Learning Deep Architectures

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Deep Architectures Work Well

- Beating shallow neural networks on vision and NLP tasks
- Beating SVMs on visions tasks from pixels (and handling dataset sizes that SVMs cannot handle in NLP)
- Reaching state-of-the-art performance in NLP
- Beating deep neural nets without unsupervised component
- Learn visual features similar to V1 and V2 neurons
Deep Motivations

- Brains have a deep architecture
- Humans organize their ideas hierarchically, through composition of simpler ideas
- Insufficiently 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
Locally Capture the Variations

- $*$ = training example
- true function: unknown
- learnt = interpolated

Prediction $f(x)$ at test point $x$
Easy with Few Variations

\[ * = \text{example (x,y)} \]

true unknown function

learned function: prediction = f(x)
The Curse of Dimensionality

To generalise locally, need representative exemples for all possible variations!
Limits of Local Generalization: Theoretical Results

(Bengio & Delalleau 2007)

- **Theorem:** Gaussian kernel machines need at least $k$ examples to learn a function that has $2k$ zero-crossings along some line.

- **Theorem:** For a Gaussian kernel machine to learn some maximally varying functions over $d$ inputs require $O(2^d)$ examples.
Curse of Dimensionality When Generalizing Locally on a Manifold
How to Beat the Curse of Many Factors of Variation?

Compositionality: exponential gain in representational power

- Distributed representations
- Deep architecture
Distributed Representations

- Many neurons active simultaneously
- Input represented by the activation of a set of features that are not mutually exclusive
- Can be exponentially more efficient than local representations
Local vs Distributed

regions defined by learned prototypes

LOCAL PARTITION

DISTRIBUTED PARTITION
Neuro-cognitive inspiration

- Brains use a distributed representation
- Brains use a deep architecture
- Brains heavily use unsupervised learning
- Brains learn simpler tasks first
- Human brains developed with society / culture / education
Deep Architecture in the Brain

- Retina
- Area V1
- Area V2
- Area V4

- Pixels
- Edge detectors
- Primitive shape detectors
- 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.
- Want to learn / discover these concepts.
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
Feature and Sub-Feature Sharing

- Different tasks can share the same high-level feature
- Different high-level features can be built from the same set of lower-level features
- More levels = up to exponential gain in representational efficiency
Architecture Depth

Depth = 3

Depth = 4
Deep Architectures are More Expressive

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 compactly represented with k layers may require exponential size with k-1 layers
Sharing Components in a Deep Architecture

Polynomial expressed with shared components:

Polynomial expressed with shared components:

advantage of depth may grow exponentially
How to train Deep Architecture?

- Great expressive power of deep architectures
- How to train them?
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) → Supervised deep neural network
Good Old Multi-Layer Neural Net

- Each layer outputs vector $z_k = \text{sigm}(b_k + W_k z_{k-1})$ from $z_{k-1}$ of previous layer with params $b_k$ (vector) and $W_k$ (matrix).

- Output layer predicts parametrized distribution of target variable $Y$ given input $x$. 

[Diagram of a multi-layer neural network showing layers and connections with $z_0 = x$.]
Training Multi-Layer Neural Nets

- Outputs: e.g. multinomial for multiclass classification with softmax output units

$$z_{ki} = \frac{e^{b_{ki} + W_{ki}' z_{k-1}}}{\sum_j e^{b_{kj} + W_{kj}' z_{k-1}}}$$

- Parameters are trained by gradient-based optimization of training criterion involving conditional log-likelihood, e.g.

$$- \log P(Y = y|x) = - \log z_{ky}$$
Effect of Unsupervised Pre-training

AISTATS’2009
Effect of Depth

w/o pre-training

with pre-training

Graphs showing the effect of depth on test classification error (percent) for different numbers of layers.
Boltzmann Machines and MRFs

- Boltzmann machines:  
  \[ P(x) = \frac{1}{Z} e^{-\text{Energy}(x)} = e^{c^T x + x^T W x} \]
  (Hinton 84)

- Markov Random Fields:
  \[ P(x) = \frac{1}{Z} e^{\sum_i w_i f_i(x)} \]

- More interesting with latent variables!
Restricted Boltzman Machine

- The most popular building block for deep architectures

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

- Bipartite undirected graphical model
RBM with (image, label) visible units

- Can predict a subset $y$ of the visible units given the others $x$
- Exactly if $y$ takes only few values
- Gibbs sampling o/w
RBMs are Universal Approximators
(LeRoux & Bengio 2008, Neural Comp.)

