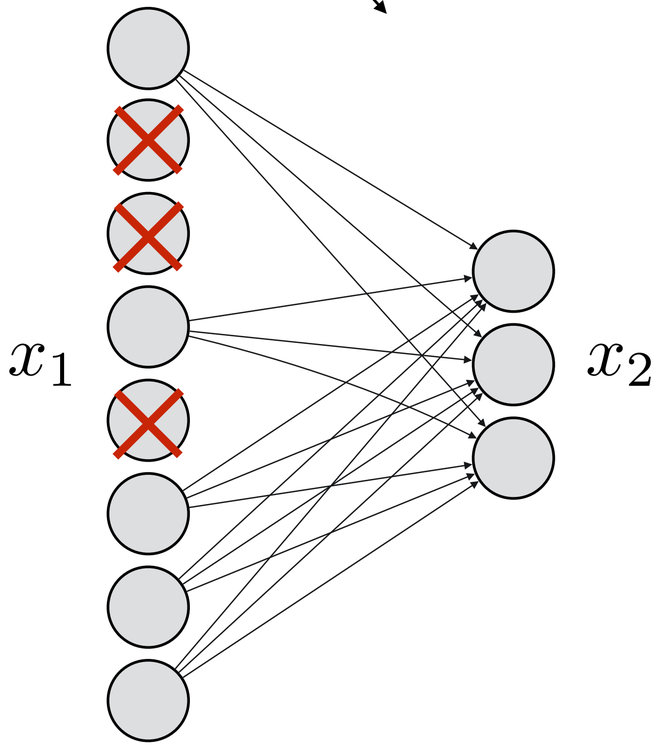
Structured Bayesian sparsification

No outgoing edges
⇒ remove neuron



Weight matrix W



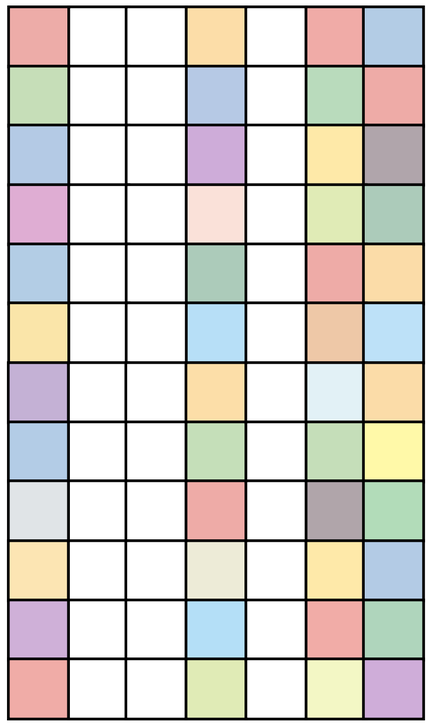
Computational graph

Benefits of structured sparsification:

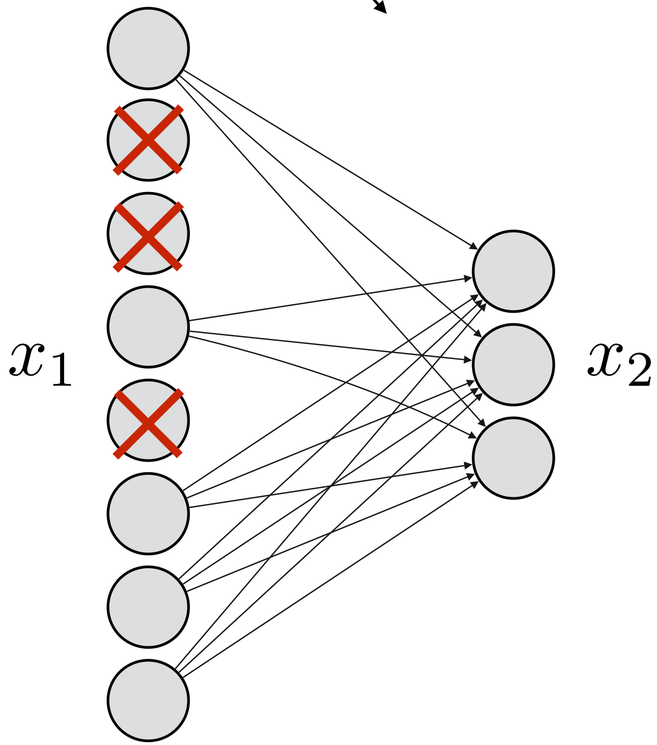
- more efficient compression
- speed-up of forward pass (faster testing stage)

