Learning and Inference in Deep, Unsupervised Neural Networks

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Aalto University
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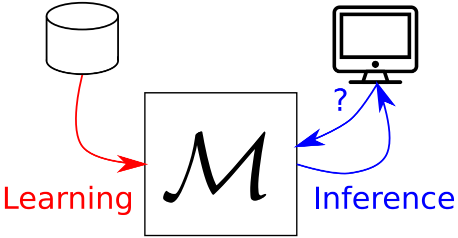
Boltzmann machines? I remember working on them in 80s and 90s..

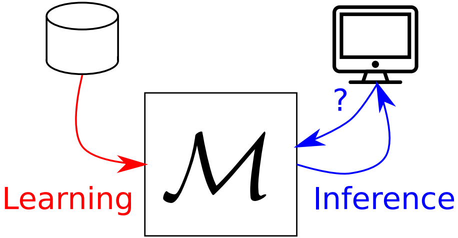
– Anonymous, 2011
paraphrased

Machine Learning in a Single Slide



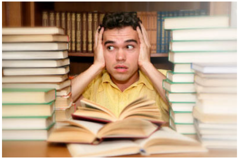
1. Let the model $\mathcal{M}$ *learn* the data D
2. Let the model $\mathcal{M}$ *infer* unknown quantities

Examples

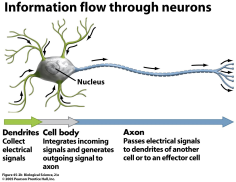


Data	Query
Movie Ratings	Will a user X like a movie Y?
Tagged Images	Is a cat in this image?
Transcribed Speech	What is this person saying?
Parallel Corpora	What is “moi” in English?

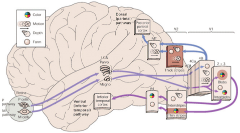
Deep Learning in a Single Slide



Learn massive data

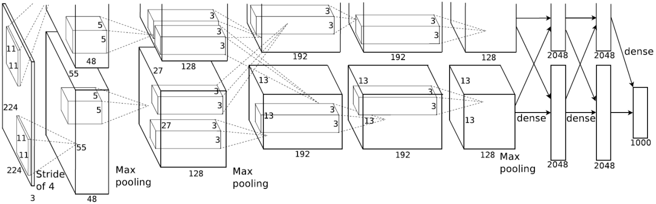


simple functions



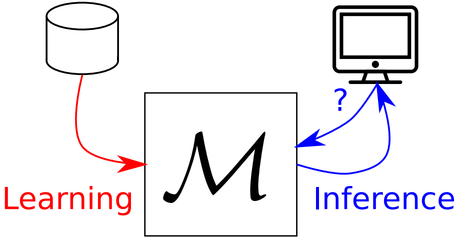
(Van Essen&Gallant, 1994)

Multi-layered



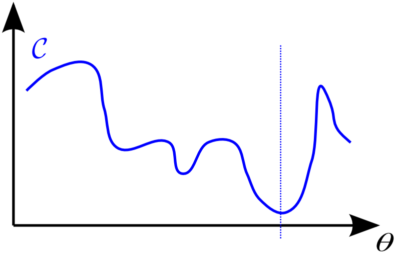
(Krizhevsky et al., 2012)

Challenges in Machine Learning



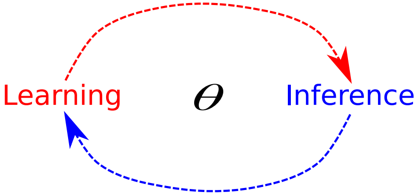
1. Learning is *not* trivial
2. Learning and inference are *not* separate

Learning Difficulties



- True cost $\mathcal{C}$ is *not* available: Only empirical cost $\tilde{\mathcal{C}}$ available
- Often, non-convex optimization with many local/apparent minima
- Impractical to compute either $\mathcal{C}$ or $\tilde{\mathcal{C}}$, as $|D| \to \infty$

Vicious Cycle or Virtuous Cycle?