- Adding one hidden unit (with proper choice of parameters) guarantees increasing likelihood
- With enough hidden units, can perfectly model any discrete distribution
- RBMs with variable nb of hidden units = non-parametric
- Optimal training criterion for RBMs which will be stacked into a DBN is not the RBM likelihood
RBM Conditionals Factorize

\[
P(h | x) = \frac{\exp(b'x + c'h + h'Wx)}{\sum_{\tilde{h}} \exp(b'x + c'\tilde{h} + \tilde{h}'Wx)} \\
= \frac{\prod_i \exp(c_i h_i + h_i W_i x)}{\prod_i \sum_{\tilde{h}_i} \exp(c_i \tilde{h}_i + \tilde{h}_i W_i x)} \\
= \prod_i \frac{\exp(h_i (c_i + W_i x))}{\sum_{\tilde{h}_i} \exp(\tilde{h}_i (c_i + W_i x))} \\
= \prod_i P(h_i | x).
\]
With $h_i \in \{0, 1\}$, recall $\text{Energy}(x, h) = -b'x - c'h - h'Wx$

$$P(h_i = 1| x) = \frac{e^{1c_i + 1W_i x + \text{other terms}}}{e^{1c_i + 1W_i x + \text{other terms}} + e^{0c_i + 0W_i x + \text{other terms}}}$$

$$= \frac{e^{c_i + W_i x}}{e^{c_i + W_i x} + 1}$$

$$= \frac{1}{1 + e^{-c_i - W_i x}}$$

$$= \text{sigm}(c_i + W_i x).$$

since $\text{sigm}(a) = \frac{1}{1+e^{-a}}$. 
RBM Hidden Units Carve Input Space
Gibbs Sampling in RBMs

\[ h_1 \sim P(h \mid x_1) \]

\[ x_2 \sim P(x \mid h_1) \]

\[ h_2 \sim P(h \mid x_2) \]

\[ x_3 \sim P(x \mid h_2) \]

\[ h_3 \sim P(h \mid x_3) \]

P(h \mid x) and P(x \mid h) factorize

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

- Easy inference
- Convenient Gibbs sampling

\[ x \rightarrow h \rightarrow x \rightarrow h \ldots \]
Problems with Gibbs Sampling

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

RBM trained by CD on MNIST

Chains from random state

Chains from real digits
RBM Free Energy

- Free Energy = equivalent energy when marginalizing

$$P(x, h) = \frac{e^{-\text{Energy}(x, h)}}{Z}$$

- Can be computed exactly and efficiently in RBMs

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

- Marginal likelihood $P(x)$ tractable up to partition function $Z$

$$\text{FreeEnergy}(x) = -b'x - \sum_i \log \sum_h e^{h_i(c_i + W_i x)}$$
Factorization of the Free Energy

Let the energy have the following general form:

\[ \text{Energy}(\mathbf{x}, h) = -\beta(\mathbf{x}) + \sum_i \gamma_i(\mathbf{x}, h_i) \]

Then

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

\[
= \frac{1}{Z} \sum_{h_1} \sum_{h_2} \cdots \sum_{h_k} e^{\beta(\mathbf{x}) - \sum_i \gamma_i(\mathbf{x}, h_i)} = \frac{1}{Z} \sum_{h_1} \sum_{h_2} \cdots \sum_{h_k} e^{\beta(\mathbf{x})} \prod_i e^{-\gamma_i(\mathbf{x}, h_i)}
\]

\[
= \frac{e^{\beta(\mathbf{x})}}{Z} \sum_{h_1} e^{-\gamma_1(\mathbf{x}, h_1)} \sum_{h_2} e^{-\gamma_2(\mathbf{x}, h_2)} \cdots \sum_{h_k} e^{-\gamma_k(\mathbf{x}, h_k)}
\]

\[
= \frac{e^{\beta(\mathbf{x})}}{Z} \prod_i \sum_{h_i} e^{-\gamma_i(\mathbf{x}, h_i)}
\]