Structured Bayesian sparsification

No outgoing edges
⇒ remove neuron



Weight matrix W

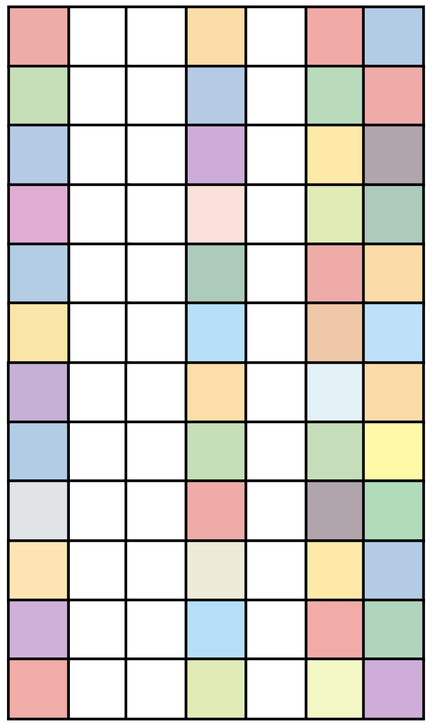


Computational graph

$$x_2 = \sigma(W x_1 + b)$$

Structured Bayesian sparsification

No outgoing edges
⇒ remove neuron



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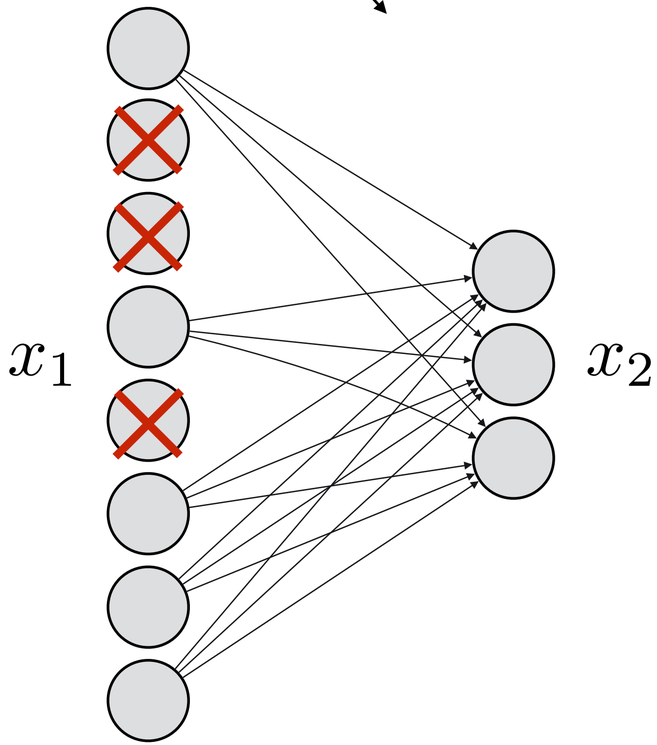


Computational graph

$$x_2 = \sigma(W x_1 + b)$$

Multiply x_1 by group variable z:

