Uncertainty estimation via Stochastic Batch Normalization

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Kirill Neklyudov, Dmitry Vetrov

Batch Normalization recap

Train phase

$$\mathrm{BN}^{\mathrm{train}}_{\gamma,\beta}(x_i) = \frac{x_i - \mu(\mathcal{B})}{\sqrt{\sigma^2(\mathcal{B}) + \epsilon}} \cdot \gamma + \beta$$

$$\mu(\mathcal{B}) = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\sigma^2(\mathcal{B}) = \frac{1}{N}\sum_{i=1}^{N} (x_i - \mu(\mathcal{B}))^2$$

“Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift”, Sergey Ioffe, Christian Szegedy 2015

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Test phase

$$\mathrm{BN}^{\mathrm{test}}_{\gamma,\beta}(x_i) = \frac{x_i - \hat{\mu}}{\sqrt{\hat{\sigma}^2 + \epsilon}} \cdot \gamma + \beta$$

$\hat{\mu}, \hat{\sigma^2}$ exponential smoothed statistics:

$$\hat{\mu} \leftarrow \alpha\,\hat{\mu} + (1-\alpha)\,\mu(\mathcal{B})$$

$$\hat{\sigma}^2 \leftarrow \alpha\,\hat{\sigma}^2 + (1-\alpha)\,\sigma^2(\mathcal{B})$$

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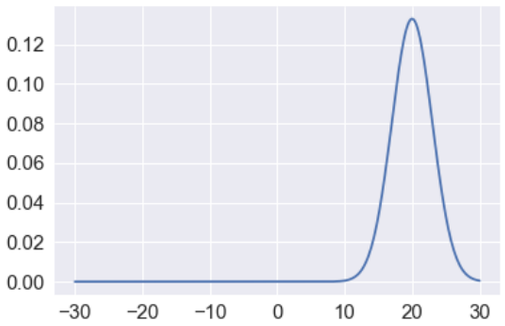
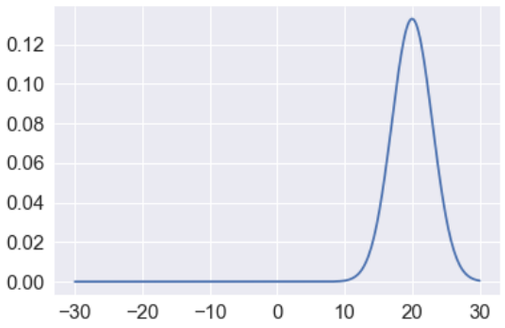
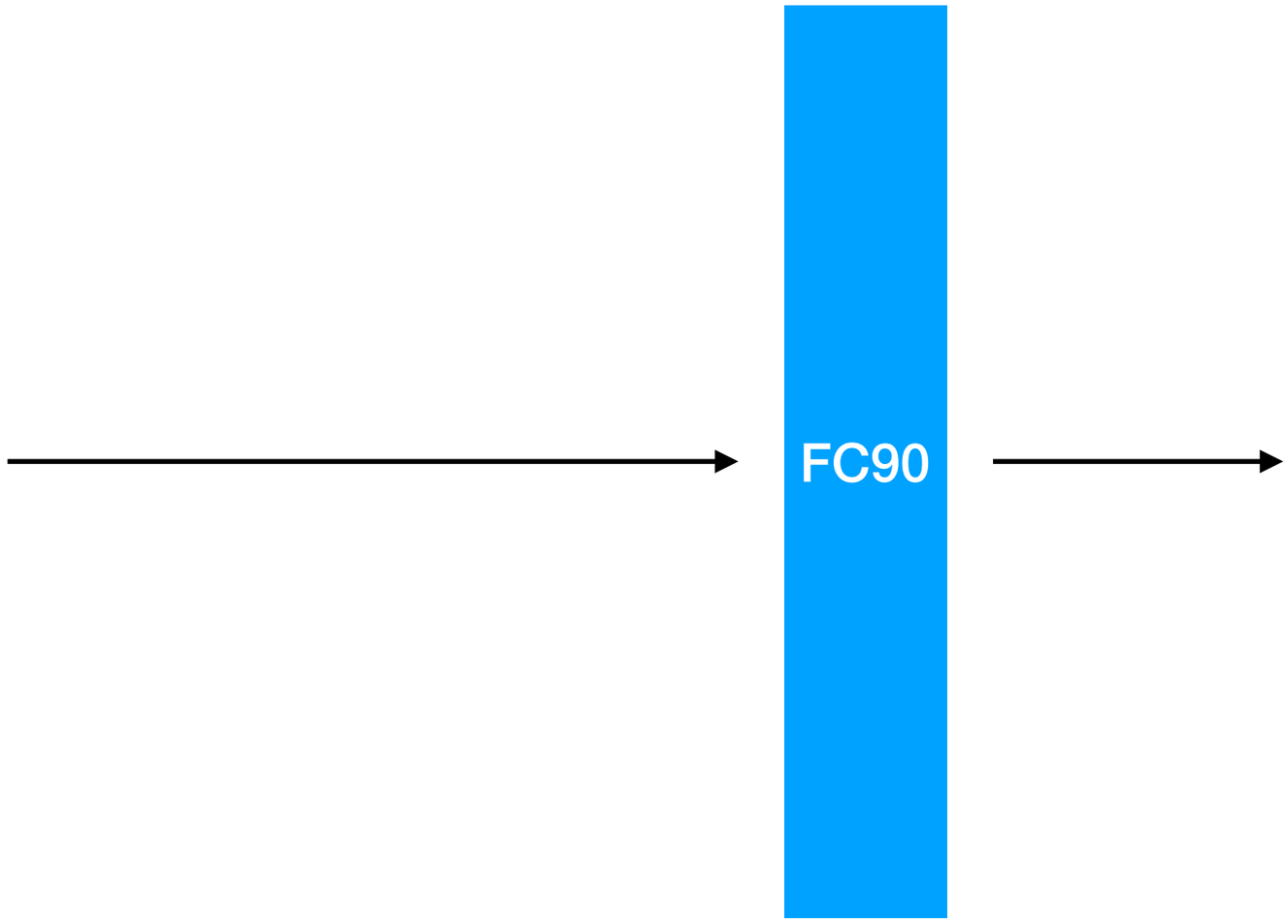
Batch Normalization recap