Example: MLE for feedforward neural networks

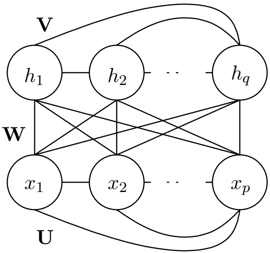
$$\min_{\boldsymbol{\theta}} \mathcal{C}(\boldsymbol{\theta}) \approx \min_{\boldsymbol{\theta}} \tilde{\mathcal{C}}(\boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} -\frac{1}{N} \sum_{(\mathbf{x},t)\in D} \log p(y = t \mid \mathbf{x}, \boldsymbol{\theta})$$

What gets worse with *deep* learning?

- Learning
  - No access to $\mathcal{C}$, but only to $\tilde{\mathcal{C}}$
  - Highly entangled inference and learning
  - **High-dimensional**
  - **Non-convex with a lot of local (apparent) minima**
  - **Intractable to compute even** $\tilde{\mathcal{C}}$, because $|D| \to \infty$
- Inference
  - **No analytical expression**, often
  - **Intractable to compute**, often
  - Difficult to analyze and understand

Deep, Unsupervised Neural Networks
Boltzmann Machines and Autoencoders

Boltzmann Machines



Popular variants:

- If $\mathbf{V} = \mathbf{0}$ and $\mathbf{U} = \mathbf{0}$, restricted Boltzmann machine (RBM)
- If $\mathbf{U} = \mathbf{0}$ and layered $\mathbf{h}$, deep Boltzmann machine (DBM)

1. Negative energy over $\mathbf{x}$ and $\mathbf{h}$:

$$-E(\mathbf{x}, \mathbf{h} \mid \boldsymbol{\theta}) = \mathbf{b}^\top \mathbf{x} + \mathbf{c}^\top \mathbf{h} + \mathbf{x}^\top \mathbf{W} \mathbf{h} + \frac{1}{2} \mathbf{x}^\top \mathbf{U} \mathbf{x} + \frac{1}{2} \mathbf{h}^\top \mathbf{V} \mathbf{h}$$

2. Probability over $\mathbf{x}$ and $\mathbf{h}$:

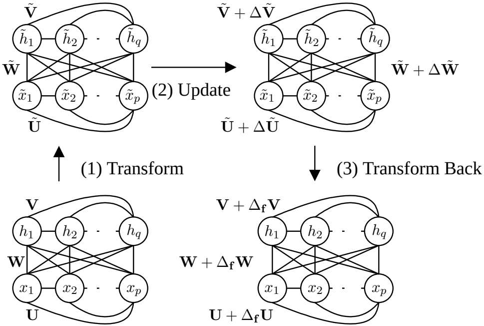
$$p(\mathbf{x}, \mathbf{h} \mid \boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \exp\left\{-E\left(\mathbf{x}, \mathbf{h} \mid \boldsymbol{\theta}\right)\right\}$$

3. Learn $p(\mathbf{x})$ by maximizing

$$\mathcal{L}(\boldsymbol{\theta}) = \mathbb{E}_{\mathbf{x} \in D}\left[\log \frac{1}{Z(\boldsymbol{\theta})} \sum_{\mathbf{h}} e^{-E(\mathbf{x}, \mathbf{h} \mid \boldsymbol{\theta})}\right]$$

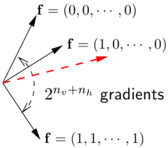
with stochastic gradient descent

Learning: Observations

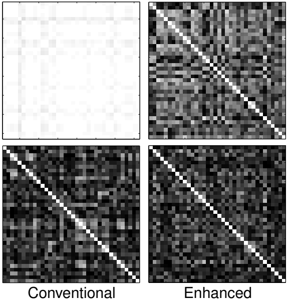


- Invariant to bit-flipping transformation
- 2^{p+q} descent directions
- leading to (potentially all) different solutions
- Which direction?
- How to tractably decide?