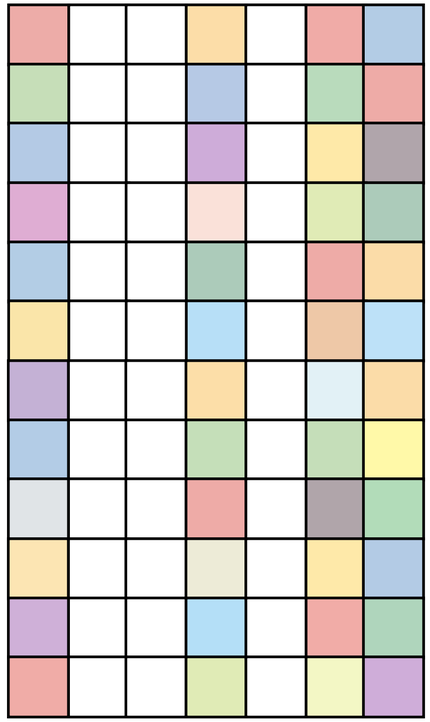
$$x_2 = \sigma(W(x_1 \odot z) + b)$$

zero component in z ⇒
no outgoing edges ⇒
remove neuron

Louizos, Christos et al. Bayesian compression for deep learning. NIPS 2017

Structured Bayesian sparsification: training

No outgoing edges
⇒ remove neuron



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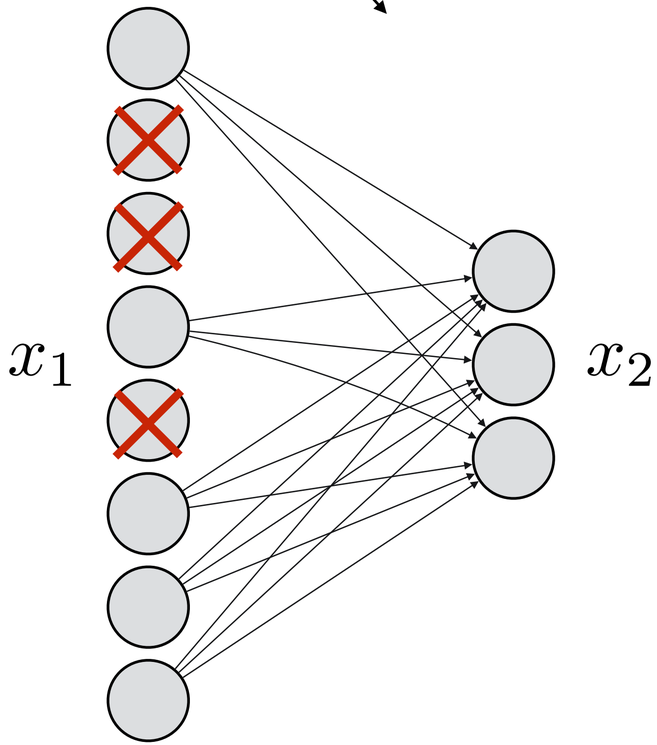

Computational graph

$$x_2 = \sigma(W(x_1 \odot z) + b)$$

minor modification of computational graph

Treat z in **the same way** as W :

- Log-uniform prior on z and on W
- Normal approx. posterior for both
- RT & LRT for W
- RT for z (LRT is not needed)

A bit more mathematical motivation

Let's choose standard normal prior on W :

$$x_2 = \sigma(W(x_1 \odot z) + b) \qquad p(z_i) \propto \frac{1}{|z_i|}; \quad p(w_{ij}) = \mathcal{N}(0, 1)$$

independent

Louizos, Christos et al. Bayesian compression for deep learning. NIPS 2017

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independent

$$p(\underbrace{w_{ij} z_i}_{\tilde{w}_{ij}} | z_i) = \mathcal{N}(0, z_i^2)$$

Louizos, Christos et al. Bayesian compression for deep learning. NIPS 2017

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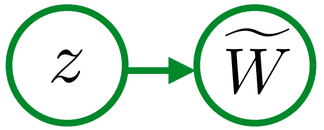
independent

Equivalent model:

$$x_2 = \sigma(\widetilde{W}x_1 + b) \qquad p(z_i) \propto \frac{1}{|z_i|}; \quad p(\tilde{w}_{ij}|z_i) = \mathcal{N}(0, z_i^2)$$



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Louizos, Christos et al. Bayesian compression for deep learning. NIPS 2017

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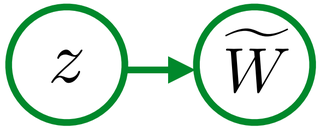


dependent!

