Theoretical Remarks on Deep Belief Networks

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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

1. Justify the CD criterion with theoretical results
2. Take advantage of the knowledge of the final number of layers in the DBN
Why CD is a good thing?

\[ p(h^1) \] is the marginal associated to the RBM.
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\[ \text{the best weights are those who maximize} \]

\[ ML = \sum_v p_0(v) \log \left( \sum_{h^1} p(v, h^1) \right) \]
**Why CD is a good thing?**

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2. The best weights are those who maximize
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   \]
3. Maximizing ML leads to good features.
Why CD is a good thing?

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2. the best weights are those who maximize
   \[ ML = \sum_v p_0(v) \log \left( \sum_{h^1} p(v, h^1) \right) \]
3. maximizing ML leads to good features
4. CD is faster than ML
What are the “problems” of CD?

\[ p(h^1) \text{ is NOT the marginal associated to the RBM} \]
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\[ p(h^1) \text{ is NOT the marginal associated to the RBM} \]

\[ \text{CD is a “trick” to speed up training and reduce variance} \]
Why the greedy procedure?

1. There are strong dependencies between $W^1$, $W^2$, ...
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2. The obtained solution leads to good features
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1. There are strong dependencies between $W^1$, $W^2$, ...
2. The obtained solution leads to good features

- Could we remove the dependencies between the $W$'s?
The variational bound

Variational bound:

\[ p(v) \geq C(W^1) + \sum_{h^1} \sum_{v_0} p_0(v_0) Q(h^1|v_0) \log p(h^1) \]

\[ p^*(h^1) = \sum_{v_0} p_0(v_0) Q(h^1|v_0) \]
The variational bound

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The variational bound

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  \[ p(v) \geq C(W^1) + \sum_{h^1} \sum_{v_0} p_0(v_0) Q(h^1 | v_0) \log p(h^1) \]
  \[ p^*(h^1) = \sum_{v_0} p_0(v_0) Q(h^1 | v_0) \]

- Given \( p(h^1) \), \( W^1 \) is independent from the other \( W \)
- What is the best \( W^1 \)?
Optimal model distribution

\[ p^*(h^1) = \sum_{v_0} p_0(v_0) Q(h^1|v_0) \]

\[ p^*(v) = \sum_{h^1} p^*(h^1) P(v|h^1) \]

\[ p^*(v) = \sum_{h^1} \sum_{v_0} p_0(v_0) Q(h^1|v_0) P(v|h^1) \]
One-step RBM

\[ v_0 \xrightarrow{W} h^1 \xrightarrow{W^T} v_1 \]
One-step RBM

\[ p^*(v_1) = \sum_{h^1} \sum_{v_0} p_0(v_0) Q(h^1|v_0) P(v_1|h^1) \]
One-step RBM

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2. \( p^*(v_1) = p_1(v_1) \)
3. Minimizing the likelihood is minimizing \( KL(p_0||p_1) \)
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4. \( KL(p_0||p_1) \approx KL(p_0||p_\infty) - KL(p_1||p_\infty) \)
One-step RBM

\[ p^*(v_1) = \sum_{h^1} \sum_{v_0} p_0(v_0) Q(h^1 | v_0) P(v_1 | h^1) \]

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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 \( p_\infty \) \( \implies \) fast!
And then?

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Continue until the last layer.
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2. Let’s try to be as close as $p^*(h^1)$ as possible.
3. $p^*(h^1)$ is exactly what we obtain if we clamp the empirical distribution and go through $W^1$.
4. Continue until the last layer.
5. Train it using CD (it is a usual RBM).
A few problems

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2. Minimizing $KL(p^*(h^1) \| p(h^1))$ does not guarantee to improve the variational bound

• Could we adapt that framework such that the guarantee remains?
Using a very big top hidden layer

**VeryBigLayer**

\[ W^{\ell+1} \]

\[ h^{\ell} \]

Any marginal on \( h^{\ell} \)

\[ W^1 \]

\[ \vdots \]

\[ W^1 \]

\[ V \]
Using a very big top hidden layer

Any marginal on $h^\ell$

Maximizing the likelihood of the data needs minimizing $KL (p_0^\ell || p_0) \rightarrow W^1$

1. VeryBigLayer

$W^{\ell+1}$

$h^\ell$

$W^1$

...
Using a very big top hidden layer (2)

Compute $p_0^1(h^1)$ from $p_0^0(v)$ and $W^1$
Using a very big top hidden layer (2)

VeryBigLayer

\[ W^{\ell+1} \]

\[ h^\ell \]

\[ W^2 \]

\[ \vdots \]

\[ W^2 \]

\[ h^1 \]

1. Compute \( p_0^1(h^1) \) from \( p_0^0(v) \) and \( W^1 \)

2. Minimize \( KL(p_0^1(h^1) || p_{\ell-1}^1(h^1)) \)
Using a very big top hidden layer (2)

1. Compute $p_0^1(h^1)$ from $p_0^0(v)$ and $W_1^1$
2. Minimize $KL(p_0^1(h^1) || p_{\ell-1}^1(h^1))$
3. Iterate
Layers are regularizers

VeryBigLayer

\[ W^{\ell+1} \]

\[ h^\ell \]

\[ W^1 \]

\[ \vdots \]

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\[ h^1 \]

We have any marginal on \( h^\ell \)
Layers are regularizers

VeryBigLayer

\[ W^{\ell+1} \]
\[ h^{\ell} \]
\[ W^1 \]
\[ h^1 \]

1. We have any marginal on \( h^\ell \)
2. This architecture suggests memorizing high-level features
Layers are regularizers

VeryBigLayer

$W^{\ell+1} \uparrow$

$h^\ell$

$W^1 \downarrow$

$h^1$

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3. To sample, you just need to do a forward-backward pass
Layers are regularizers

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\[ h^\ell \]

\[ W^1 \]

\[ h^1 \]

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2. This architecture suggests memorizing high-level features
3. To sample, you just need to do a forward-backward pass
4. Going through the layers adds noise and regularizes
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  2. Do we have the same guarantee as with ML?
  3. What is the set of distributions we can model with a $\ell$-layer DBN?
  4. Why do I keep getting results opposed to what Geoff finds?