Learning: Enhanced Gradient



Covariance of Weight Updates



- Importance/weight of each direction $\nabla_{\mathbf{f}} \mathcal{L}$

$$\prod_{k=1}^{n_v+n_h} \langle x_k \rangle_{\mathrm{dm}}^{f_k} \left(1 - \langle x_k \rangle_{\mathrm{dm}}\right)^{1-f_k}$$

- Weighted sum of all possible updates

$$\nabla_e w_{ij} = \mathrm{Cov}_{\mathrm{d}}\left(x_i, h_j\right) - \mathrm{Cov}_{\mathrm{m}}\left(x_i, h_j\right)$$

$$\nabla_e b_i = \langle x_i \rangle_{\mathrm{d}} - \langle x_i \rangle_{\mathrm{m}} - \sum_j \langle h_j \rangle_{\mathrm{dm}} \nabla_e w_{ij}$$

$$\nabla_e c_j = \langle h_j \rangle_{\mathrm{d}} - \langle h_j \rangle_{\mathrm{m}} - \sum_i \langle x_i \rangle_{\mathrm{dm}} \nabla_e w_{ij}$$

Learning vs. Inference

- Boltzmann machine learning requires inference.

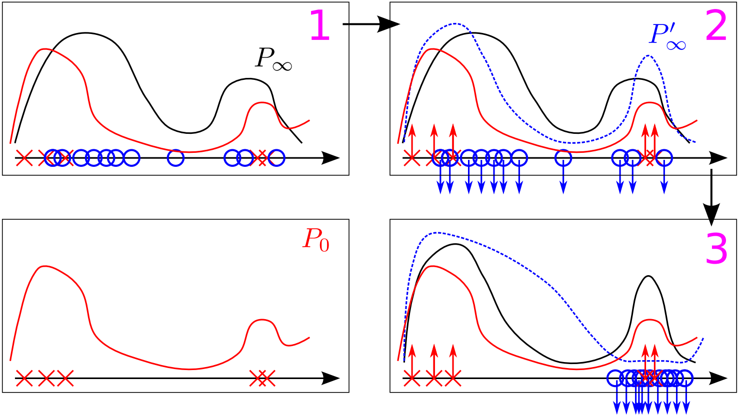
$$\nabla_e w_{ij} = \mathrm{Cov_d}\left(x_i, h_j\right) - \mathrm{Cov_m}\left(x_i, h_j\right)$$

- *What is the covariance between x_i and h_j with the current $\boldsymbol{\theta}$?*
  - NP-Hard problem even in the case of RBMs (Long&Servedio, 2010)
  - Monte Carlo approximation with persistent MCMC

$$\mathrm{Cov_m}\left(x_i, h_j\right) \approx \left(\frac{1}{N}\sum_{n=1}^{N} x_i^{(n)} h_j^{(n)}\right) - \left(\frac{1}{N}\sum_{n=1}^{N} x_i^{(n)}\right)\left(\frac{1}{N}\sum_{n=1}^{N} h_j^{(n)}\right)$$

  - Gibbs sampling

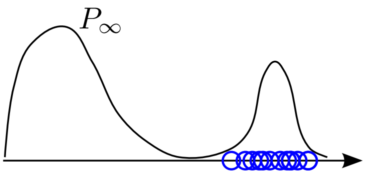
Learning vs. Inference: Vicious Cycle

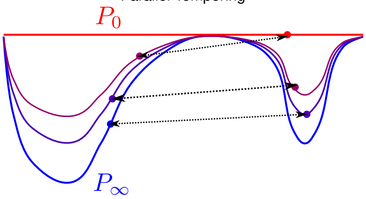


Failed inference (sampling) breaks learning

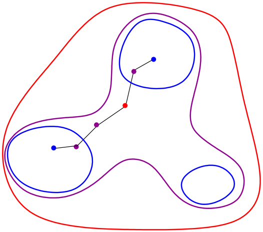
$\rightarrow$ *Good MCMC sampler is needed!*

Inference: Better MCMC Sampler





- MCMC with a *local* jump cannot easily escape an isolated mode

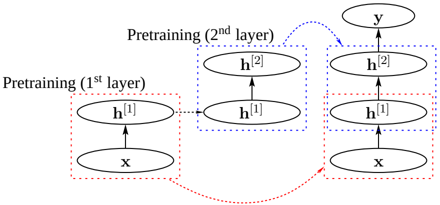


Parallel Tempering

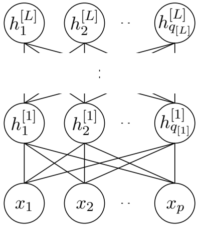
- Parallel chains between P_0 and P_∞
- Jump via tempered chains
- Better exploration of the state space

From an RBM to a *deeper* neural network..

