Batch-normalized Deep Boltzmann Machines

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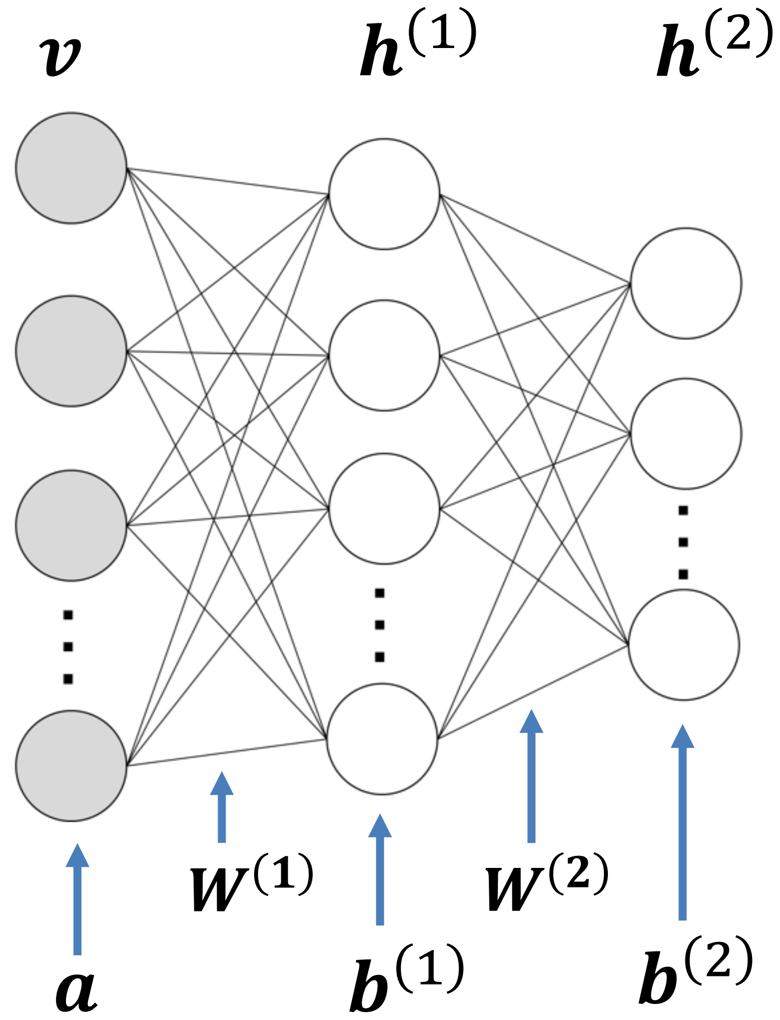
Outline

- Deep Boltzmann Machines (DBMs)
- Problem statement
- Batch normalized DBMs (BNDBMs)
- Experiments
- Conclusion

Deep Boltzmann Machines (DBM)

- Energy-based generative model
  - probabilistic modeling *(Salakhudinov and Hinton, 2009)*
  - feature extraction *(Montavon et al., 2012).*
- Consider a **binary** DBM:
  - 1 visible layer $\boldsymbol{v} \in \{0,1\}^M$
  - 2 hidden layers $\boldsymbol{h} = \{\boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}\}$
    - $h^{(1)} \in \{0,1\}^{K_1}$
    - $h^{(2)} \in \{0,1\}^{K_2}$



Deep Boltzmann Machines (DBM)

Definition: Energy function

$$E\left(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}; \Psi\right) = -\boldsymbol{a}^{\top}\boldsymbol{v} - \boldsymbol{b}^{(1)\top}\boldsymbol{h}^{(1)} - \boldsymbol{b}^{(2)\top}\boldsymbol{h}^{(2)} - \boldsymbol{v}^{\top}\boldsymbol{W}^{(1)}\boldsymbol{h}^{(1)} - \boldsymbol{h}^{(1)\top}\boldsymbol{W}^{(2)}\boldsymbol{h}^{(2)}$$

Joint distribution:

$$p\left(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}; \Psi\right) = \frac{e^{-E\left(\boldsymbol{v}, \boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}; \Psi\right)}}{\mathcal{Z}(\Psi)}$$

