Theoretical Remarks on Deep Belief Networks

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Disclaimer

All the theoretical results presented here go against Geoff's intuitions. As there is a strong prior on where the truth lies, this presentation should be considered as pure entertainment.

Motivation

- Justify the CD criterion with theoretical results
- Take advantage of the knowledge of the final number of layers in the DBN

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Why CD is a good thing?



• $p(\mathbf{h}^1)$ is the marginal associated to the RBM.

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- Ithe best weights are those who maximize

$$\mathit{ML} = \sum_{\mathbf{v}} p_0(\mathbf{v}) \log \left(\sum_{\mathbf{h}^1} p\left(\mathbf{v}, \mathbf{h}^1
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Why CD is a good thing?



- p(h¹) is the marginal associated to the RBM.
 - the best weights are those who maximize

$$\mathit{ML} = \sum_{\mathbf{v}} p_0(\mathbf{v}) \log \left(\sum_{\mathbf{h}^1} p\left(\mathbf{v}, \mathbf{h}^1
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maximizing ML leads to good features

Why CD is a good thing?



What are the "problems" of CD?





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What are the "problems" of CD?







p(h¹) is NOT the marginal associated to the RBM
CD is a "trick" to speed up training and reduce variance

 W^1



Why the greedy procedure?

() There are strong dependencies between W^1 , W^2 , ...

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Why the greedy procedure?

- **(**) There are strong dependencies between W^1 , W^2 , ...
- The obtained solution leads to good features

Why the greedy procedure?

- **(**) There are strong dependencies between W^1 , W^2 , ...
- The obtained solution leads to good features
- Could we remove the dependencies between the W's?

The variational bound



The variational bound



The variational bound



Optimal model distribution

$$p^{*}(\mathbf{h}^{1}) = \sum_{\mathbf{v}_{0}} p_{0}(\mathbf{v}_{0})Q(\mathbf{h}^{1}|\mathbf{v}_{0})$$

$$p^{*}(\mathbf{v}) = \sum_{\mathbf{h}^{1}} p^{*}(\mathbf{h}^{1})P(\mathbf{v}|\mathbf{h}^{1})$$

$$p^{*}(\mathbf{v}) = \sum_{\mathbf{h}^{1}} \sum_{\mathbf{v}_{0}} p_{0}(\mathbf{v}_{0})Q(\mathbf{h}^{1}|\mathbf{v}_{0})P(\mathbf{v}|\mathbf{h}^{1})$$

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One-step RBM



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One-step RBM



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One-step RBM



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One-step RBM



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- Solution Minimizing the likelihood is minimizing $KL(p_0||p_1)$

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One-step RBM



- $p^*(\mathbf{v}_1) = \sum_{\mathbf{h}^1} \sum_{\mathbf{v}_0} p_0(\mathbf{v}_0) Q(\mathbf{h}^1 | \mathbf{v}_0) P(\mathbf{v}_1 | \mathbf{h}^1)$
- **2** $p^*(\mathbf{v}_1) = p_1(\mathbf{v}_1)$
- Solution Minimizing the likelihood is minimizing $KL(p_0||p_1)$
- $KL(p_0||p_1) \approx KL(p_0||p_\infty) KL(p_1||p_\infty)$

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One-step RBM



- $p^*(\mathbf{v}_1) = \sum_{\mathbf{h}^1} \sum_{\mathbf{v}_0} p_0(\mathbf{v}_0) Q(\mathbf{h}^1 | \mathbf{v}_0) P(\mathbf{v}_1 | \mathbf{h}^1)$
- 2 $p^*(\mathbf{v}_1) = p_1(\mathbf{v}_1)$
- Solution Minimizing the likelihood is minimizing $KL(p_0||p_1)$
- $KL(p_0||p_1) \approx KL(p_0||p_\infty) KL(p_1||p_\infty)$
- **()** Exact gradient does not depend on $p_{\infty} \Longrightarrow$ fast !

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And then?



 $W^\ell \ddagger$



If we had the best marginal p*(h¹), we'd have the perfect W¹

 $W^{\ell-1}$



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And then?