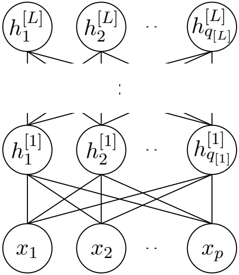
Deep Belief Network
(Pretrained MLP)



Deep Boltzmann Machine



Deep Boltzmann Machines



- *Undirected* Hierarchical Model
- Negative Energy

$$
\begin{aligned}
-E(\mathbf{x}, \mathbf{h} \mid \boldsymbol{\theta}) = \\
&\mathbf{b}^\top \mathbf{x} + \mathbf{c}_{[1]}^\top \mathbf{h}_{[1]} + \mathbf{x}^\top \mathbf{W} \mathbf{h}_{[1]} \\
&+ \sum_{l=2}^{L} \left(\mathbf{c}_{[l]}^\top \mathbf{h}_{[l]} + \mathbf{h}_{[l-1]}^\top \mathbf{U}_{[l-1]} \mathbf{h}_{[l]} \right)
\end{aligned}
$$

- The further away a layer from **x**, the more abstract concept the layer learns
- Hierarchical representation with both bottom-up and top-down signals

Learning: Depressing Observation

Observation: Lack of Structures in Deeper Hidden Layers

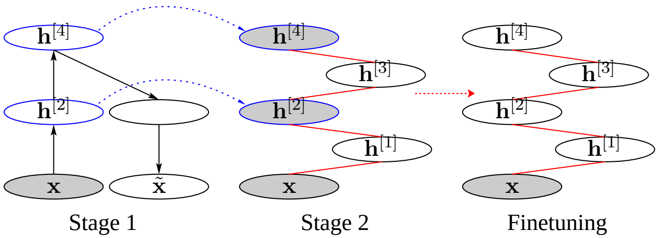
Which direction does learning move toward? – matching data and model statistics

$$\frac{\partial \mathcal{L}(\boldsymbol{\theta})}{\partial u_{ij}^{[l]}} \propto \left\langle h_i^{[l]} h_j^{[l+1]} \right\rangle_{p(\mathbf{h}|\mathbf{v},\boldsymbol{\theta})p_D(\mathbf{v})} - \left\langle h_i^{[l]} h_j^{[l+1]} \right\rangle_{p(\mathbf{v},\mathbf{h}|\boldsymbol{\theta})}$$

What happens if $p(\mathbf{h} \mid \mathbf{v}, \boldsymbol{\theta})$ does not have *any* structure?

- Learning will *not* utilize deeper layers easily
- Especially severe at the intial stage of learning

Learning: Hierarchical structure *borrowed* from DBN



Stage 1 Recursively train a stack of RBMs to get $Q(\mathbf{h}_- \mid \mathbf{x})$

Stage 2 Train a large RBM $\iff$ Maximize the variational lower-bound of DBM

$$\mathbb{E}_{D(\mathbf{v})}\left[\log p(\mathbf{v}^{(n)} \mid \boldsymbol{\theta})\right] \geq \mathbb{E}_{D(\mathbf{v})Q(\mathbf{h}_-)}\left[\log \sum_{\mathbf{h}_+} e^{\left\{-E(\mathbf{v}^{(n)},\mathbf{h}_-,\mathbf{h}_+)\right\}}\right] + \mathcal{H}(Q) - \log Z(\boldsymbol{\theta})$$

Q: Have I worked on anything other than Boltzmann machines?