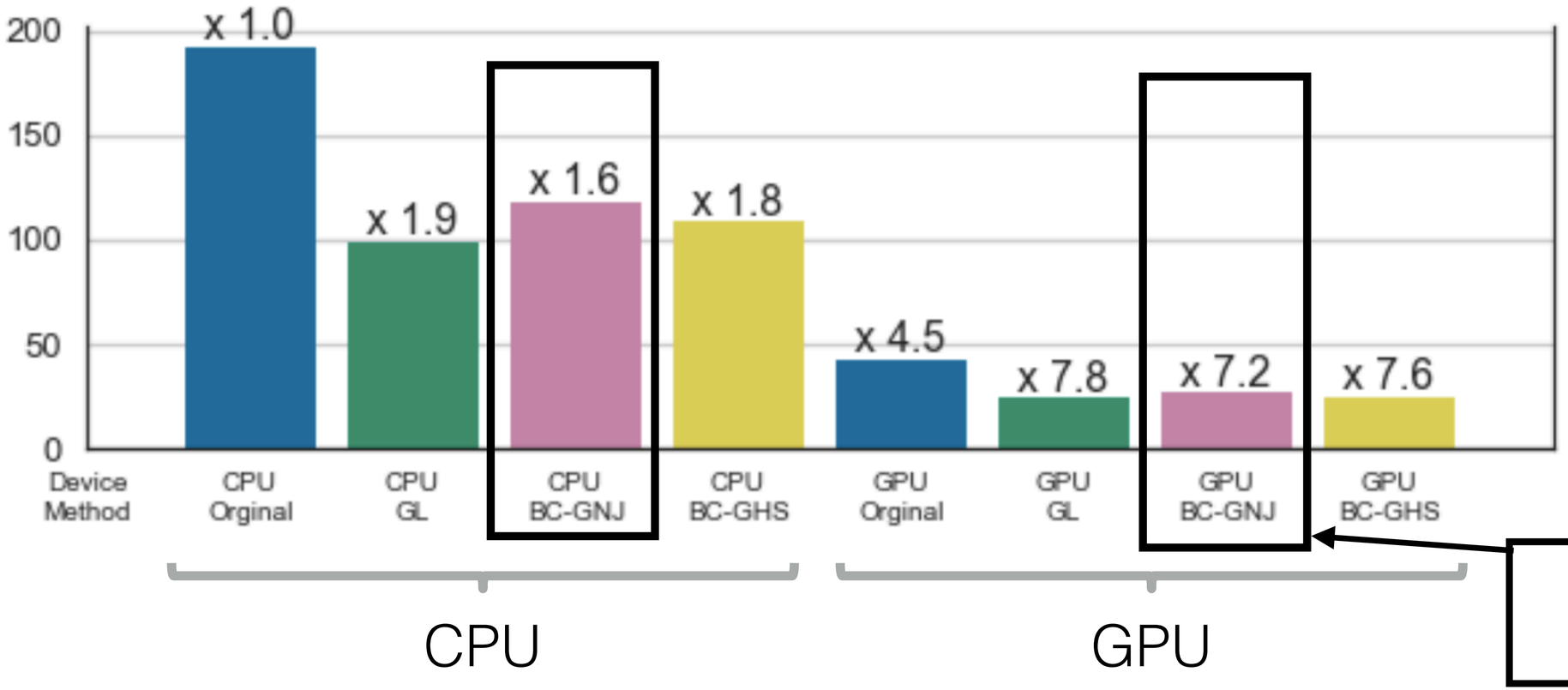
$$p(\tilde{w}_{ij}) \propto \int \frac{1}{|z_i|}\mathcal{N}(0, z_i^2)dz_i = \frac{1}{|\tilde{w}_{ij}|}$$