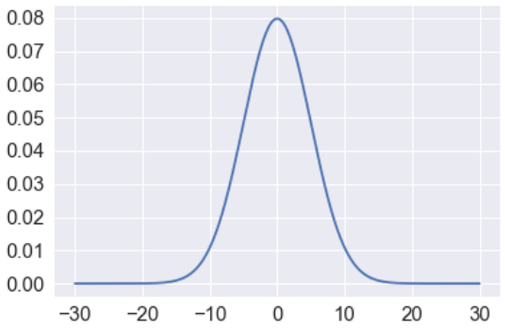
Batch Normalization recap

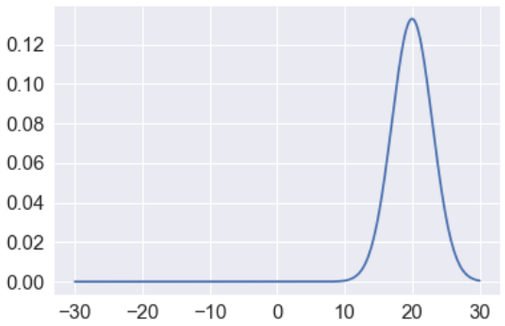


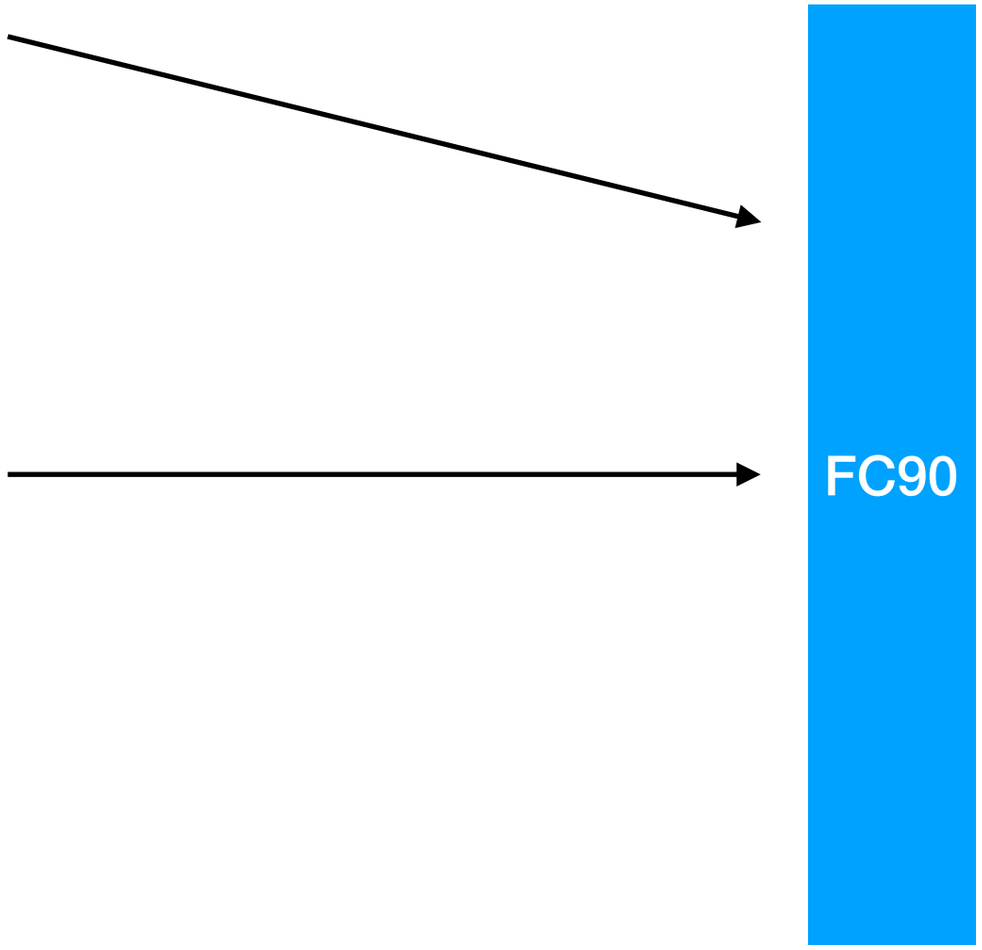


Fail

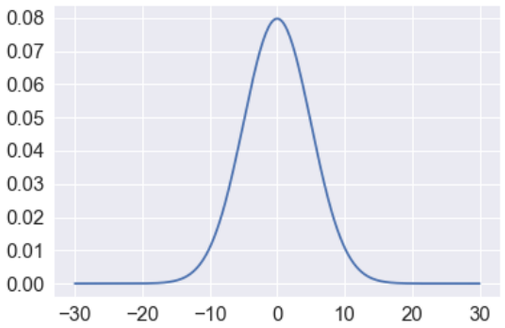
Batch Normalization recap

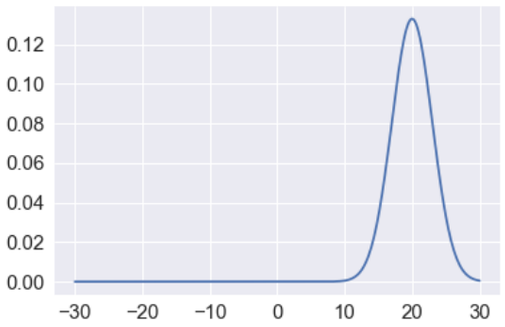