\[
\text{FreeEnergy}(\mathbf{x}) = - \log P(\mathbf{x}) - \log Z = -\beta(\mathbf{x}) - \sum_i \log \sum_{h_i} e^{-\gamma_i(\mathbf{x}, h_i)}
\]
Energy-Based Models Gradient

\[ P(x) = \frac{e^{-\text{Energy}(x)}}{Z} \]

\[ Z = \sum_x e^{-\text{Energy}(x)} \]

\[ \frac{\partial \log P(x)}{\partial \theta} = -\frac{\partial \text{Energy}(x)}{\partial \theta} - \frac{\partial \log Z}{\partial \theta} \]

\[ \frac{\partial \log Z}{\partial \theta} = \frac{\partial \log \sum_x e^{-\text{Energy}(x)}}{\partial \theta} \]

\[ = \frac{1}{Z} \frac{\partial \sum_x e^{-\text{Energy}(x)}}{\partial \theta} \]

\[ = -\frac{1}{Z} \sum_x e^{-\text{Energy}(x)} \frac{\partial \text{Energy}(x)}{\partial \theta} \]

\[ = -\sum_x P(x) \frac{\partial \text{Energy}(x)}{\partial \theta} \]
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:

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

- 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: start negative Gibbs chain at observed x, run k Gibbs steps

Persistent CD: 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: Deterministic near-chaos dynamical system defines both learning and sampling

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)

$h \sim P(h | x)$

$\begin{array}{c}
\text{Observed } x \\
\text{positive phase}
\end{array}$

$k = 2 \text{ steps}$

$\begin{array}{c}
\text{Sampled } x' \\
\text{negative phase}
\end{array}$

$h' \sim P(h | x')$

Free Energy

push down

$x$

push up

$x'$
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
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
Herding MRFs

- Consider 0-temperature MRF with state $s$ and weights $w$

- Fully observed case, observe values $s^+$, dynamical system where $s^-$ and $W$ evolve

- Then statistics of samples $s^-$ match the data's statistics, even if approximate max, as long as $w$ remains bounded

\[
\ell = E_{data \ s^+} [\sum_i w_i f_i(s^+)] - \max_s \sum_i w_i f_i(s)
\]

\[
s^- \leftarrow \arg\max_s \sum_i w_i f_i(s)
\]

\[
w \leftarrow w + E_{data \ s^+} [f(s^+)] - f(s^-)
\]

\[
E_{samples \ s^-} [f(s^-)] = E_{data \ s^+} [f(s^+)]
\]
Herding RBMs

- Hidden part $h$ of the state $s = (x,h)$
- Binomial state variables $s_i \in \{-1, 1\}$
- Statistics $f$
  
  $S_i, S_i S_j$
- Optimize $h$ given $x$ in positive phase
  
  $\ell = E_{data \times}{[\max_h \sum_i w_i f_i(x^+, h)]} - \max_s \sum_i w_i f_i(s)$
  
  $s^- \leftarrow \text{argmax}_s \sum_i w_i f_i(s)$
  
  $w \leftarrow w + \frac{\left( E_{data \times}{[\max_h \sum_i f_i(x^+, h)]} - f(s^-) \right)}{\text{number of training examples}}$

- In practice, greedy maximization works, exploiting RBM structure
Fast Mixing with Herding

FPCD

Herding

![Graph showing comparison between FPCD, Herding, WHerd, FCD, and CD over number of samples with coverage on the y-axis and number of samples on the x-axis.]
The Sampler as a Generative Model

- Instead of the traditional clean separation between model and sampling procedure
- Consider the overall effect of combining some adaptive procedure with a sampling procedure as the generative model
- Can be evaluated as such (without reference to some underlying probability model)

Training data \((x, y)\) → \(\text{Sampled data } y\) → \(\text{Query inputs } x\)
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 $T=1$.