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 $W^\ell \ddagger$



- If we had the best marginal $p^*(\mathbf{h}^1)$, we'd have the perfect W^1
- 2 Let's try to be as close as $p^*(\mathbf{h}^1)$ as possible

 W^1



And then?



 $W^\ell \ddagger$



- If we had the best marginal $p^*(\mathbf{h}^1)$, we'd have the perfect W^1
- 2 Let's try to be as close as $p^*(\mathbf{h}^1)$ as possible
- p*(h¹) is exactly what we obtain if we clamp the empirical distribution and go through W¹

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- Continue until the last layer



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- 2 Let's try to be as close as $p^*(\mathbf{h}^1)$ as possible
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- Continue until the last layer
- Train it using CD (it is a usual RBM)

A few problems

• $p^*(\mathbf{h}^1)$ is obtained using the variational bound and not the true likelihood

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- p* (h¹) is obtained using the variational bound and not the true likelihood
- Minimizing $KL(p^*(\mathbf{h}^1) || p(\mathbf{h}^1))$ does not guarantee to improve the variational bound

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A few problems

- p* (h¹) is obtained using the variational bound and not the true likelihood
- Ominimizing $KL(p^*(\mathbf{h}^1) || p(\mathbf{h}^1))$ does not guarantee to improve the variational bound
- Could we adapt that framework such that the guarantee remains?

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Using a very big top hidden layer



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Using a very big top hidden layer

 $W^{\ell+1}$

 W^1

 W^1



- **()** Any marginal on \mathbf{h}^{ℓ}
- Solution Maximizing the likelihood of the data needs minimizing $\mathcal{K}L\left(p_{0}^{0}||p_{\ell}^{0}\right)\longrightarrow \mathcal{W}^{1}$



Using a very big top hidden layer (2)

VeryBigLayer

 $W^{\ell+1}$



• Compute $p_0^1(\mathbf{h}^1)$ from $p_0^0(\mathbf{v})$ and W^1

 W^2

 W^2



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Using a very big top hidden layer (2)

VeryBigLayer

 $W^{\ell+1}$



 W^2

• Compute $p_0^1(\mathbf{h}^1)$ from $p_0^0(\mathbf{v})$ and W^1 • Minimize $KL\left(p_0^1(\mathbf{h}^1)||p_{\ell-1}^1(\mathbf{h}^1)\right)$

 W^2



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Using a very big top hidden layer (2)

VeryBigLayer

 $W^{\ell+1}$

 W^2

 M^2



- **(**) Compute $p_0^1(\mathbf{h}^1)$ from $p_0^0(\mathbf{v})$ and W^1
- **2** Minimize $KL\left(p_0^1(\mathbf{h}^1)||p_{\ell-1}^1(\mathbf{h}^1)\right)$
- Iterate

$$h^1$$

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Layers are regularizers



 $W^{\ell+1}$

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• We have any marginal on \mathbf{h}^{ℓ}

 W^1

 W^1



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Layers are regularizers

VeryBigLayer

 $W^{\ell+1}$.

$$\mathbf{h}^{\ell}$$

 W^1

 W^1

- **(**) We have any marginal on \mathbf{h}^{ℓ}
- ② This architecture suggests memorizing high-level features



Layers are regularizers

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VeryBigLayer

 $W^{\ell+1}$

$$\mathbf{h}^{\ell}$$

 $W^1 \downarrow$: $W^1 \downarrow$

 h^1

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This architecture suggests memorizing high-level features

To sample, you just need to do a forward-backward pass

Layers are regularizers

VeryBigLayer

 $W^{\ell+1}$



 W^{1}

- ${f 0}$ We have any marginal on ${f h}^\ell$
 - This architecture suggests memorizing high-level features
 - To sample, you just need to do a forward-backward pass
 - Going through the layers adds noise and regularizes



Summary and Conclusion

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 - A new ungreedy training procedure for the DBN
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 - Can we use the ML instead of the variational bound to find p* (hⁱ)?
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 - $\textcircled{\sc 0}$ What is the set of distributions we can model with a $\ell\text{-layer}$ DBN?
 - Why do I keep getting results opposed to what Geoff finds?