Marginal distributions:

$$p\left(\boldsymbol{v}, \boldsymbol{h}^{(1)}; \Psi\right)$$

$$p\left(\boldsymbol{h}^{(1)}, \boldsymbol{h}^{(2)}; \Psi\right)$$

$$p\left(\boldsymbol{v}, \boldsymbol{h}^{(2)}; \Psi\right)$$

Conditional distributions:

$$p\left(\boldsymbol{v} | \boldsymbol{h}^{(1)}; \Psi\right)$$

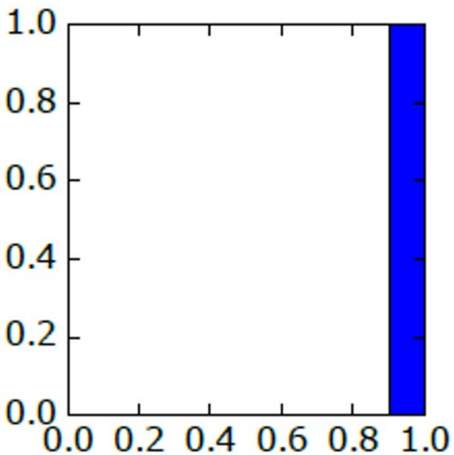
$$p\left(\boldsymbol{h}^{(1)} | \boldsymbol{v}, \boldsymbol{h}^{(2)}; \Psi\right)$$

$$p\left(\boldsymbol{h}^{(2)} | \boldsymbol{h}^{(1)}; \Psi\right)$$

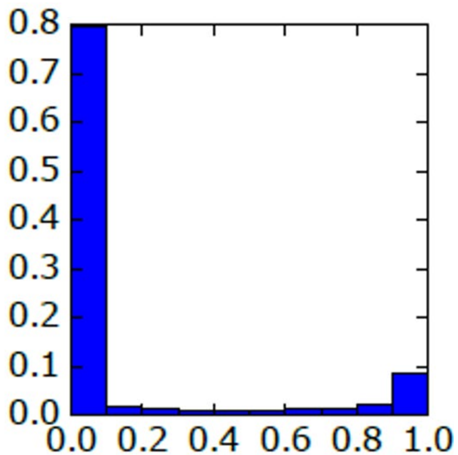
Problem: Internal Covariance Shift

- Hidden states:
  - Degenerate into 0 or 1
  - Not diverse

Hidden Layer 1's states

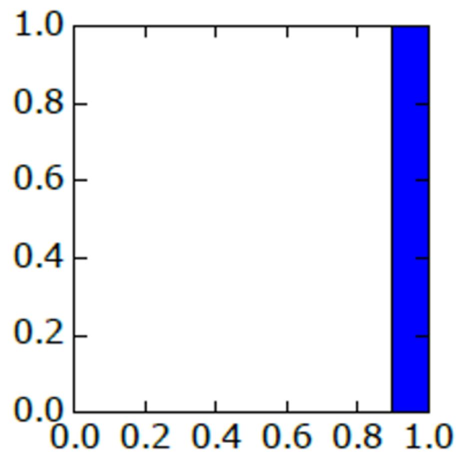


Unit 11

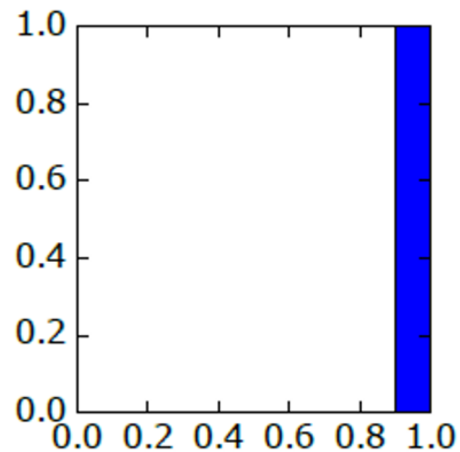


Unit 79

Hidden Layer 2 's states



Unit 17



Unit 100

Idea

- DBM training is also affected by Internal Covariance Shift
- Internal Covariance Shift is successfully solved for CNNs using Batch Normalization [1]
- Not investigated in DBMs

➔ This work:

