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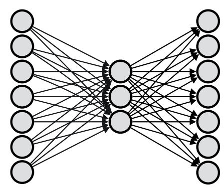
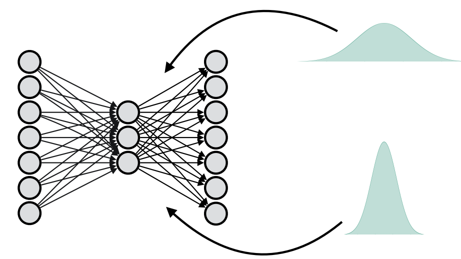
Bayesian sparsification of neural networks

2021

Slides are partially based on lectures of Dmitry Vetrov, Dmitry Kropotov and Kirill Struminsky, deepbayes.ru/2018

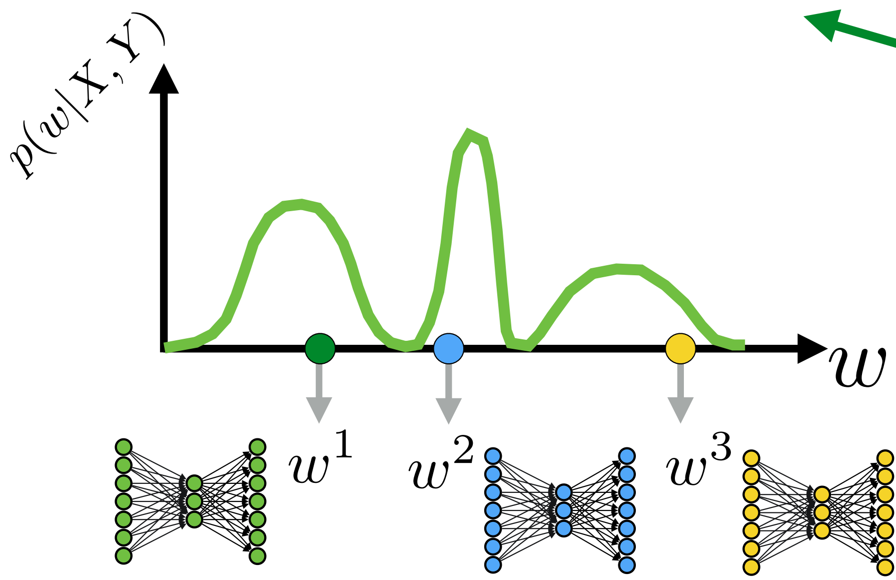
Bayesian neural networks

	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 $p(w \mid X, Y)$
Prediction on new object x_* :	$p(y_* \mid x_*, w_{MP})$	$\mathbb{E}_{p(w \mid X, Y)} p(y_* \mid x_*, w)$

Prediction with Bayesian neural network

Prediction on a new object x_*:

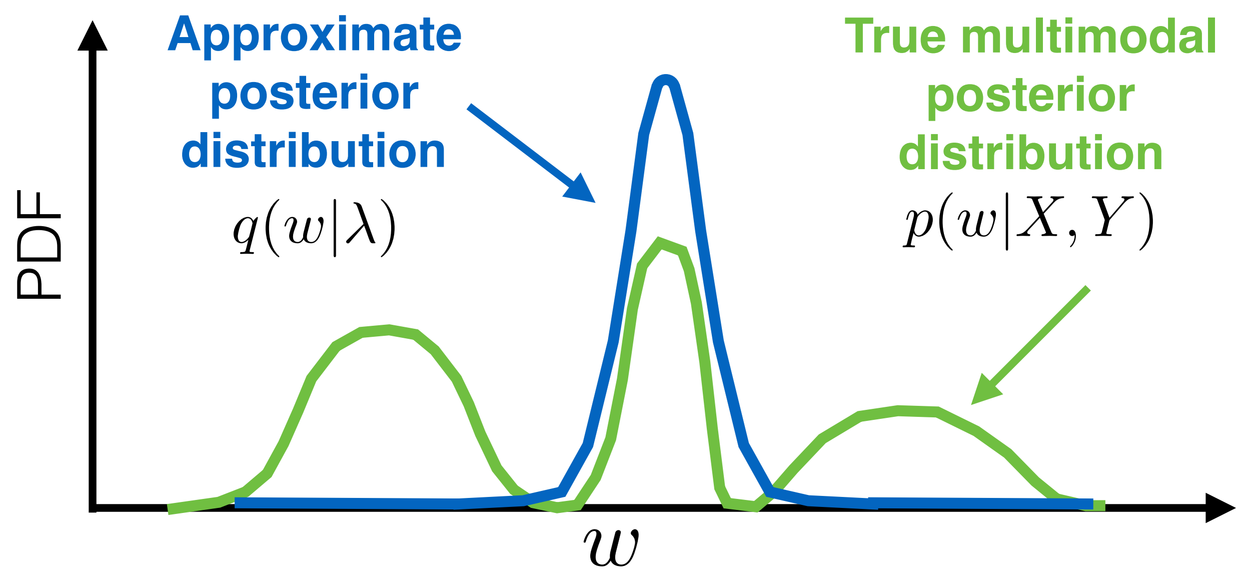
$$\mathbb{E}_{p(w|X,Y)} p(y_*|x_*, w) \approx \frac{1}{K} \sum_{k=1}^{K} p(y_*|x_*, w^k), \quad w^k \sim p(w|X,Y)$$