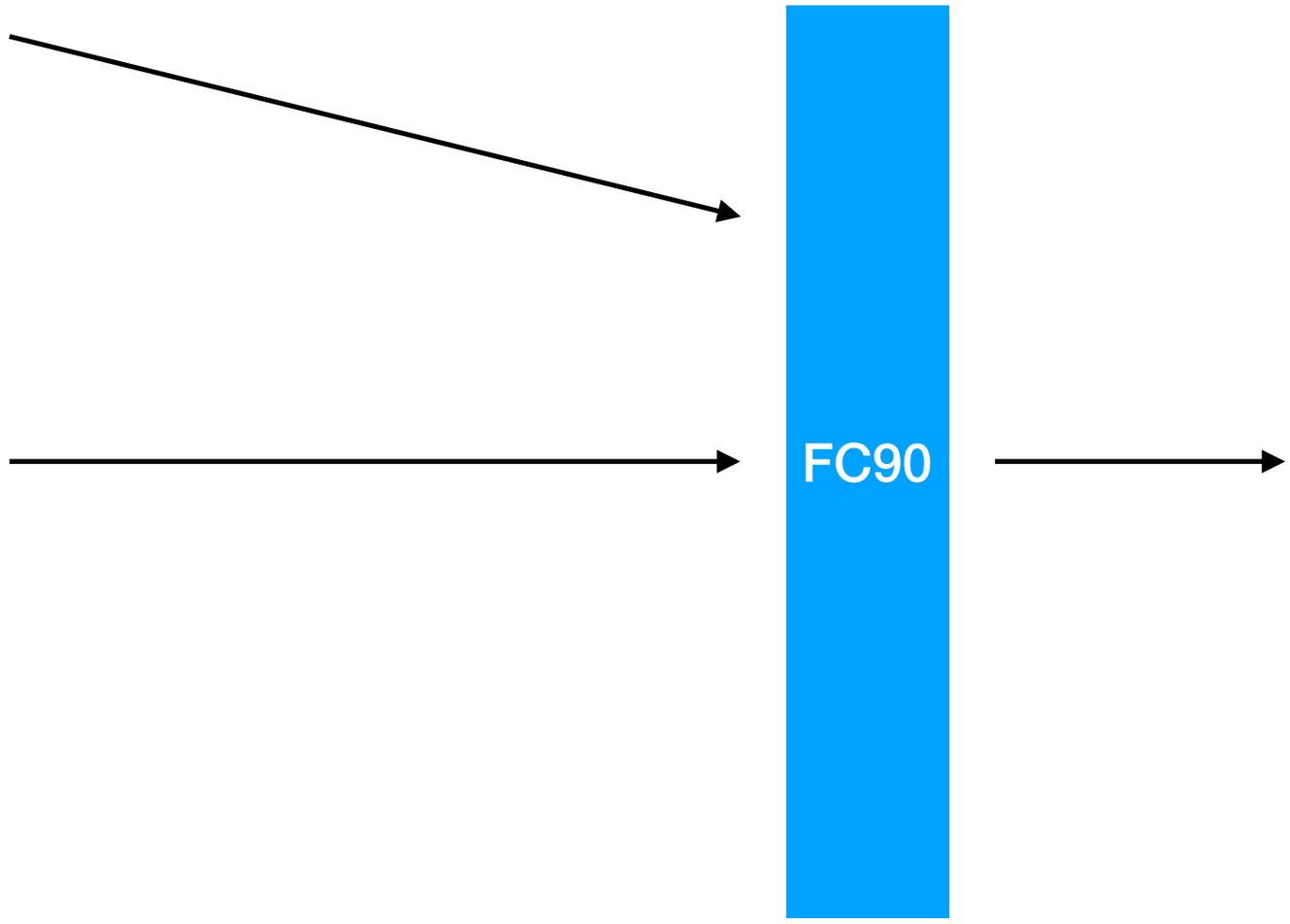




Batch Normalization recap







Fail

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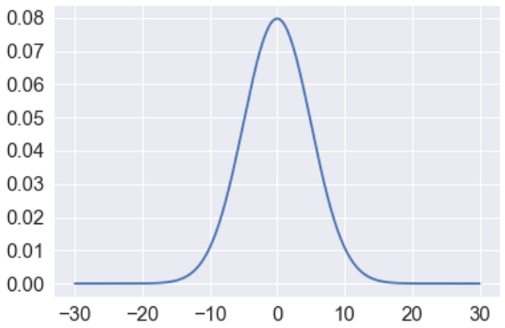
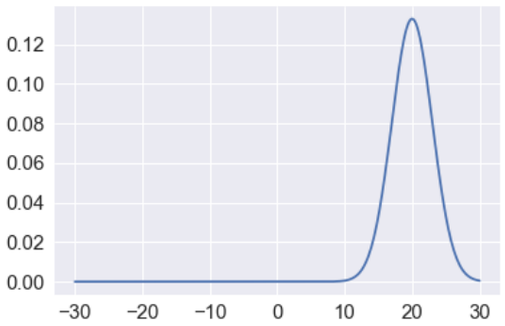
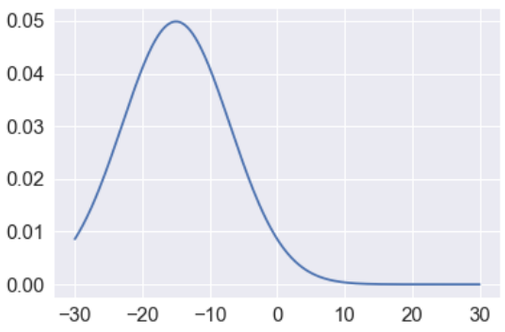
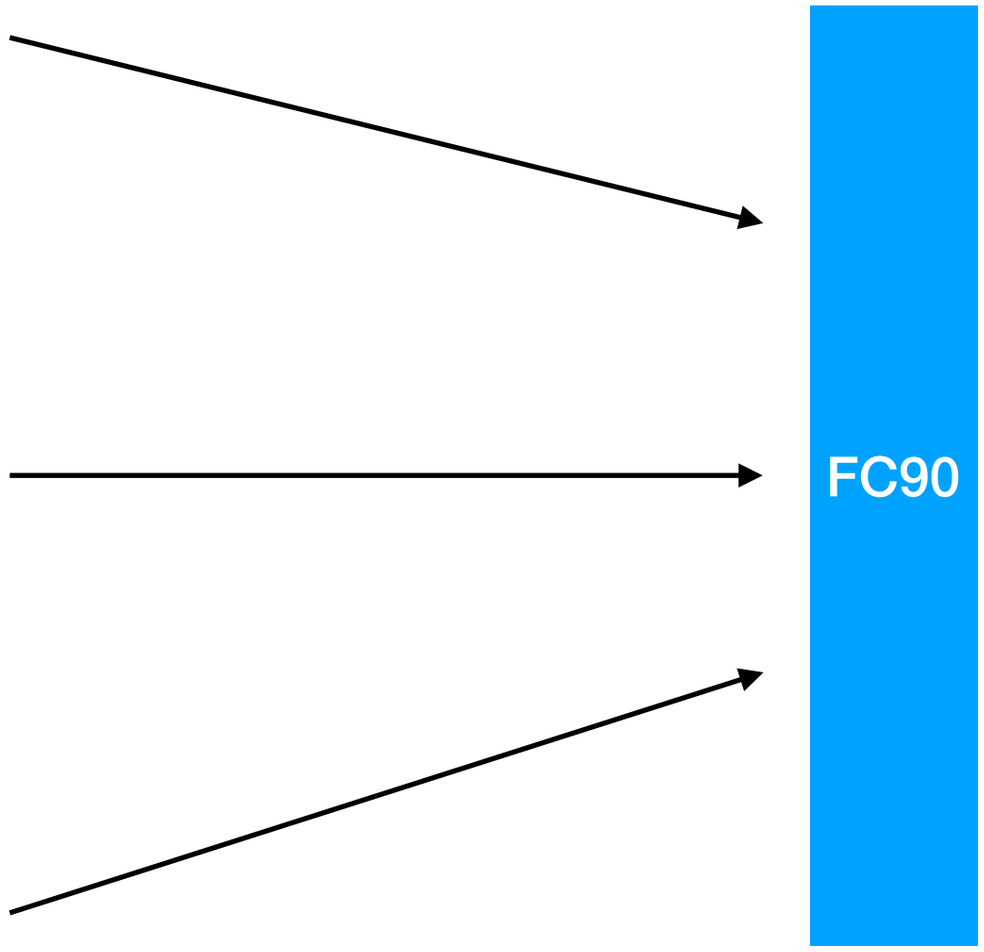