$\boxed{\text{Investigate Batch Normalization for DBMs}}$

[1] *(Ioffe and Szegedy, 2015)*

Batch-normalization

- Batch Normalization ($\mathcal{B}$)
  - normalizes every dimension i of an input vector $\boldsymbol{x}$
  - normalized vector with zero-mean and unit-variance
  - scaled by γ_i and shifted by β_i

$$\mathcal{B}(x_i) = \gamma_i \frac{x_i - \mathbb{E}[x_i]}{\sqrt{\mathrm{Var}(x_i) + \epsilon}} + \beta_i$$

γ_i: scale parameter
β_i: shift parameter

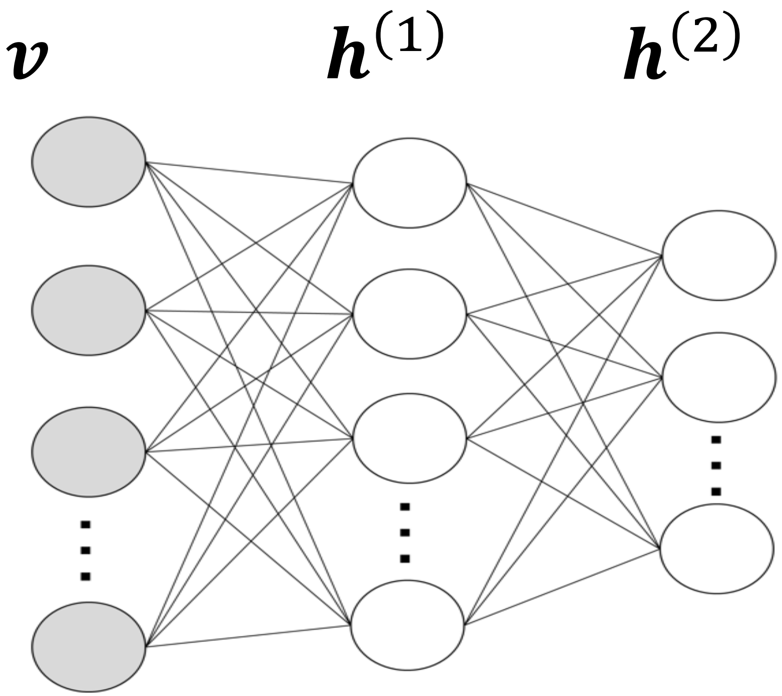
BN in DBMs: challenges

- BN in CNNs (deterministic networks)
  - Add one line of code

```
# code snippet using TensorFlow BN
training = tf.placeholder(tf.bool)
x = tf.layers.dense(input_x, units=100)
x = tf.layers.batch_normalization(x, training=training)
x = tf.nn.relu(x)
```

- BN in DBMs (probabilistic networks)
  - Add one line of code → incorrect
  - Why?

BN in DBMs: challenges



- Conditional distributions:
  - show how the information is passed between layers

$p(\boldsymbol{v}|\boldsymbol{h}^{(1)})$

$p(\boldsymbol{h}^{(1)}|\boldsymbol{v},\boldsymbol{h}^{(2)})$

$p(\boldsymbol{h}^{(2)}|\boldsymbol{h}^{(1)})$

$$\begin{cases} \mu_i^{(2)} = \sigma(b_i^{(2)} + \boldsymbol{h}^{(1)\top}\boldsymbol{w}_{.i}^{(1)}) \\ h_i^{(2)} \sim \text{Bernoulli}(\mu_i^{(2)}) \end{cases}$$

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

BN in DBMs: challenges

- Conditional distribution:
  - show how the information is passed between layers
  - BN in DBM: new conditional distribution

$$\mu_i^{(2)} = \sigma(b_i^{(2)} + \boldsymbol{h}^{(1)\top}\boldsymbol{w}_{.i}^{(1)})$$

$$\downarrow$$

$$\mu_i^{(2)} = \sigma(\mathcal{B}(b_i^{(2)} + \boldsymbol{h}^{(1)\top}\boldsymbol{w}_{.i}^{(1)}))$$

$$p(\boldsymbol{h}^{(2)}|\boldsymbol{h}^{(1)}) \begin{cases} \mu_i^{(2)} = \sigma(b_i^{(2)} + \boldsymbol{h}^{(1)\top}\boldsymbol{w}_{.i}^{(1)}) \\ h_i^{(2)} \sim \mathrm{Bernoulli}(\mu_i^{(2)}) \end{cases} \qquad \sigma(x) = \frac{1}{1+e^{-x}}$$