average net's output across several weight samples

Training Bayesian neural networks

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

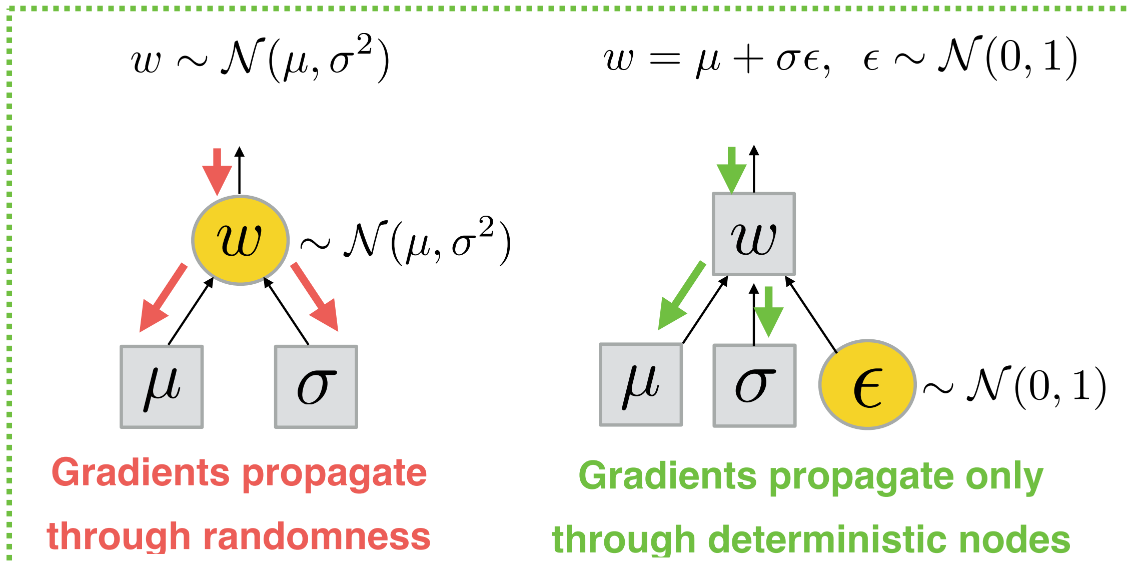


Reparametrization trick

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

$$\sum_{j=1}^{m} \log p(y^{i_j}|x^{i_j}, w = f(\lambda, \epsilon^j)),$$

$$\epsilon^j \sim p(\epsilon) \qquad i_j \sim \mathrm{Unif}(1, \dots, N)$$



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 $p(w)$

Training:

- Choose particular family for approximate posterior $q(w|\lambda)$
- How to compute the KL-divergence (regularizer) ?