### Sample Generation Procedure

<table>
<thead>
<tr>
<th>Training Procedure</th>
<th>TMCMC</th>
<th>Gibbs (random start)</th>
<th>Gibbs (test start)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TMCMC</td>
<td>215.45 ± 2.24</td>
<td>88.43 ± 2.75</td>
<td>60.04 ± 2.88</td>
</tr>
<tr>
<td>PCD</td>
<td>44.70 ± 2.51</td>
<td>-28.66 ± 3.28</td>
<td>-175.08 ± 2.99</td>
</tr>
<tr>
<td>CD</td>
<td>-2165 ± 0.53</td>
<td>-2154 ± 0.63</td>
<td>-842.76 ± 6.17</td>
</tr>
</tbody>
</table>
Deep Belief Networks

- DBN = sigmoidal belief net with RBM joint for top two layers
  
  \[ P(x, h^1, \ldots, h^\ell) = P(h^{\ell-1}, h^\ell) \left( \prod_{k=1}^{\ell-2} P(h^k|h^{k+1}) \right) P(x|h^1) \]

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

- Level k given level k+1 = same parametrization as RBM conditional: stacking RBMs \(\rightarrow\) DBN
From RBM to DBN

- RBM specifies $P(v,h)$ from $P(v|h)$ and $P(h|v)$
- Implicitly defines $P(v)$ and $P(h)$
- Keep $P(v|h)$ from 1st RBM and replace $P(h)$ by the distribution generated by 2nd level RBM
Deep Belief Networks

- Easy approximate inference
  - $P(h_{k+1} \mid h_k)$ approximated from the associated RBM
  - Approximation because $P(h_{k+1})$ differs between RBM and DBN

- Training:
  - Variational bound justifies greedy layerwise training of RBMs
    \[
    \log P(x) \geq H_{Q(h \mid x)} + \sum_h Q(h \mid x) \left( \log P(h) + \log P(x \mid h) \right)
    \]
  - How to train all levels together?
Deep Boltzman 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
Deep Convolutional Architectures

Mostly from Le Cun’s group (NYU), also Ng (Stanford): state-of-the-art on MNIST digits, Caltech-101 objects, faces
Convolutional DBNs
(Lee et al, ICML’2009)
Back to Greedy Layer-Wise Pre-Training

Stacking Restricted Boltzmann Machines (RBM) $\rightarrow$ Deep Belief Network (DBN) $\rightarrow$ Supervised deep neural network
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

Greedy layer-wise unsupervised pre-training also works with auto-encoders
Auto-encoders and CD

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

\[
\frac{\partial \log P(x_1)}{\partial \theta} = \sum_{s=1}^{t-1} \left( E \left[ \frac{\partial \log P(x_s|h_s)}{\partial \theta} \bigg| x_1 \right] + E \left[ \frac{\partial \log P(h_s|x_{s+1})}{\partial \theta} \bigg| x_1 \right] \right) + E \left[ \frac{\partial \log P(x_t)}{\partial \theta} \bigg| x_1 \right]
\]  

(Bengio & Delalleau 2009)
Credit propagation methods, commonly referred to as greedy layerwise supervised training, are 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 (e.g. set 25% of inputs to 0)
- Reconstruct the uncorrupted input
- Use uncorrupted encoding as input to next level
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
- Generative model is semi-parametric

[Graph showing online classification error over number of examples seen for different configurations of stack layers and pre-training techniques.]
Denoising Auto-Encoders: Benchmarks

<table>
<thead>
<tr>
<th>basic: subset of MNIST digits. (10 000 training samples)</th>
</tr>
</thead>
<tbody>
<tr>
<td>rot: applied random rotation (angle between 0 and 2π radians)</td>
</tr>
<tr>
<td>bg-rand: background made of random pixels (value in 0…255)</td>
</tr>
<tr>
<td>bg-img: background is random patch from one of 20 images</td>
</tr>
<tr>
<td>rot-bg-img: combination of rotation and background image</td>
</tr>
<tr>
<td>rect: discriminate between tall and wide rectangles.</td>
</tr>
<tr>
<td>rect-img: same but rectangles are random image patches</td>
</tr>
<tr>
<td>convex: discriminate between convex and non-convex shapes.</td>
</tr>
</tbody>
</table>
## Denoising Auto-Encoders: Results