BN in DBMs: challenges

Definition: Energy function E

↓

Joint distribution

↓

Marginal distributions

↓

$\boxed{\text{Conditional distributions}}$

- Conditional distribution:
  - show how the information is passed between layers
  - BN in DBM: **new** conditional distribution

➔ New energy function
  - change the whole model

Batch-normalized DBMs (BNDBMs)

- Standard energy function E (DBMs):

$$E\left(\boldsymbol{v},\boldsymbol{h}^{(1)},\boldsymbol{h}^{(2)};\boldsymbol{\Psi}\right)=-\boldsymbol{a}^{\top}\boldsymbol{v}-\boldsymbol{b}^{(1)\top}\boldsymbol{h}^{(1)}-\boldsymbol{b}^{(2)\top}\boldsymbol{h}^{(2)}-\boldsymbol{v}^{\top}\boldsymbol{W}^{(1)}\boldsymbol{h}^{(1)}-\boldsymbol{h}^{(1)\top}\boldsymbol{W}^{(2)}\boldsymbol{h}^{(2)}$$

- Proposed energy function E_{BN} (BNDBMS)

$$E_{BN}\left(v,\boldsymbol{h}^{(1)},\boldsymbol{h}^{(1)};\boldsymbol{\Gamma}\right)=-\sum_{i=1}^{M}a_i v_i-\sum_{l=1}^{2}\sum_{j=1}^{K_l}\left(\bar{\gamma}_j^{(l)}\bar{b}_j^{(l)}+\bar{\beta}_j^{(l)}\right)h_j^{(l)}$$
$$-\sum_{i=1}^{M}\sum_{j=1}^{K_1}\bar{\gamma}_j^{(1)}v_i w_{ij}^{(1)}h_j^{(1)}-\sum_{i=1}^{K_1}\sum_{j=1}^{K_2}\bar{\gamma}_i^{(1)}\,\bar{\gamma}_j^{(2)}h_i^{(1)}w_{ij}^{(2)}h_j^{(2)}$$

$\bar{\gamma}_i^{(l)}$ and $\bar{\beta}_i^{(l)}$: BN coefficients of the i^{th} neuron at the l^{th} layer

Batch-normalized DBMs (BNDBMs)

- Batch-normalized conditional distributions

$$p\left(v_m = 1 \middle| \boldsymbol{h}^{(1)}\right) = \sigma\left(a_m + \sum_{j=1}^{K_1} \bar{\gamma}_j^{(1)} w_{mj}^{(1)} h_j^{(1)}\right)$$

(No BN at visible layer)

$$p(h_n^{(1)} = 1|\boldsymbol{h}^{(2)}) = \sigma\left(\mathcal{B}_1(t_n^{(1)})\right)$$

$$t_n^{(1)} = b_n^{(1)} + \sum_{j=1}^{M} v_j \; w_{jn}^{(1)} + \sum_{j=1}^{K_2} \bar{\gamma}_j^{(2)} w_{nj}^{(2)} h_j^{(2)}$$

layer's input

$$p(h_n^{(2)} = 1|\boldsymbol{h}^{(1)}) = \sigma\left(\mathcal{B}_2(t_n^{(2)})\right)$$

$$t_n^{(2)} = b_n^{(2)} + \sum_{j=1}^{K_1} \bar{\gamma}_j^{(1)} h_j^{(1)} w_{jn}^{(2)}$$

layer's input

BNDBM – Model learning

- BNDBM training
  - same as vanilla DBMs
  - maximizing data log-likelihood

- Gradient of the log-likelihood

$$\boldsymbol{\nabla_{\Gamma} \log \mathcal{L}} = \mathbb{E}_{\text{data}}\left[-\frac{\partial E_{BN}}{\partial \Gamma}\right] - \mathbb{E}_{\text{model}}\left[-\frac{\partial E_{BN}}{\partial \Gamma}\right]$$