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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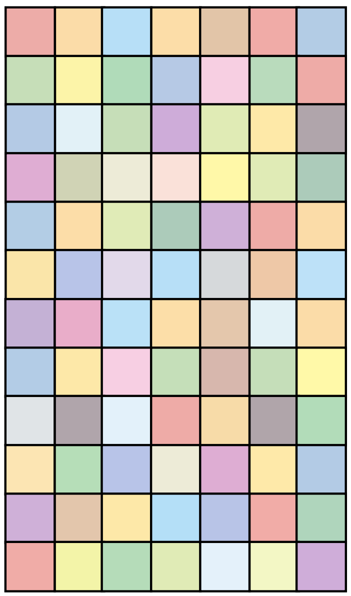
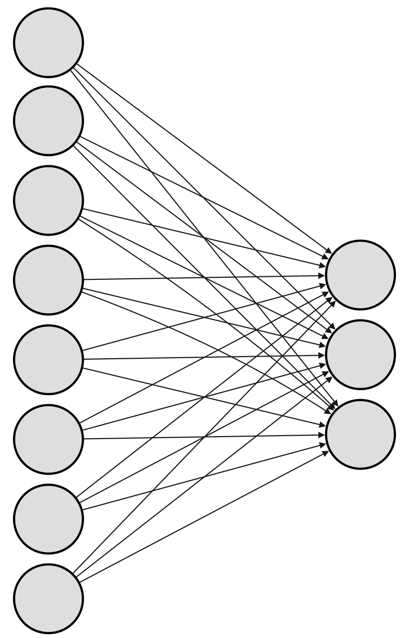
- One of the solutions — sparsification