SparseVD model!
But with structured sparsity

Louizos, Christos et al. Bayesian compression for deep learning. NIPS 2017

Structured Bayesian sparsification: results

Speed-up of forward pass (testing stage) for Lenet-5-Caffe



Louizos, Christos et al. Bayesian compression for deep learning. NIPS 2017

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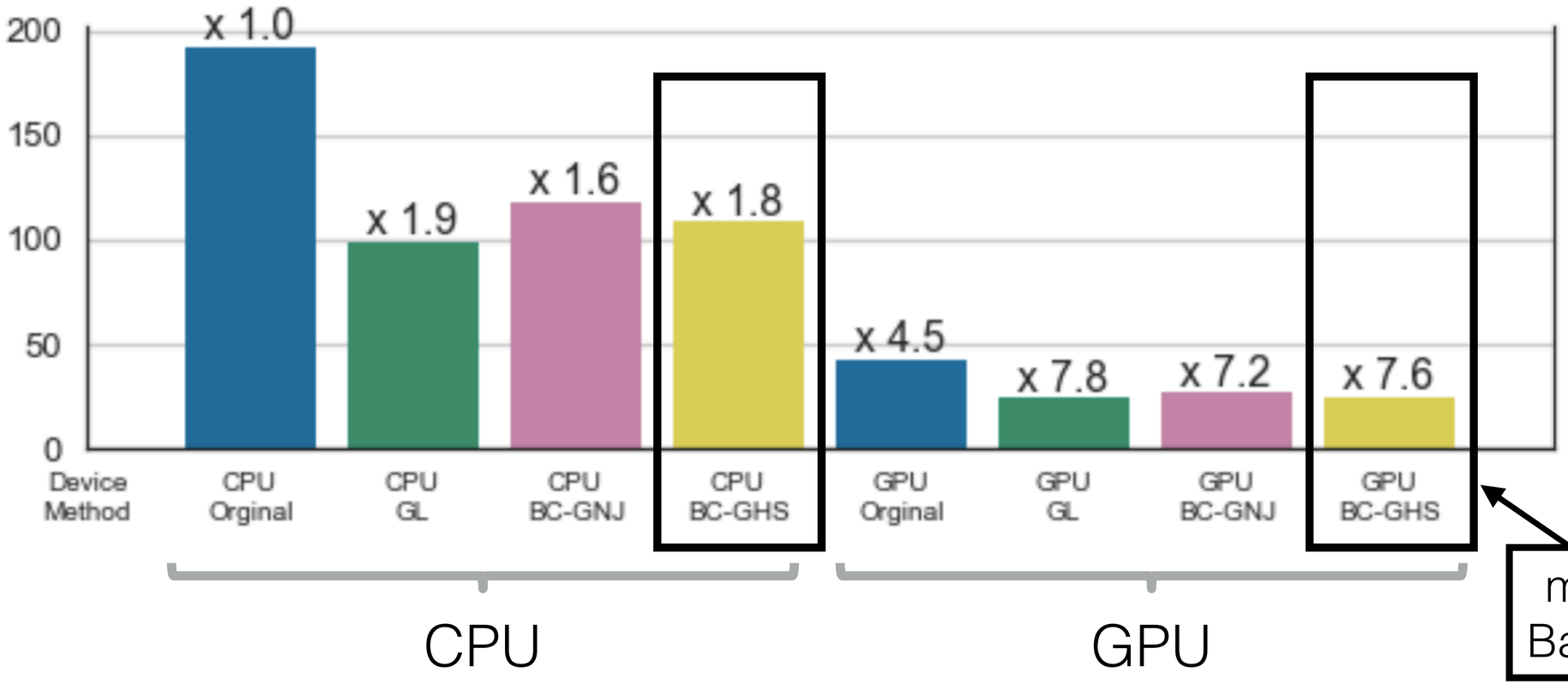


Louizos, Christos et al. Bayesian compression for deep learning. NIPS 2017

What’s next?

- SparseVD for RNNs
- Structured Bayesian sparsification
- How does it all works on large datasets and networks

Two popular frameworks for sparsification

Magnitude pruning	**Bayesian sparsification**
A lot of method hyperparameters	(Almost) no method hyperparameters
Need to choose training schedule	Need to choose training schedule
non-Bayesian	Bayesian!

The state of sparsity in deep neural networks

- Recent (2019) work on comparing different (unstructured) sparsification techniques on **large** datasets and models:
  - Transformer for neural machine translation (WMT 2014 English-to-German)
  - ResNet-50 for ImageNet
- Open-source code and top performing model checkpoints for reproducibility
- **Thousands** of experiments!