- Parameters Γ update

$$\Gamma = \Gamma + \eta \Delta \Gamma$$

Experiments

- **Datasets**: MNIST[1], Fashion-MNIST[2] and Caltech 101 Silhouette[3]
- **Network structures**: 784-500-100 and 784-500-500[4]
- **Training methods:**
  - Persistent Contrastive Divergence[5] (PCD)
  - Contrastive Divergence[6] (CD) without sampling step
- **Training settings**:
  - Batch size: 100, #Gibbs chains: 100, learning rate: 0.01, epochs: 500
  - BN parameters: learnable γ and $\beta = 0$

[1](Lecun et al., 1998), [2] (Xiao et al., 2017) , [3] (Marlin et al., 2010), [4](Montavon and Muller, 2012; Melchior et al., 2016), [5](Tieleman, 2008), [6](Hinton, 2002)

Experiments: Classification

- Classification evaluation:
  - train DBMs in unsupervised manner (without label information)
  - use the last hidden layer as features
  - train a Logistic Regression classifier
- Run 10 times

Experiments: Classification

Classification ↑	PCD (500-100)			PCD (500-500)			CD^{prob}(500-100)		
Pretraining	**DBM**	**cDBM**	**BNDBM**	**DBM**	**cDBM**	**BNDBM**	**DBM**	**cDBM**	**BNDBM**
MNIST	94.81 ±0.58	93.89 ±0.19	**95.37** ±0.19	96.68 ±0.36	96.63 ±0.15	**96.80** ±0.11	11.35 ±0.00	85.56 ±3.25	**90.31** ±0.002
Fashion-MNIST	81.27 ±1.07	73.60 ±2.7	**81.66** ±0.76	69.88 ±8.79	83.07 ±0.40	**84.70** ±0.38	15.92 ±6.60	71.97 ±2.12	**72.67** ±2.59
Caltech 101 Silhouette	65.27 ±0.24	58.39 ±0.58	**65.63** ±0.25	66.54 ±0.65	65.96 ±0.42	**69.20** ±0.45	28.08 ±3.13	54.40 ±0.99	**62.94** ±0.19
No pretraining	**DBM***	**cDBM***	**BNDBM***	**DBM***	**cDBM***	**BNDBM***	**DBM***	**cDBM***	**BNDBM***
MNIST	11.35 ±0.00	84.35 ±2.13	**93.81** ±0.58	12.22 ±2.74	94.05 ±0.08	**96.50** ±0.11	25.32 ±11.84	61.84 ±3.42	**85.73** ±0.81
Fashion-MNIST	16.14 ±9.91	71.64 ±1.15	**76.26** ±1.20	35.66 ±8.39	**82.27** ±0.27	78.75 ±0.99	12.31 ±0.66	68.25 ±3.19	**71.92** ±1.09
Caltech 101 Silhouette	19.77 ±4.78	54.70 ±0.78	**59.45** ±1.20	23.65 ±1.20	64.63 ±8.12	**66.80** ±0.69	35.34 ±3.98	55.95 ±0.79	**60.99** ±0.31
Our average improvement	**vs DBM**	**vs cDBM**		**vs DBM**	**vs cDBM**		**vs DBM**	**vs cDBM**	
Pretraining	0.44	5.60		5.86	1.67		56.95	4.76	
No pretraining	60.75	6.28		56.86	0.38		48.56	10.87	

➔ Better classification accuracy

*: no pretraining
Bold: best number
Underlined: next best

positive signs: better
negative signs: worse

Experiments: Reconstruction

- Reconstruction improvement evaluation
  - DBM/cDBM's reconstruction error - BNDBM's reconstruction error

Reconstruction	PCD (500-100)		PCD (500-500)		CD^{prob}(500-100)	
Average improvement	**vs DBM**	**vs cDBM**	**vs DBM**	**vs cDBM**	**vs DBM**	**vs cDBM**
Pretraining	-1.13	-1.50	-0.59	-0.64	**0.29**	**1.55**
No pretraining	-0.98	-1.86	**1.02**	-1.34	**0.06**	**3.57**