Neural network

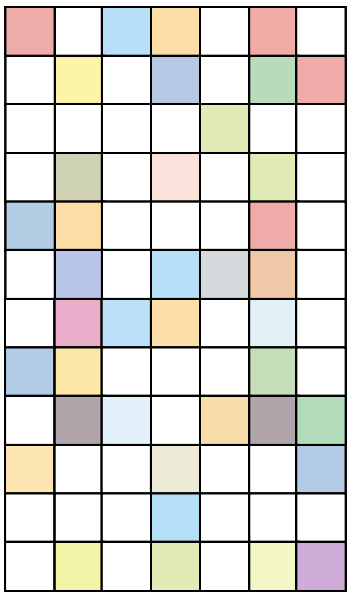


Weight matrix W



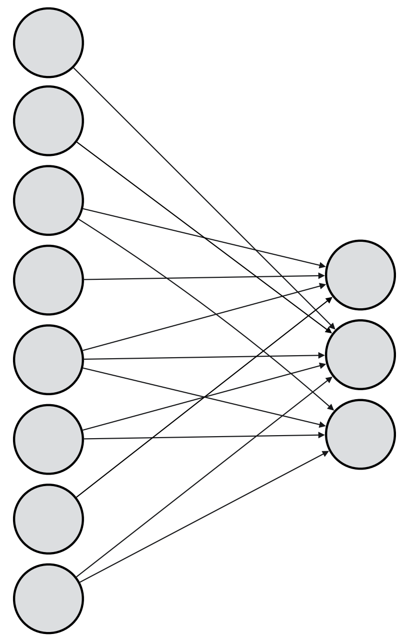
Computational graph

Sparse neural network



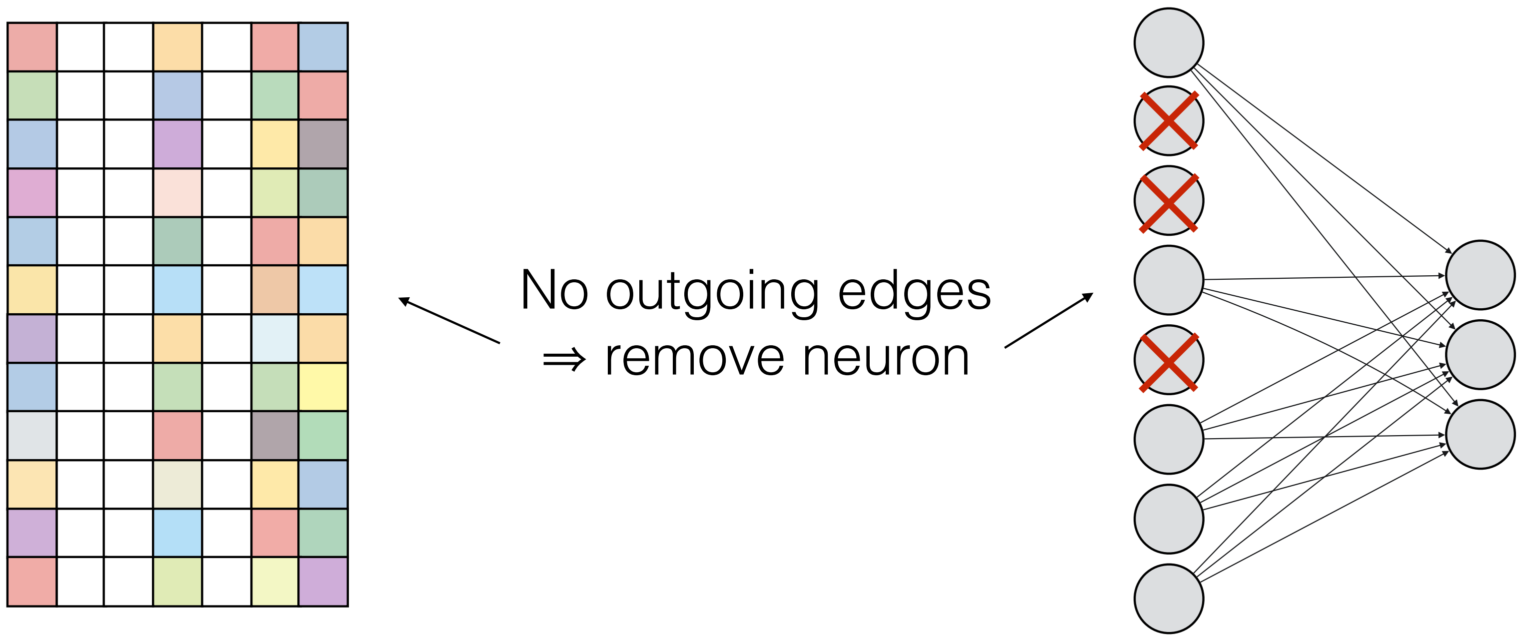
Weight matrix W

A lot of weights
set to zero



Computational graph

Structured sparsity



Weight matrix W

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)

Sparse variational dropout

Prior: ?

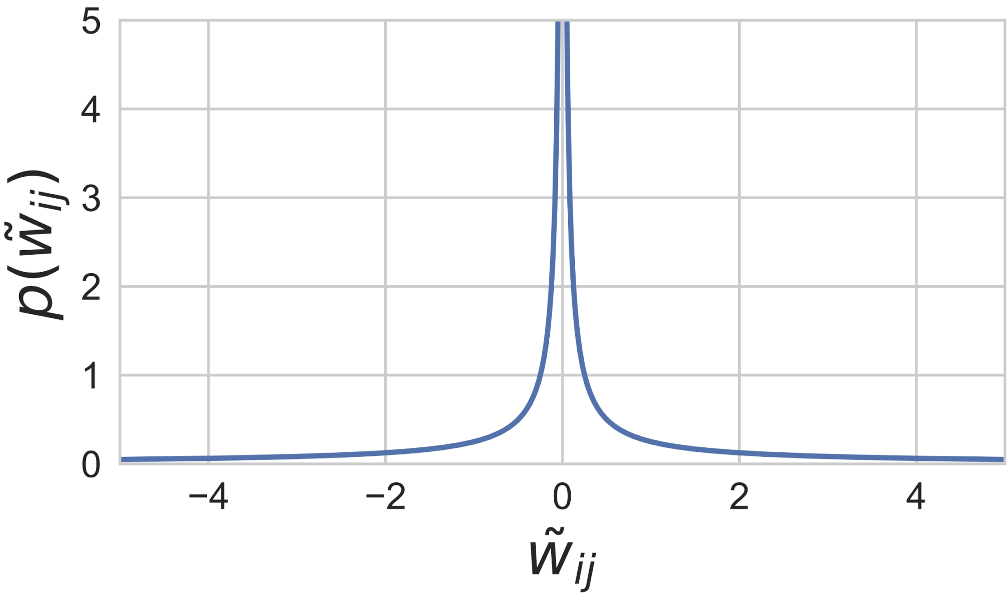
Approximate posterior: ?

Approximate KL-divergence: ?

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

Sparse variational dropout

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



Favors removing noisy weights!

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

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

Approximate KL-divergence: ?

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

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

Approximate KL-divergence: ?