Gale, Trevor et al. The State of Sparsity in Deep Neural Networks. Arxiv, 2019

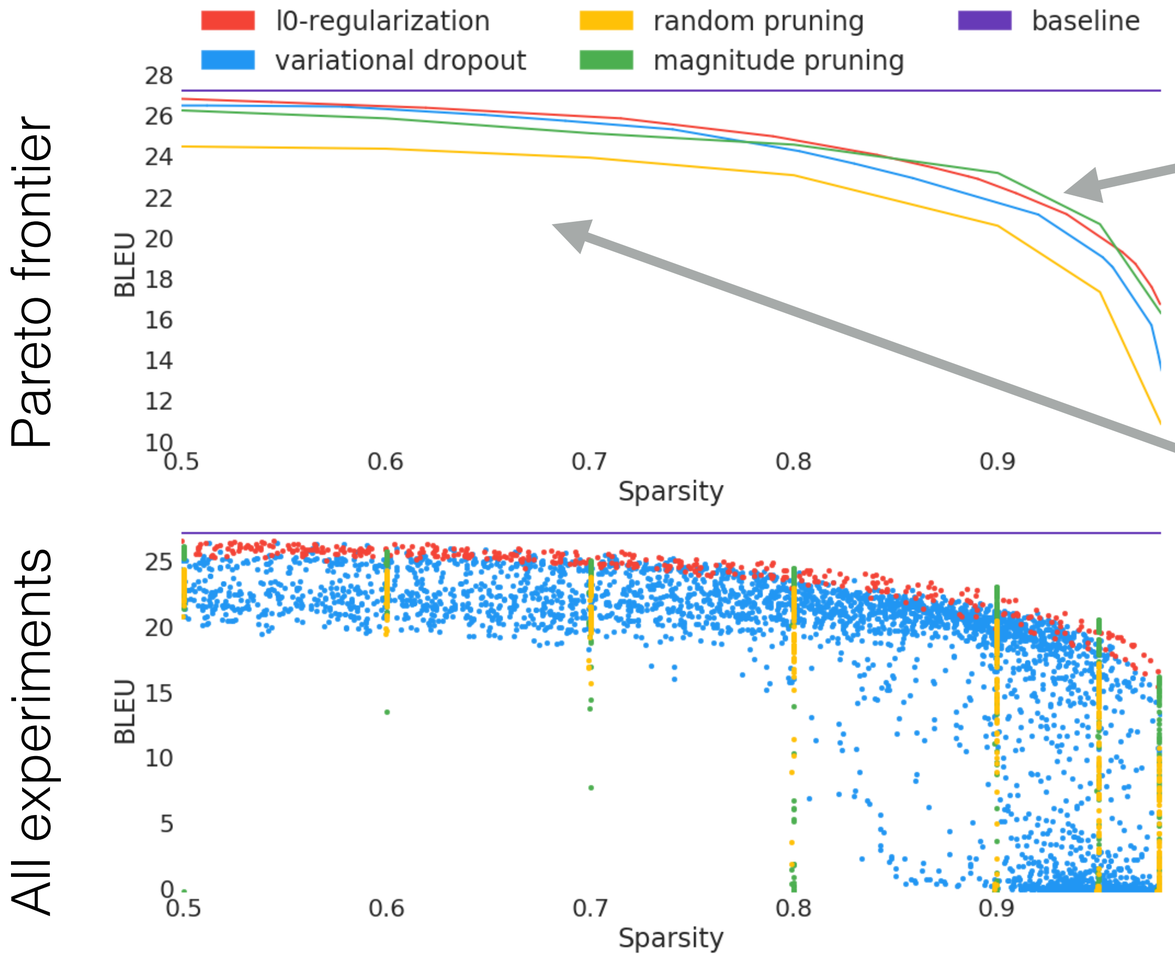
Hyperparameters for both tasks

- Hyperparameters tuned in Sparse variational dropout:
  - KL-divergence weight & annealing schedule (not grounded theoretically, but works in practice)
  - Sparsification threshold

- Hyperparameters tuned in Magnitude pruning:
  - target sparsity
  - starting iteration of the sparsification process
  - ending iteration of the sparsification process
  - frequency of pruning steps

Gale, Trevor et al. The State of Sparsity in Deep Neural Networks. Arxiv, 2019

Transformer for neural machine translation



Magnitude pruning outperforms SparseVD a bit for high compression ratio

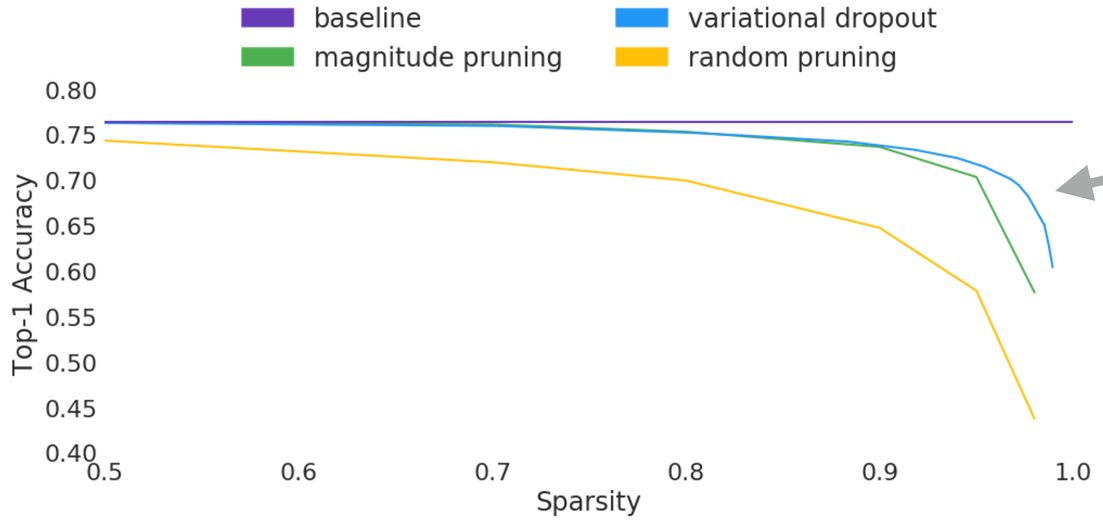
L0-regularization (another Bayesian approach) outperform others for small compression ratio