Bold/positive values: better

➔ Comparable reconstruction

1) Training facilitation

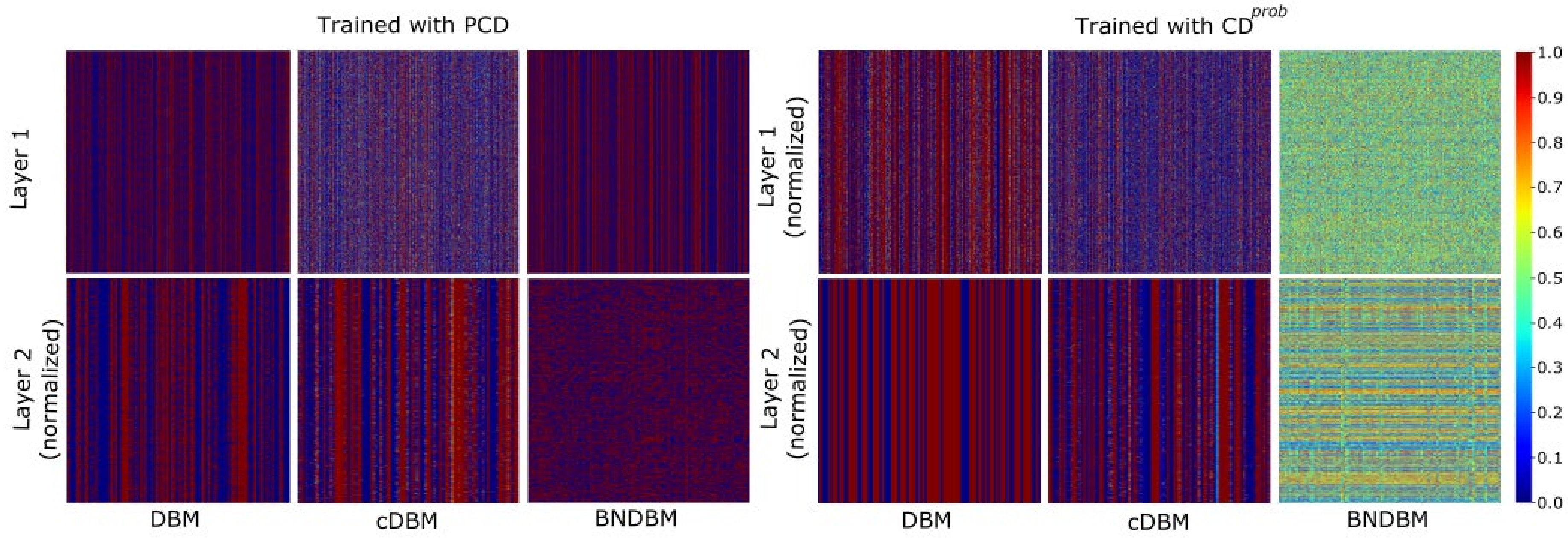
- DBMs and cDBMs
  - require pretraining
  - unsuccessfully train DBMs without pretraining
- BNDBMs
  - train without pretraining
  - 5.84% better than no-pretraining cDBMs

→ easy to train

Classification ↑	PCD (500-100)		
Pretraining	**DBM**	**cDBM**	**BNDBM**
MNIST	94.81 ±0.58	93.89 ±0.19	**95.37** ±0.19
Fashion-MNIST	81.27 ±1.07	73.60 ±2.7	**81.66** ±0.76
Caltech 101 Silhouette	65.27 ±0.24	58.39 ±0.58	**65.63** ±0.25
No pretraining	**DBM***	**cDBM***	**BNDBM**
MNIST	11.35 ±0.00	84.35 ±2.13	**93.81** ±0.58
Fashion-MNIST	16.14 ±9.91	71.64 ±1.15	**76.26** ±1.20
Caltech 101 Silhouette	19.77 ±4.78	54.70 ±0.78	**59.45** ±1.20
Our average improvement	**vs DBM**	**vs cDBM**	
Pretraining	0.44	5.60	
No pretraining	60.75	6.28	

2) Feature representation improvement

- 10,000 MNIST test samples vs hidden units (network 500-100)



- DBMs and cDBMs
  - vertical homogeneous strips → neurons respond to all data in a similar way
- BNDBMs
  - random/heterogeneous patterns → neurons are distinguishing data samples

→richer and more distinctive representation

Conclusion

- **Finding**
  - Internal Covariance Shift in DBM training
- **Solution**
  - Derive Batch Normalization for DBM
    - Via new energy function E_{BN}
- **Experiments**
  - Better classification and comparable reconstruction
  - Meaningful learning representations
  - No pretraining required
- **Analysis**: How to use BN in DBM efficiently (*more details in paper*)

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Question

THANK YOU