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Approximating KL-divergence

Remember: training Bayesian neural networks — optimizing ELBO:

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

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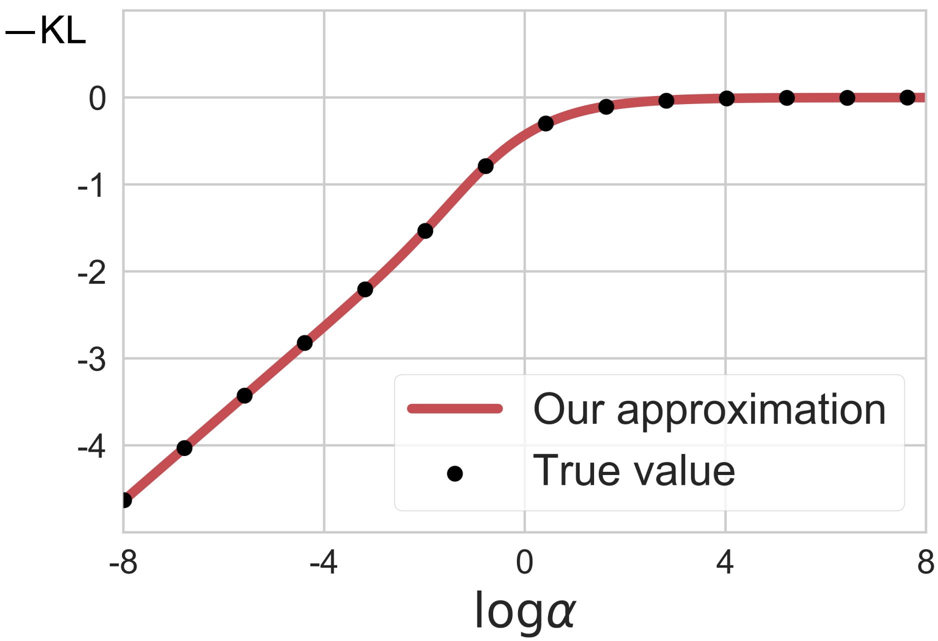
Approximating KL-divergence
(fully factorized)



$$-KL(q(w_{ij}|\mu_{ij},\sigma_{ij}) \,\|\, p(w_{ij})) \approx$$
$$\approx k_1 \sigma(k_2 + k_3 \log \alpha_{ij})) - 0.5 \log(1 + \alpha_{ij}^{-1}) + \mathrm{C}$$
$$k_1 = 0.63576 \qquad k_2 = 1.87320 \qquad k_3 = 1.48695$$
$$\alpha_{ij} = \frac{\sigma_{ij}^2}{\mu_{ij}^2}$$

- KL depends only on α_{ij}
- Favors large α_{ij} $\Rightarrow$ removing noisy weights

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Sparse variational dropout

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

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

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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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:

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

Final algorithm

Training on a mini-batch X with labels Y:

1. Sample weights: $w_{ij} = \mu_{ij} + \epsilon_{ij}\sigma_{ij}, \quad \epsilon_{ij} \sim \mathcal{N}(0,1)$
2. Forward pass: $Y_{\text{pred}} = NN(X, w, b)$
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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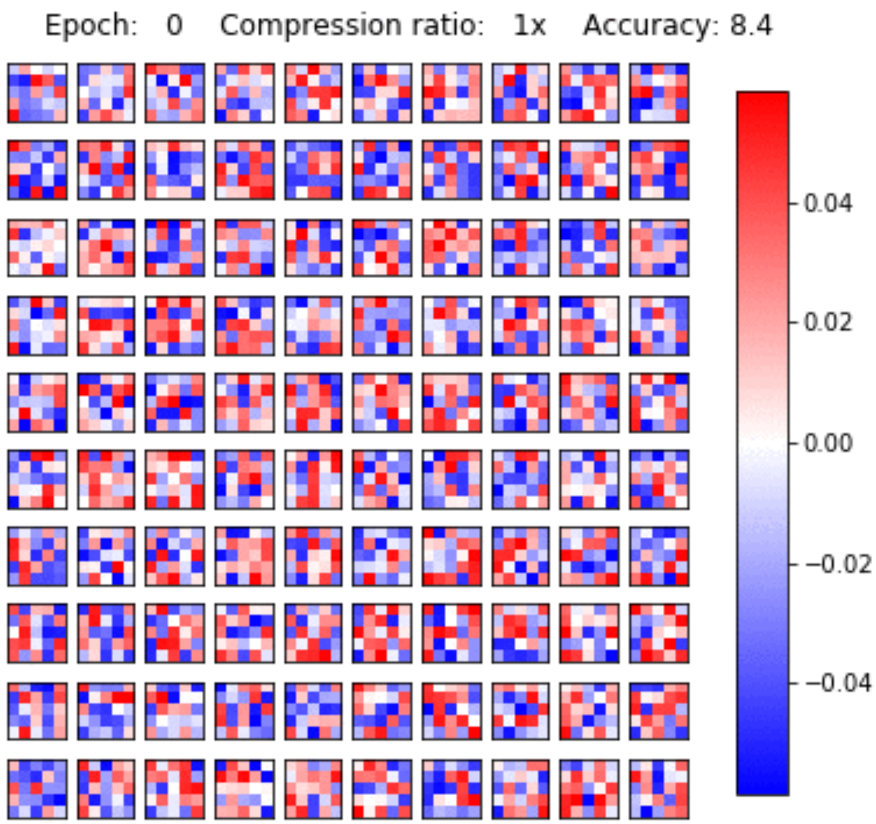
Prediction for a mini-batch X :

