Learning Deep Architectures

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Deep Motivations

- Brains have a deep architecture
- Humans organize their ideas hierarchically, through composition of simpler ideas
- Unsufficiently deep architectures can be exponentially inefficient
- Distributed (possibly sparse) representations are necessary to achieve non-local generalization, exponentially more efficient than 1-of-N enumeration latent variable values
- Multiple levels of latent variables allow combinatorial sharing of statistical strength
Deep Architecture in the Brain

- Retina
  - Area V1
    - Pixels
    - Edge detectors
  - Area V2
    - Primitive shape detectors
  - Area V4
    - Higher level visual abstractions
Deep Architecture in our Mind

- Humans organize their ideas and concepts hierarchically.
- Humans first learn simpler concepts and then compose them to represent more abstract ones.
- Engineers break-up solutions into multiple levels of abstraction and processing.

It would be nice to learn / discover these concepts (knowlege engineering failed because of poor introspection?)
Architecture Depth

Depth = 4

Depth = 3
Good News, Bad News

Theoretical arguments: deep architectures can be

2 layers of

- logic gates
- formal neurons
- RBF units

= universal approximator

Theorems for all 3:
(Hastad et al 86 & 91, Bengio et al 2007)

Functions representable compactly with $k$ layers may require exponential size with $k-1$ layers
The Deep Breakthrough

- Before 2006, training deep architectures was unsuccessful, except for convolutional neural nets


Greedy Layer-Wise Pre-Training

Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)
Deep Architectures and Sharing Statistical Strength, Multi-Task Learning

- Generalizing better to new tasks is crucial to approach AI
- Deep architectures learn good intermediate representations that can be shared across tasks
- A good representation is one that makes sense for many tasks
Restricted Boltzmann Machines

- The most popular building block for deep architectures
- Bipartite undirected graphical model.
  \( x = \text{observed}, \ h = \text{hidden} \)

\[
P(x, h) = \frac{1}{Z} e^{-\text{Energy}(x, h)} = \frac{1}{Z} e^{b^T h + c^T x + h^T W x}
\]

- \( P(h \mid x) \) and \( P(x \mid h) \) factorize:
  - Easy inference
  - Convenient Gibbs sampling \( x \rightarrow h \rightarrow x \rightarrow h \ldots \)

- In practice, Gibbs sampling does not always mix well...

RBM trained by CD on MNIST

Chains from random state

Chains from real digit
Boltzmann Machine Gradient

\[ P(x) = \frac{1}{Z} \sum_h e^{-\text{Energy}(x,h)} = \frac{1}{Z} e^{-\text{FreeEnergy}(x)} \]

- Gradient has two components:
  - 'positive phase'
  - 'negative phase'

\[
\frac{\partial \log P(x)}{\partial \theta} = \frac{\partial \text{FreeEnergy}(x)}{\partial \theta} + \sum_x P(\tilde{x}) \frac{\partial \text{FreeEnergy}(\tilde{x})}{\partial \theta} \\
= - \sum_h P(h|x) \frac{\partial \text{Energy}(x,h)}{\partial \theta} + \sum_{\tilde{x}, \tilde{h}} P(\tilde{x}, \tilde{h}) \frac{\partial \text{Energy}(\tilde{x}, \tilde{h})}{\partial \theta}
\]

- In RBMs, easy to sample or sum over \( h \mid x \):
- Difficult part: sampling from \( P(x) \), typically with a Markov chain
Training RBMs

- Contrastive Divergence (CD-k): start negative Gibbs chain at observed $x$, run $k$ Gibbs steps.

- Persistent CD (PCD): run negative Gibbs chain in background while weights slowly change

- Fast PCD: two sets of weights, one with a large learning rate only used for negative phase, quickly exploring modes

- Herding (see Max Welling’s ICML, UAI and workshop talks)

- Tempered MCMC: use higher temperature to escape modes
Contrastive Divergence

- Contrastive Divergence (CD-k): start negative phase block Gibbs chain at observed x, run k Gibbs steps (Hinton 2002)

\[ h \sim P(h | x) \]

\[ h' \sim P(h | x') \]