<table>
<thead>
<tr>
<th>Problem</th>
<th>$\text{SVM}_{rbf}$</th>
<th>DBN-1</th>
<th>DBN-3</th>
<th>SAA-3</th>
<th>$\text{SdA-3 (}\nu\text{)}$</th>
<th>$\text{SVM}_{rbf}(\nu)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>basic</td>
<td>3.03±0.15</td>
<td>3.94±0.17</td>
<td>3.11±0.15</td>
<td>3.46±0.16</td>
<td>2.80±0.14 (10%)</td>
<td>3.07 (10%)</td>
</tr>
<tr>
<td>rot</td>
<td>11.11±0.28</td>
<td>14.69±0.31</td>
<td>10.30±0.27</td>
<td>10.30±0.27</td>
<td>10.29±0.27 (10%)</td>
<td>11.62 (10%)</td>
</tr>
<tr>
<td>bg-rand</td>
<td>14.58±0.31</td>
<td>9.80±0.26</td>
<td>6.73±0.22</td>
<td>11.28±0.28</td>
<td>10.38±0.27 (40%)</td>
<td>15.63 (25%)</td>
</tr>
<tr>
<td>bg-img</td>
<td>22.61±0.37</td>
<td>16.15±0.32</td>
<td>16.31±0.32</td>
<td>23.00±0.37</td>
<td>16.68±0.33 (25%)</td>
<td>23.15 (25%)</td>
</tr>
<tr>
<td>rot-bg-img</td>
<td>55.18±0.44</td>
<td>52.21±0.44</td>
<td>47.39±0.44</td>
<td>51.93±0.44</td>
<td>44.49±0.44 (25%)</td>
<td>54.16 (10%)</td>
</tr>
<tr>
<td>rect</td>
<td>2.15±0.13</td>
<td>4.71±0.19</td>
<td>2.60±0.14</td>
<td>2.41±0.13</td>
<td>1.99±0.12 (10%)</td>
<td>2.45 (25%)</td>
</tr>
<tr>
<td>rect-img</td>
<td>24.04±0.37</td>
<td>23.69±0.37</td>
<td>22.50±0.37</td>
<td>24.05±0.37</td>
<td>21.59±0.36 (25%)</td>
<td>23.00 (10%)</td>
</tr>
<tr>
<td>convex</td>
<td>19.13±0.34</td>
<td>19.92±0.35</td>
<td>18.63±0.34</td>
<td>18.41±0.34</td>
<td>19.06±0.34 (10%)</td>
<td>24.20 (10%)</td>
</tr>
</tbody>
</table>
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 $P(y \mid x)$

- **Optimization hypothesis:**
  - Unsupervised initialization near better local minimum of $P(y \mid x)$
  - 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/o 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 $\# \text{ samples} \to \infty$, training err. = online err. = generalization err.
- Without unsup. pre-training: can’t exploit capacity to capture complexity in target function from training data.
Pre-training lower layers more critical

Verifies that what matters is not just the marginal distribution over initial weight values

(Histogram init.)
The Credit Assignment Problem

- Even with the correct gradient, lower layers (far from the prediction, close to input) are the most difficult to train

- Lower layers benefit most from unsupervised pre-training
  - Local unsupervised signal = extract / disentangle factors
  - Temporal constancy
  - Mutual information between multiple modalities

- Credit assignment / error information not flowing easily?

- Related to difficulty of credit assignment through time?
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
Semi-Supervised Embedding

- Use pairs (or triplets) of examples which are known to represent nearby concepts (or not)

- Bring closer the intermediate representations of supposedly similar pairs, push away the representations of randomly chosen pairs

- (Weston, Ratle & Collobert, ICML’2008): improved semi-supervised learning by combining unsupervised embedding criterion with supervised gradient
Slow Features

- Successive images in a video = similar
- Randomly chosen pair of images = dissimilar
- Slowly varying features are likely to represent interesting abstractions
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
Order & Selection of Examples Matters

- 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
Continuation Methods

Heavily smoothed objective = surrogate criterion

Track local minima

Easy to find minimum

Final solution

Target objective
Curriculum Learning as Continuation

- Sequence of training distributions
- Initially peaking on easier / simpler ones
- Gradually give more weight to more difficult ones until reach target distribution
Take-Home Messages

- Break-through in learning complicated functions: deep architectures with distributed representations
- Multiple levels of latent variables: potentially exponential gain in statistical sharing
- Main challenge: training deep architectures
- RBMs allow fast inference, stacked RBMs / auto-encoders have fast approximate inference
- 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?
- Capturing scene structure and sequential structure?
Thank you for your attention!

- Questions?
- Comments?