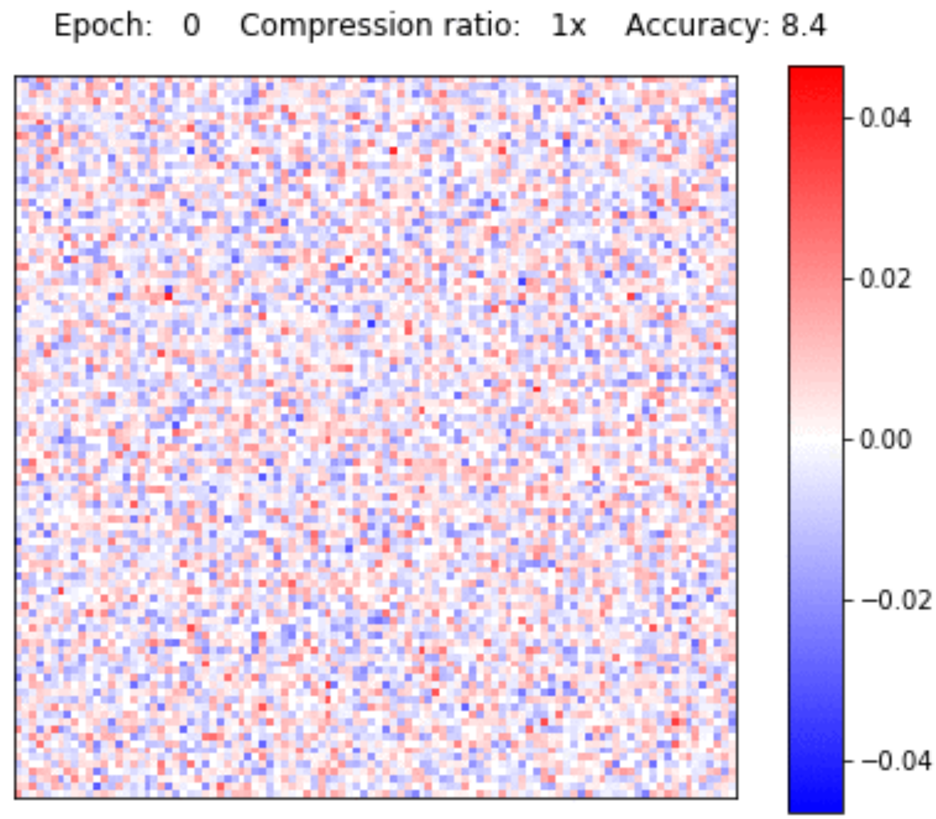
Return $Y_{\text{pred}} = NN(X, \mu, b)$