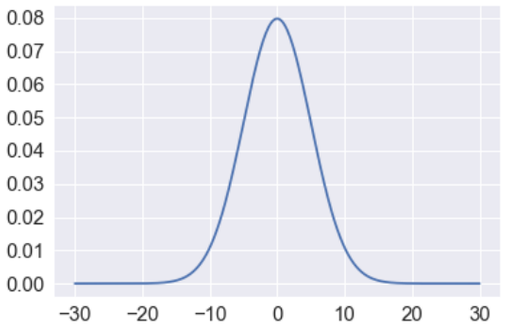


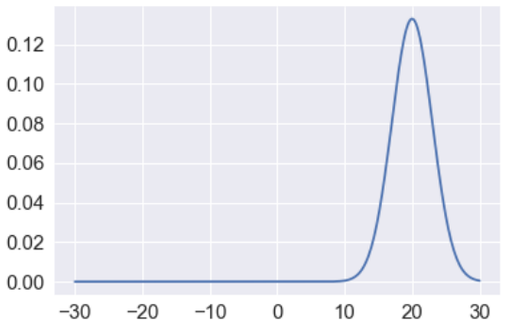


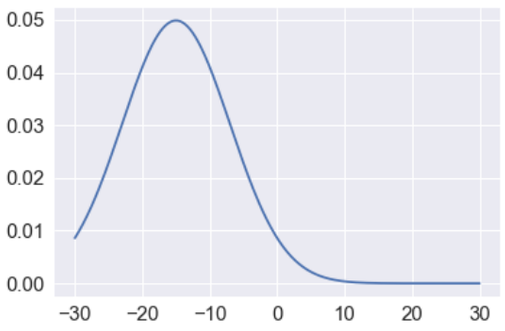


Fail

Batch Normalization recap

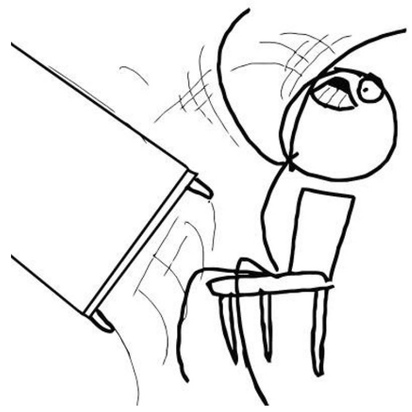




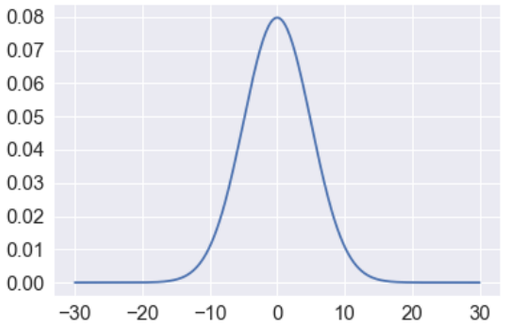


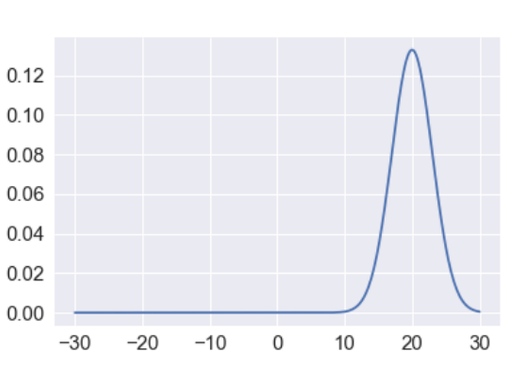
FC90

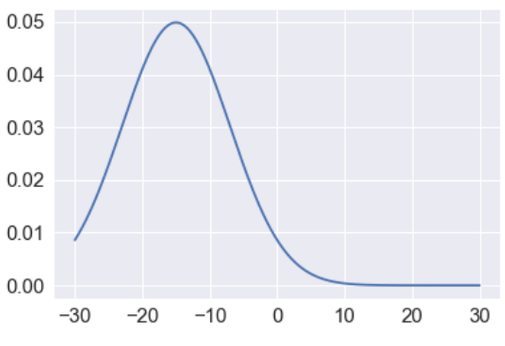
Fail



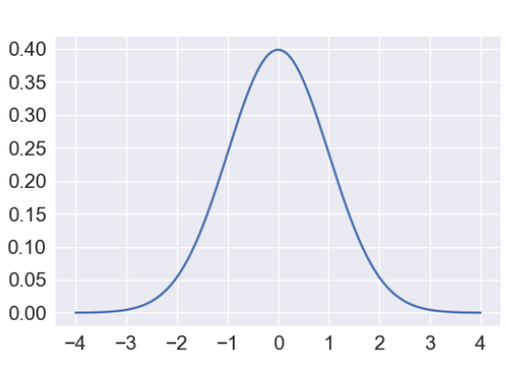
Batch Normalization recap







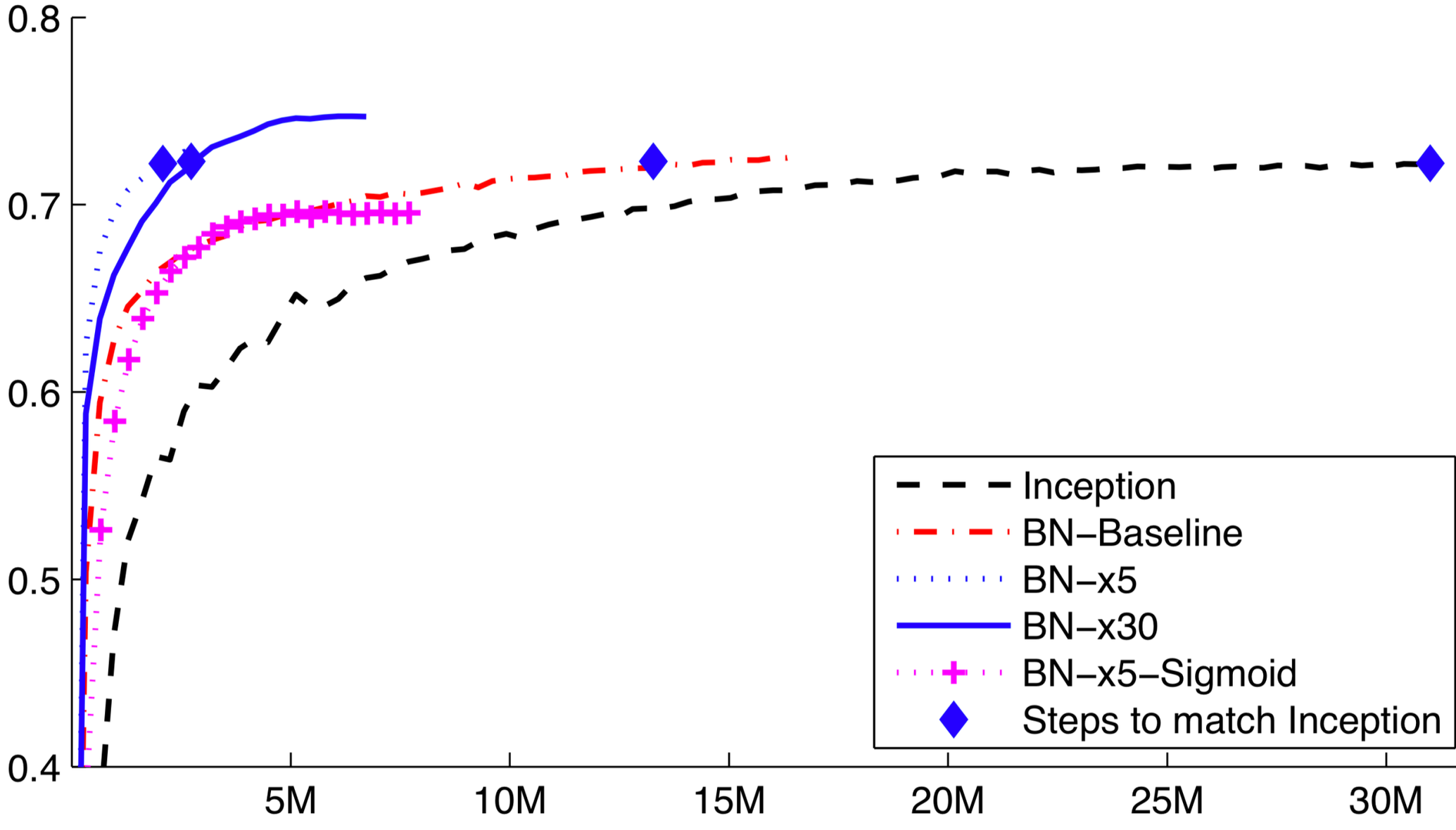
BN



FC90

Success

Batch Normalization recap



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Batchnorm: Probabilistic View

$$\mathrm{BN}^{\mathrm{train}}_{\gamma,\beta}(x_i) = \frac{x_i - \mu(\mathcal{B})}{\sqrt{\sigma^2(\mathcal{B}) + \epsilon}} \cdot \gamma + \beta$$

Batchnorm: Probabilistic View

$$\mathrm{BN}^{\mathrm{train}}_{\gamma,\beta}(x_i) = \frac{x_i - \mu(\mathcal{B})}{\sqrt{\sigma^2(\mathcal{B}) + \epsilon}} \cdot \gamma + \beta$$

Forward pass depends on an entire mini-batch by statistics:

$$p_\theta(y_i \mid x_i, \mathcal{B}_{\setminus i}) = p_\theta(y_i | x_i, \mu(\mathcal{B}), \sigma(\mathcal{B}))$$

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The random choice of a mini-batch induce distribution over statistics:

$$p_\theta(\mu, \sigma | x_i) = \mathbb{E}_{\mathcal{B}_{\setminus i}}\, p_\theta(\mu, \sigma \mid x_i, \mathcal{B}_{\setminus i}) = \mathbb{E}_{\mathcal{B}_{\setminus i}}\, \delta_{\mu(\mathcal{B})}(\mu)\delta_{\sigma(\mathcal{B})}(\sigma)$$

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Marginal likelihood:

$$p_\theta(y|x) = \mathbb{E}_{p_\theta(\mu,\sigma|x)} p_\theta(y|x,\mu,\sigma)$$

Batchnorm: Probabilistic View

MLE optimization problem:

$$\mathcal{L}(\theta) = \sum_{i=1}^{N} \log p_\theta(y_i|x_i) = \sum_{i=1}^{N} \log \mathbb{E}_{p_\theta(\mu,\sigma|x_i)}\, p_\theta(y_i|x_i,\mu,\sigma)$$