FreeEnergy

push down

push up
Persistent CD

- Persistent CD (PCD): run negative Gibbs chain in background while weights slowly change (Younes 2000, Tieleman 2008)
  - Guarantees (Younes 89,2000; Yuille 2004)
  - If learning rate decreases in $1/t$, chain mixes before parameters change too much, chain stays converged when parameters change.

\[ h \sim P(h \mid x) \]

Observed $x$ (positive phase)
**Persistent CD with large learning rate**

- Negative phase samples quickly push up the energy of wherever they are and quickly move to another mode.
Persistent CD with large step size

- Negative phase samples quickly push up the energy of wherever they are and quickly move to another mode.
Persistent CD with large learning rate

- Negative phase samples quickly push up the energy of wherever they are and quickly move to another mode.
Fast Persistent CD and Herding

- Exploit impressively faster mixing achieved when parameters change quickly (large learning rate) while sampling
- Fast PCD: two sets of weights, one with a large learning rate only used for negative phase, quickly exploring modes
- Herding (see Max Welling’s ICML, UAI and workshop talks): 0-temperature MRFs and RBMs, only use fast weights

![FPCD](image1.png) ![Herding](image2.png)
Tempered MCMC

- Annealing from high-temperature worked well for estimating log-likelihood (AIS)
- Consider multiple chains at different temperatures and reversible swaps between adjacent chains
- Higher temperature chains can escape modes
- Model samples are from $T=1$

<table>
<thead>
<tr>
<th>Training procedure</th>
<th>Sample generation procedure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TMCMC</td>
</tr>
<tr>
<td>TMCMC</td>
<td>215.45 ± 2.24</td>
</tr>
<tr>
<td>PCD</td>
<td>44.70 ± 2.51</td>
</tr>
<tr>
<td>CD</td>
<td>-2165 ± 0.53</td>
</tr>
</tbody>
</table>
Deep Belief Networks

- Sampling:
  - Sample from top RBM
  - Sample from level k given k+1

- Easy approximate inference

- Training:
  - Variational bound justifies greedy layerwise training of RBMs
  - How to train all levels together?

\[
\log P(x) \geq H_Q(h|x) + \sum_h Q(h|x) \left( \log P(h) + \log P(x|h) \right)
\]
Deep Boltzmann Machines
(Salakhutdinov et al, AISTATS 2009, Lee et al, ICML 2009)

- Positive phase: variational approximation (mean-field)
- Negative phase: persistent chain
- Can (must) initialize from stacked RBMs
- Improved performance on MNIST from 1.2% to .95% error
- Can apply AIS with 2 hidden layers
Estimating Log-Likelihood

- RBMs: requires estimating partition function
  - Reconstruction error provides a cheap proxy
  - log $Z$ tractable analytically for < 25 binary inputs or hidden
  - Lower-bounded (how well?) with Annealed Importance Sampling (AIS)

- Deep Belief Networks:
  - Extensions of AIS (Salakhutdinov & Murray, ICML 2008, NIPS 2008)

- Open question: efficient ways to monitor progress
Back to Greedy Layer-Wise Pre-Training

Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)
Why are classifiers obtained from DBNs working so well?

- General principles?
- Would these principles work for other single-level algorithms?
- Why does it work?
Stacking Auto-Encoders
Auto-encoders and CD

RBM log-likelihood gradient can be written as converging expansion: CD-k = 2k terms, reconstruction error ~ 1 term.

\[
\frac{\partial \log P(x_1)}{\partial \theta} = \sum_{s=1}^{t-1} \left( E \left[ \frac{\partial \log P(x_s|h_s)}{\partial \theta} \right] | x_1 \right] + E \left[ \frac{\partial \log P(h_s|x_{s+1})}{\partial \theta} \right] | x_1 \right] + E \left[ \frac{\partial \log P(x_t)}{\partial \theta} \right] | x_1 \right] \quad \text{(Bengio & Delalleau 2009)}
\]
Greedy Layerwise Supervised Training

Generally worse than unsupervised pre-training but better than ordinary training of a deep neural network (Bengio et al. 2007).
Supervised Fine-Tuning is Important

- Greedy layer-wise unsupervised pre-training phase with RBMs or auto-encoders on MNIST

- Supervised phase with or without unsupervised updates, with or without fine-tuning of hidden layers