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

Sparse variational dropout: visualization

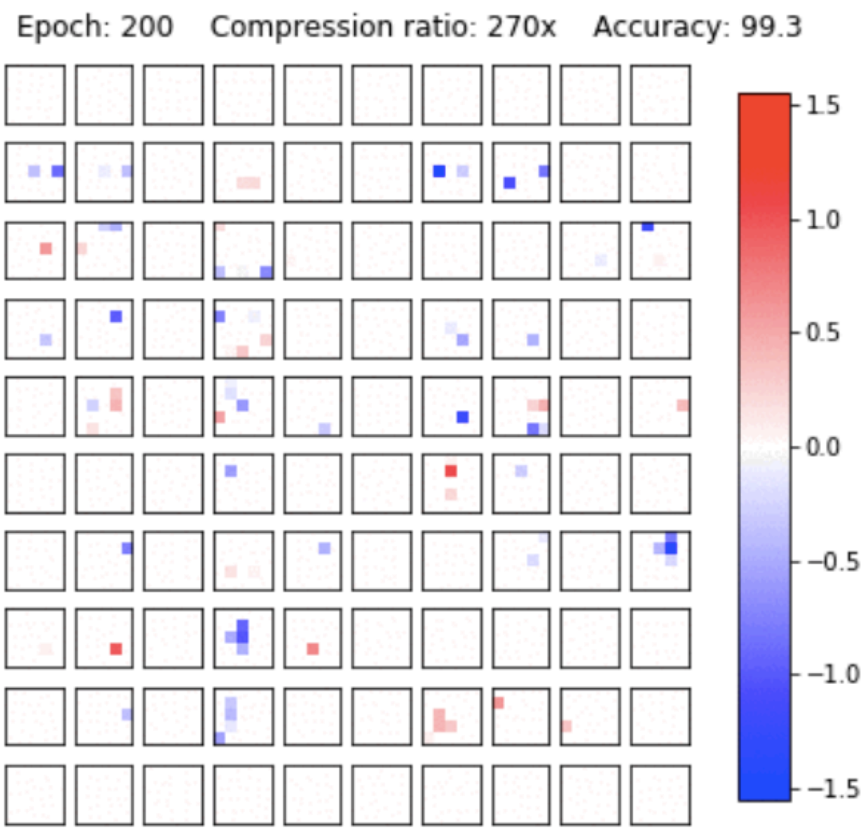


LeNet-5: convolutional layer

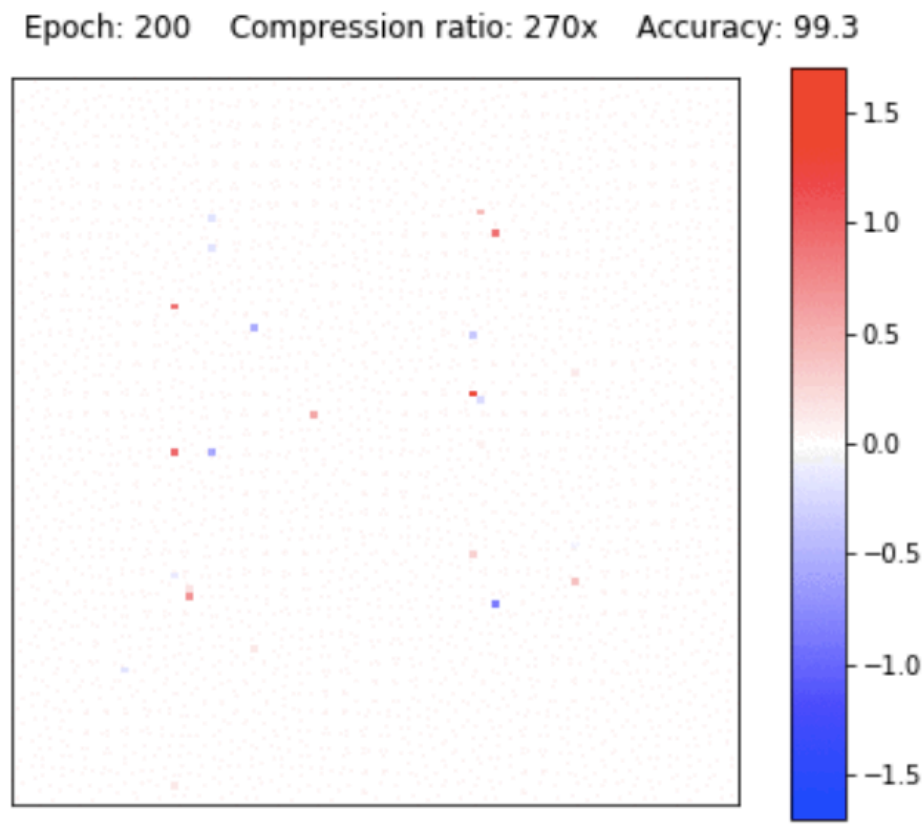


LeNet-5: fully-connected layer
(100 x 100 patch)