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Lower bound using Jensen-Shannon inequality:

$$\mathcal{L}_{\text{BN}}(\theta) = \sum_{i=1}^{N} \mathbb{E}_{\mu,\sigma} \log p_\theta(y_i|x_i,\mu,\sigma) \leq \sum_{i=1}^{N} \log \mathbb{E}_{\mu,\sigma}\, p_\theta(y_i|x_i,\mu,\sigma) = \mathcal{L}(\theta)$$

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Batch Normalization performs unbiased estimation of gradients :

$$\nabla \hat{\mathcal{L}}_{\text{BN}}(\theta) = \frac{N}{M} \sum_{i=1}^{M} \nabla \log p_\theta(y_i|x_i,\mu(\mathcal{B}),\sigma(\mathcal{B}))$$

$$\mathbb{E}_{\mathcal{B}} \nabla \hat{\mathcal{L}}_{\text{BN}}(\theta) = \mathbb{E}_{x_i} \mathbb{E}_{\mathcal{B}_{\setminus i}} \nabla \hat{\mathcal{L}}_{\text{BN}}(\theta) = \nabla \mathcal{L}_{\text{BN}}(\theta)$$

Batchnorm: Probabilistic View

$$\mathrm{BN}^{\mathrm{test}}_{\gamma,\beta}(x_i) = \frac{x_i - \hat{\mu}}{\sqrt{\hat{\sigma}^2 + \epsilon}} \cdot \gamma + \beta$$

Proper predictive distribution:

$$p_\theta(y|x) = \mathbb{E}_{p_\theta(\mu,\sigma|x)} p(y|x,\mu,\sigma)$$

However Batchnorm uses running averaged statistics $\hat{\mu}, \hat{\sigma^2}$:

$$\mathbb{E}\mu \approx \hat{\mu}, \quad \mathbb{E}\sigma \approx \hat{\sigma}$$

$$\mathbb{E}_{p_\theta(\mu,\sigma|x_i)} p(y_i|x_i,\mu,\sigma) \approx p_\theta(y|x,\mathbb{E}\mu,\mathbb{E}\sigma)$$

Batchnorm: Probabilistic View

$$p_\theta(y|x) = \mathbb{E}_{p_\theta(\mu,\sigma|x)} p(y|x,\mu,\sigma)$$

Mini-batch parametrization:

$$\mathbb{E}_{\mu,\sigma} p_\theta(y_i|x_i,\mu,\sigma) = \mathbb{E}_{\mathcal{B}_{\setminus i}}\, p_\theta(y_i|x_i,\mu(\mathcal{B}),\sigma(\mathcal{B}))$$

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Unbiased Monte Carlo estimation:

$$\mathbb{E}_{p_\theta(\mu,\sigma|x_i)}\, p_\theta(y_i|x_i,\mu,\sigma) \approx \frac{1}{S}\sum_{i=1}^{S} p_\theta(y_i|x_i,\mu(\mathcal{B}_i),\sigma(\mathcal{B}_i))$$