The relative performance of all three techniques is remarkably consistent

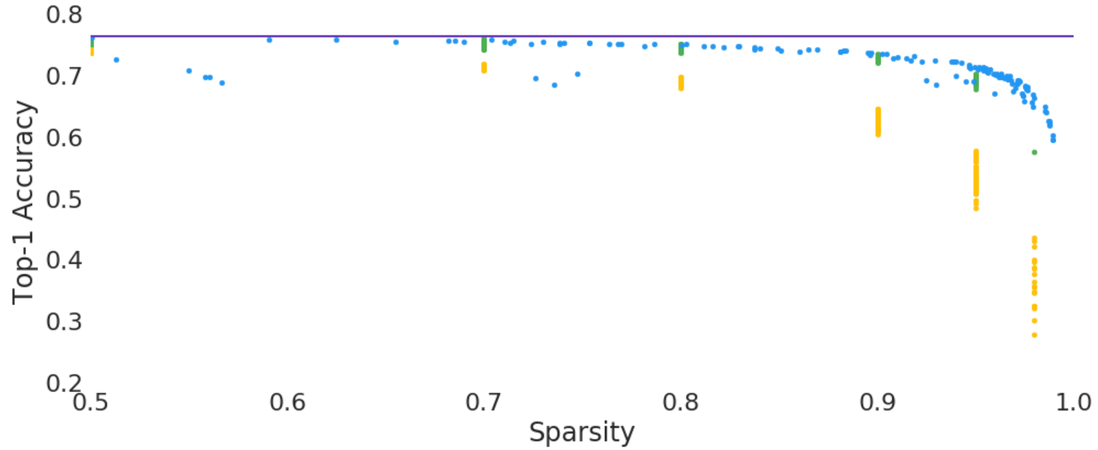
Gale, Trevor et al. The State of Sparsity in Deep Neural Networks. Arxiv, 2019

ResNet-50 for ImageNet

Pareto frontier



All experiments



SparseVD outperforms magnitude pruning for high compression ratio

The relative performance of all three techniques is remarkably consistent

Gale, Trevor et al. The State of Sparsity in Deep Neural Networks. Arxiv, 2019

Other Bayesian sparsification models

- Group horseshoe with half-Cauchy scale priors:

  more levels is model hierarchy & usually better compression

$$s \sim \mathcal{C}^+(0, \tau_0); \qquad \tilde{z}_i \sim \mathcal{C}^+(0, 1); \qquad \tilde{w}_{ij} \sim \mathcal{N}(0, 1); \qquad w_{ij} = \tilde{w}_{ij}\tilde{z}_i s$$

- L_0 regularization

  relax non-differentiable L_0 regularizer & obtain exact zero weights

$$\mathcal{R}(\boldsymbol{\theta}) = \frac{1}{N}\left(\sum_{i=1}^{N} \mathcal{L}\left(h(\mathbf{x}_i; \boldsymbol{\theta}), \mathbf{y}_i\right)\right) + \lambda\|\boldsymbol{\theta}\|_0$$

  relaxation is based on spike-and-slab prior (as well as approx. posterior)

$$p(z) = \textbf{Bernoulli}(\pi), \qquad p(\theta|z=0) = \delta(\theta), \qquad p(\theta|z=1) = \mathcal{N}(\theta|0, 1)$$

Louizos, Christos et al. Bayesian compression for deep learning. NIPS 2017
Louizos, Learning Sparse Neural Networks through L0 Regularization. ICLR 2018

Summary

- Sparsification of neural networks is an urgent industrial problem that is well solved using Bayesian deep learning
- Bayesian sparsification relies on Bayesian neural networks that provide regularization, fast ensembling, uncertainty estimation etc.
- Bayesian sparsification is a theoretically grounded approach but several tricks are needed to train the model