Sparse variational dropout: visualization



LeNet-5: convolutional layer

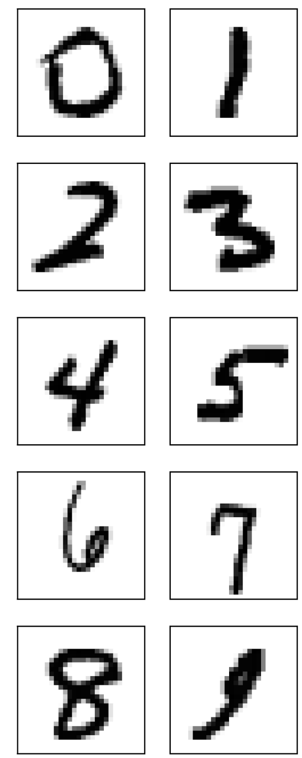


LeNet-5: fully-connected layer
(100 x 100 patch)

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

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

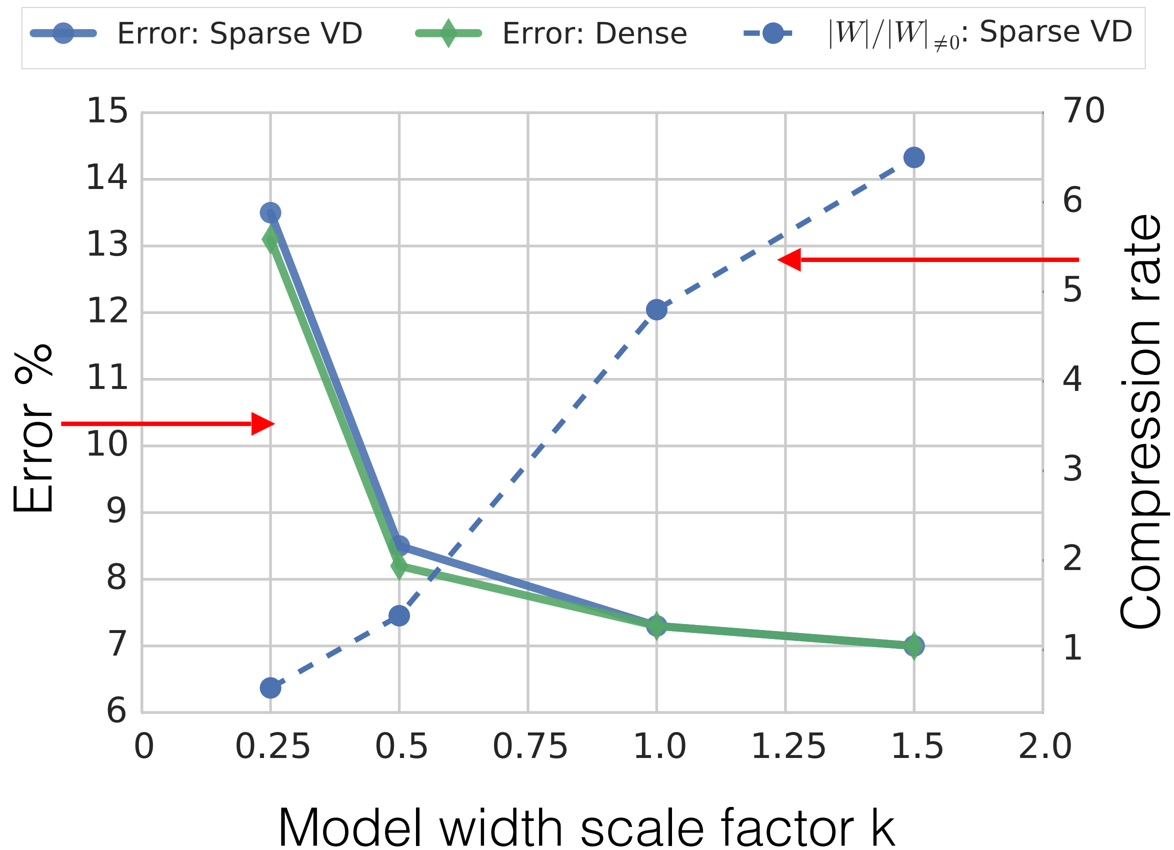
Network	Method	Error %	Sparsity per Layer %	$\frac{\lvert\mathbf{W}\rvert}{\lvert\mathbf{W}_{\neq 0}\rvert}$
LeNet-300-100	Original	1.64		1
	Pruning	1.59	$92.0 - 91.0 - 74.0$	12
	DNS	1.99	$98.2 - 98.2 - 94.5$	56
	SWS	1.94		23
(ours)	Sparse VD	1.92	$98.9 - 97.2 - 62.0$	**68**
LeNet-5-Caffe	Original	0.80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