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- S forward passes through the network
- Access to the training data during inference

Stochastic Batch Normalization

Approximate true distribution by parametric one:

$$p_\theta(\mu, \sigma \mid x_i) \approx r(\mu) r(\sigma)$$

$$r(\mu) = \mathcal{N}(\mu | \mathrm{m}_\mu, \mathrm{s}_\mu^2) \quad r(\sigma) = \mathrm{Log}\mathcal{N}(\sigma | \mathrm{m}_\sigma, \mathrm{s}_\sigma^2)$$

Stochastic Batch Normalization

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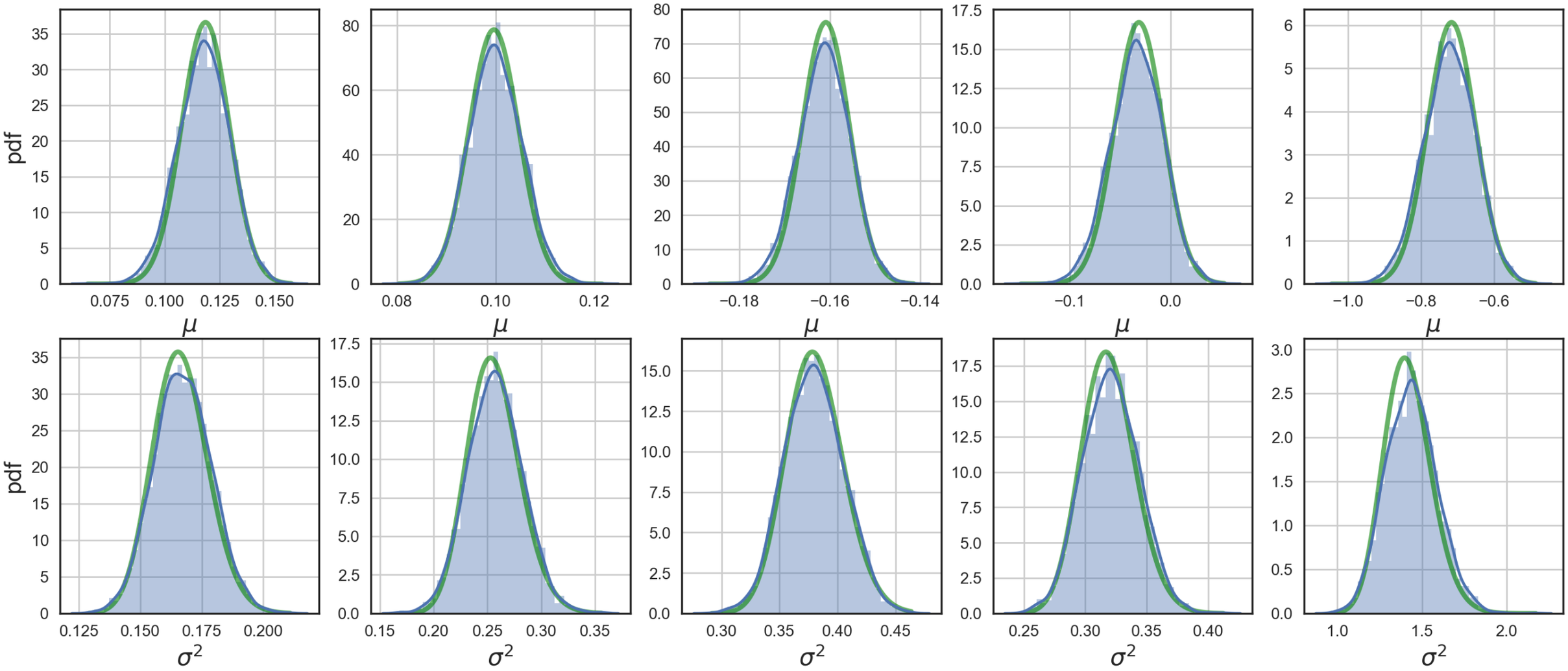
$$p_\theta(\mu, \sigma \,|\, x_i) \approx r(\mu) r(\sigma)$$

$$r(\mu) = \mathcal{N}(\mu | \mathrm{m}_\mu, \mathrm{s}_\mu^2) \quad r(\sigma) = \mathrm{Log}\mathcal{N}(\sigma | \mathrm{m}_\sigma, \mathrm{s}_\sigma^2)$$

Minimize the KL-divergency between averaged statistics distribution and approximation:

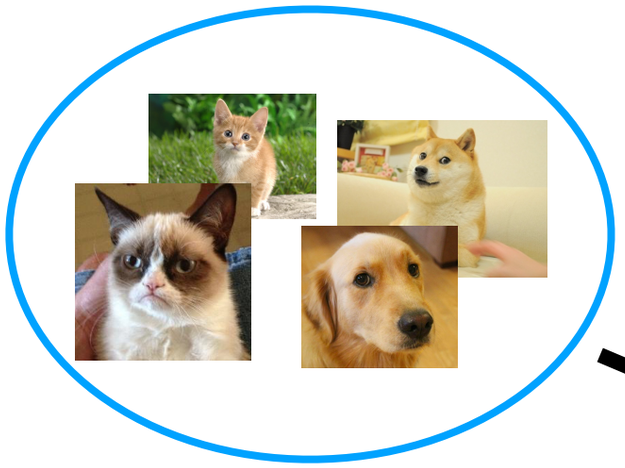
$$D_{\mathrm{KL}} \left(\frac{1}{N} \sum\nolimits_{i=1}^{N} p_\theta(\mu, \sigma \,|\, x_i) \,\middle|\middle|\, r(\mu) r(\sigma) \right) \longrightarrow \min_{m_\mu, s_\mu, m_\sigma, s_\sigma}$$