Unsupervised Learning: Encoder-Decoder Perspective

- Sparse coding:

Encoder $\mathbf{h} = \arg\min_{\mathbf{h}} \|\mathbf{x} - \mathbf{W}^\top \mathbf{h}\| + \lambda \Omega(\mathbf{h})$

Decoder $\mathbf{x} = \mathbf{W}^\top \mathbf{h}$

- Probabilistic PCA:

Encoder $\mathbb{E}[\mathbf{h}] = (\mathbf{W}^\top \mathbf{W} + \sigma^2 \mathbf{I})^{-1} \mathbf{W}^\top \mathbf{x}$

Decoder $\mathbb{E}[\mathbf{x}] = \mathbf{W}^\top \mathbf{h}$

- RBM:

Encoder $\mathbb{E}[\mathbf{h}] = \sigma(\mathbf{W}\mathbf{x} + \mathbf{c})$

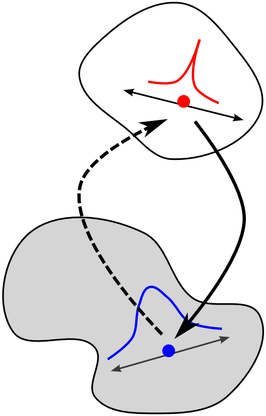
Decoder $\mathbb{E}[\mathbf{x}] = \sigma(\mathbf{W}^\top \mathbf{h} + \mathbf{b})$

- DBM:

Encoder $\boldsymbol{\mu}^{[l]} \leftarrow \sigma(\mathbf{U}_{[l]}^\top \boldsymbol{\mu}^{[l+1]} + \mathbf{U}_{[l-1]} \boldsymbol{\mu}^{[l-1]} + \mathbf{c}^{[l]}),$

$\mathbb{E}\left[\mathbf{h}^{[l]}\right] \approx \boldsymbol{\mu}^{[l]}$

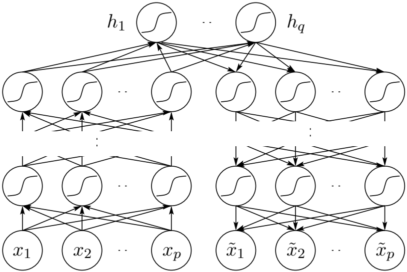
Decoder $\mathbb{E}[\mathbf{x}] = \sigma(\mathbf{W}^\top \mathbf{h}^{[1]} + \mathbf{b})$



Denoising Autoencoder: Explicit Sparsification

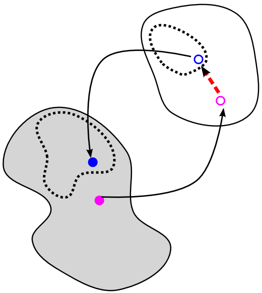
Sparse Denoising Autoencoder

- Encoder $\mathbf{h} = f(\mathbf{x}) : \mathbb{P} \to \mathbb{Q}$
- Decoder $\tilde{\mathbf{x}} = g(\mathbf{h}) : \mathbb{Q} \to \mathbb{P}$



$$\mathbb{P} = \left\{ \mathbf{x} \in \mathbb{R}^p \,\middle|\, \exists \mathbf{x}^{(n)} \in D, \|\mathbf{x} - \mathbf{x}^{(n)}\|_2^2 \leq \epsilon \right\}$$
$$\mathbb{Q} \approx \left\{ \mathbf{h} = f(\mathbf{x}) \,\middle|\, \mathbf{x} \in \mathbb{P}, \|\mathbb{E}_{\mathbf{x} \in \mathbb{P}}[h_j] - \rho\|_2^2 = 0 \right\}$$

What do we do with $\mathbf{x} \notin \mathbb{P}$?



1. Encode: $\mathbf{h} = f(\mathbf{x})$
2. Sparsify: $\tilde{\mathbf{h}} = R(\mathbf{h})$
3. Decode: $\tilde{\mathbf{x}} = g(\tilde{\mathbf{h}})$

And beyond..

- Theoretical understanding beyond universal approximator properties
- Deep learning for long sequences
- Deep learning for $p \gg n$ and $n \to 1$
- New models that tackles learning and inference directly