- Can train all RBMs at the same time, same results
Sparse Auto-Encoders

- (Ranzato et al, 2007; Ranzato et al 2008)
- Sparsity penalty on the intermediate codes
- Like sparse coding but with efficient run-time encoder
- Sparsity penalty pushes up the free energy of all configurations (proxy for minimizing the partition function)
- Impressive results in object classification (convolutional nets):
  - MNIST: .5% error = record-breaking
  - Caltech-101: 65% correct = state-of-the-art (Jarrett et al, ICCV 2009)
    similar results obtained with a convolutional DBN: (Lee et al, ICML’2009)
Denoising Auto-Encoder

- (Vincent et al, 2008)
- Corrupt the input
- Reconstruct the uncorrupted input

Hidden code (representation)

Corrupted input

Raw input

reconstruction

KL(reconstruction | raw input)
Denoising Auto-Encoder

- Learns a vector field towards higher probability regions
- Minimizes variational lower bound on a generative model
- Similar to pseudo-likelihood
Stacked Denoising Auto-Encoders

- No partition function, can measure training criterion
- Encoder & decoder: any parametrization
- Performs as well or better than stacking RBMs for unsupervised pre-training
Why is Unsupervised Pre-Training Working So Well?

- Regularization hypothesis:
  - Unsupervised component forces model close to $P(x)$
  - Representations good for $P(x)$ are good for $P(y | x)$

- Optimization hypothesis:
  - Unsupervised initialization near better local minimum of $P(y | x)$
  - Can reach lower local minimum otherwise not achievable by random initialization
Learning Trajectories in Function Space

- Each point a model in function space
- Color = epoch
- Top: trajectories w/o pre-training
- Each trajectory converges in different local min.
- No overlap of regions with and w/c pre-training
Unsupervised learning as regularizer

- Adding extra regularization (reducing # hidden units) hurts more the pre-trained models
- Pre-trained models have less variance wrt training sample
- Regularizer = infinite penalty outside of region compatible with unsupervised pre-training
Better optimization of online error

- Both training and online error are smaller with unsupervised pre-training.

- As \( \# \) samples \( \to \infty \), training err. = online err. = generalization err.

- Without unsup. pre-training: can’t exploit capacity to capture complexity in target function from training data.
Learning Dynamics of Deep Nets

Before fine-tuning

After fine-tuning
Learning Dynamics of Deep Nets

- As weights become larger, get trapped in basin of attraction (“quadrant” does not change)

- Initial updates have a crucial influence (“critical period”), explain more of the variance

- Unsupervised pre-training initializes in basin of attraction with good generalization properties
The order and selection of examples makes a difference

- Curriculum learning (Bengio et al, ICML’2009; Krueger & Dayan 2009)
- Start with easier examples
- Faster convergence to a better local minimum in deep architectures
- Also acts like a regularizer with optimization effect?
- **Influencing learning dynamics can make a big difference**

![Graph showing curriculum and no-curriculum learning](image-url)
Level-local learning is important

- Initializing each layer of an unsupervised deep Boltzmann machine helps a lot.
- Initializing each layer of a supervised neural network as an RBM helps a lot.
- Helps most the layers further away from the target.
- Not just an effect of unsupervised prior.
- Jointly training all the levels of a deep architecture is difficult.
- Initializing using a level-local learning algorithm (RBM, auto-encoders, etc.) is a useful trick.
Take-Home Messages

- Multiple levels of latent variables: potentially exponential gain in statistical sharing
- RBMs allow fast inference, stacked RBMs / auto-encoders have fast approximate inference
- Gibbs sampling in RBMs does not mix well, but sampling and learning can interact in surprisingly useful ways
- Unsupervised pre-training of classifiers acts like a strange regularizer with improved optimization of online error
- At least as important as the model: the inference approximations and the learning dynamics
Some Open Problems

- Why is it difficult to train deep architectures?
- What is important in the learning dynamics?
- How to improve joint training of all layers?
- How to sample better from RBMs and deep generative models?
- Monitoring unsupervised learning quality in deep nets?
- Other ways to guide training of intermediate representations?
THANK YOU FOR YOUR ATTENTION!

- Questions?
- Comments?