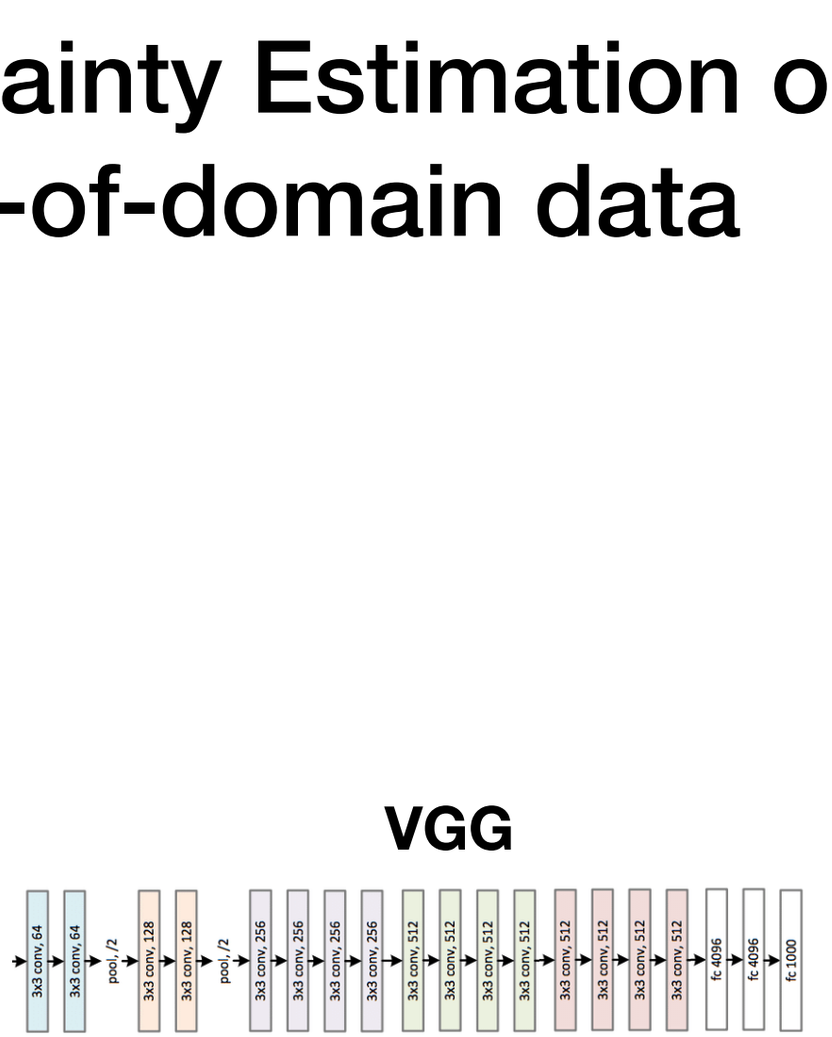
Marginals of true distribution (blue) and approximation (green)

Uncertainty Estimation on out-of-domain data

Training domain



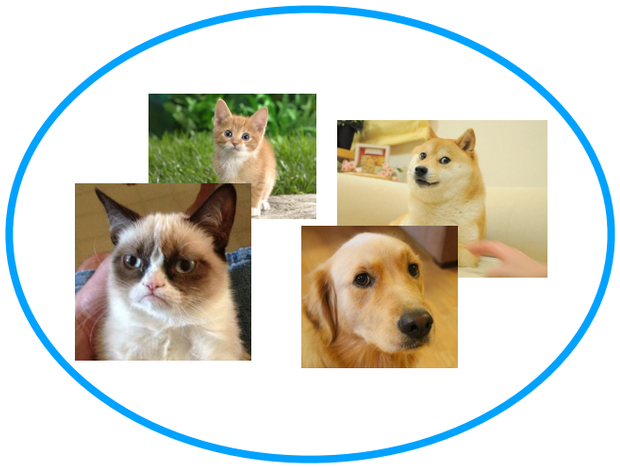
VGG



Out-of-domain data

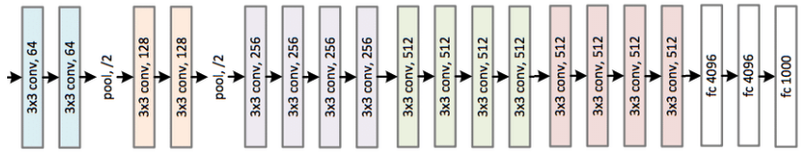
Uncertainty Estimation on out-of-domain data

Training domain



Out-of-domain data

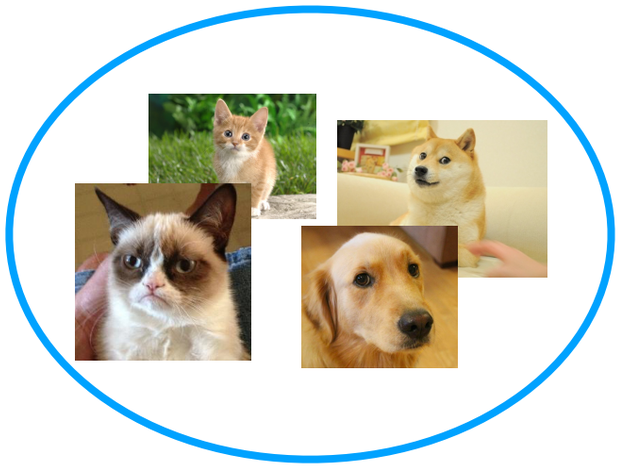
VGG



Cat **Dog**

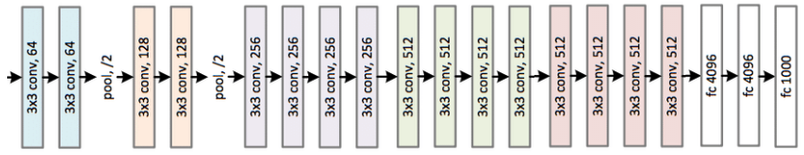
Uncertainty Estimation on out-of-domain data

Training domain



Out-of-domain data

VGG



Cat **Dog**

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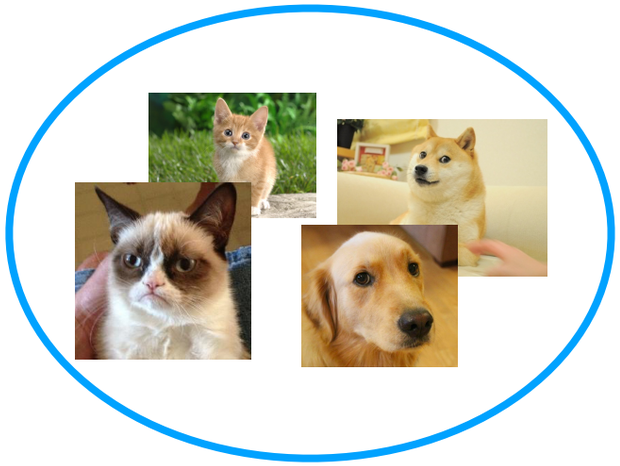
- Dropout
- MNF

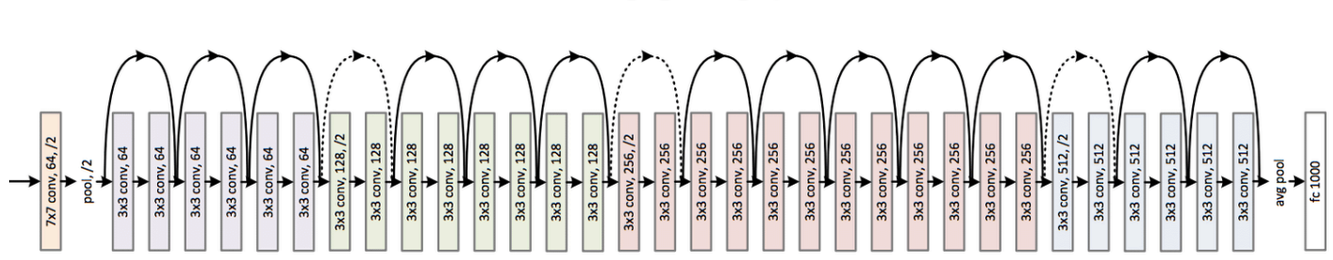
Uncertainty Estimation on out-of-domain data

Training domain



Out-of-domain data

ResNet



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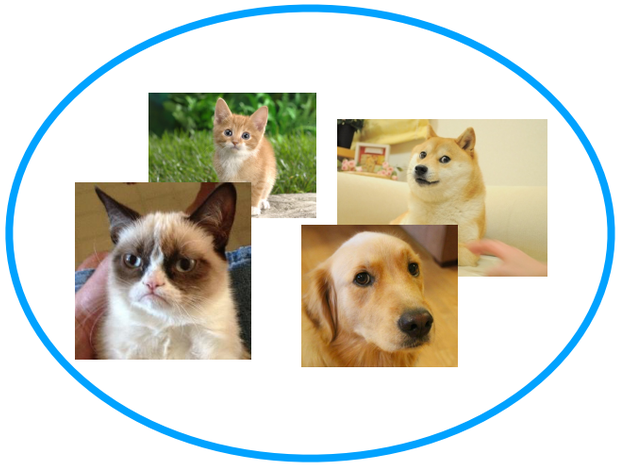
- ~~Dropout~~
- ~~MNF~~

Uncertainty Estimation on out-of-domain data

Training domain



Out-of-domain data

ResNet

Cat **Dog**

+

~~• Dropout~~
~~• MNF~~

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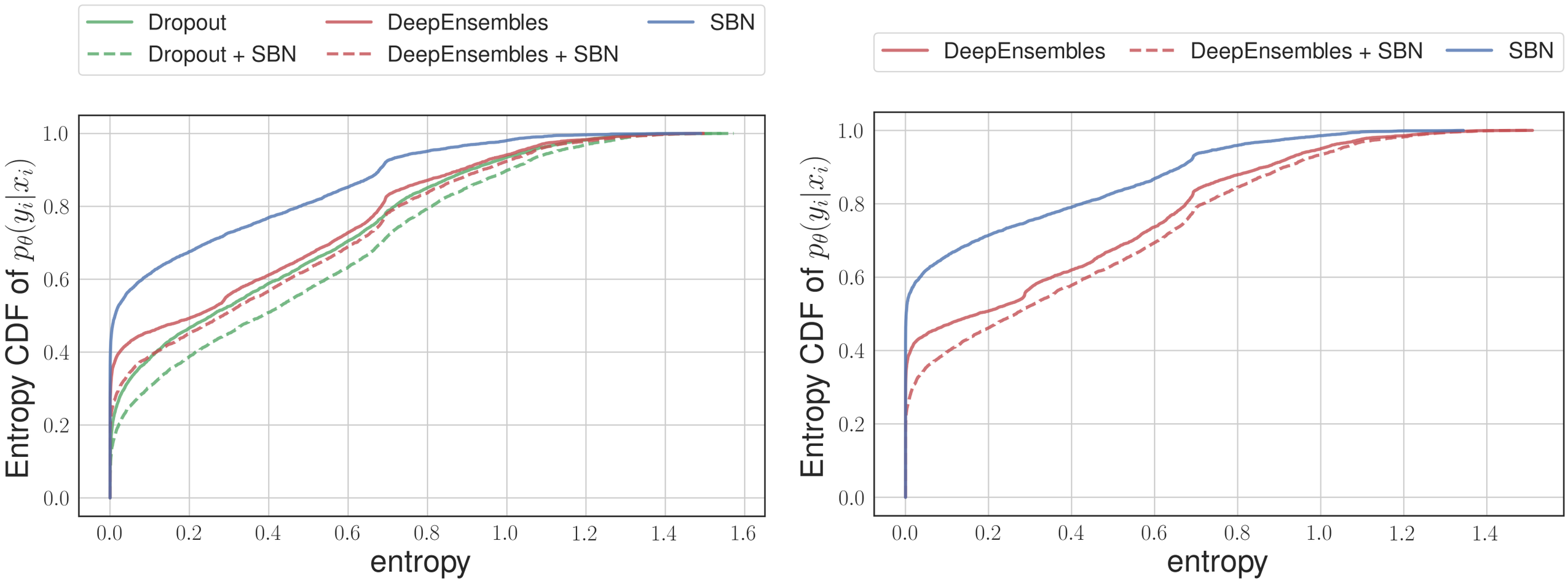
Stochastic Batch Normalization

Stochastic Batch Normalization



Empirical predictive distribution entropy CDF for CIFAR5

Stochastic Batch Normalization

Network	Method	Error%		NLL	
		No SBN	SBN	No SBN	SBN
LeNet-5 MNIST	SBN	—	0.53 ± 0.05	—	0.025 ± 0.003
	Deep Ensembles	0.43 ± 0.00	0.43 ± 0.00	0.015 ± 0.001	0.014 ± 0.001
	Dropout	0.51 ± 0.00	0.49 ± 0.00	0.016 ± 0.000	0.015 ± 0.000
VGG-11 CIFAR5	SBN	—	5.76 ± 0.00	—	0.302 ± 0.002
	Deep Ensembles	$\mathbf{5.18 \pm 0.00}$	5.23 ± 0.00	0.177 ± 0.004	$\mathbf{0.154 \pm 0.002}$
	Dropout	$\mathbf{5.32 \pm 0.00}$	5.38 ± 0.00	0.155 ± 0.001	$\mathbf{0.149 \pm 0.001}$
ResNet-18 CIFAR5	SBN	—	4.35 ± 0.17	—	0.255 ± 0.018
	Deep Ensembles	$\mathbf{3.37 \pm 0.00}$	3.34 ± 0.00	0.138 ± 0.005	$\mathbf{0.110 \pm 0.004}$

Table 1: Test errors (%) and NLL scores for known classes. MNIST for LeNet-5 and CIFAR5 for VGG-11 and ResNet-18. SBN column correspond to methods with all Batch Normalization layers replaced by ours SBN.

Uncertainty estimation via Stochastic Batch Normalization

We proposed:

- Probabilistic model for Batch Normalization.
- Scaleable approximation technique for inference phase.
- Simple and efficient method for uncertainty estimation.

- Check out our paper on arXiv: https://goo.gl/FCMTGQ
- Code available at https://goo.gl/TfMxni
- Submission on ICLR Workshop track: https://goo.gl/tvHyoy