On the Difficulty of Training 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

WHY?
V1 and V2-like Filters Learned

Slow features 1st layer

RBM 1st layer

DBN 2nd layer

Denoising auto-encoder 1st layer
Greedy Layer-Wise Pre-Training

Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)

→ Supervised deep neural network
Effect of Unsupervised Pre-training

AISTATS’2009

- 1 layer without pretraining
- 1 layer with pretraining
- 4 layers without pretraining
- 4 layers with pretraining
Effect of Depth

w/o pre-training

with pre-training

![Box plots comparing test classification error with varying number of layers for both w/o pre-training and with pre-training.]
Why are Classifiers Obtained from Unsupervised Pre-Training Working so Well?

- General principles?
- Would these principles work for other single-level algorithms?
- Explanatory hypotheses?
Greedy Layerwise Supervised Training

Generally worse than unsupervised pre-training but better than ordinary training of a deep neural network (Bengio et al. 2007).
Stacking Auto-Encoders
Auto-Encoders and CD

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

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

(Bengio & Delalleau 2009)
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
Two phases?
Pre-training + Fine-tuning

- Currently best results generally obtained when doing purely supervised fine-tuning after unsupervised pre-training
- Kind of disappointing
- Can we avoid the fine-tuning altogether?
- Can we fold both phases together? (would be very useful for online learning on huge datasets)
- Can we avoid layer-wise initialization?
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 0.5% error = record-breaking
  - Caltech-101 65% correct = state-of-the-art (Jarrett et al, ICCV 2009)
- Similar results with a sparse convolutional DBN (Lee et al, ICML'2009)
Denoising Auto-Encoder
(Vincent et al, ICML 2008)

- Corrupt the input
- Reconstruct the uncorrupted 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

Budget of 10 million iterations

Online classification error

Number of examples seen

Infinite MNIST
Learning Layer-Local Embeddings

- (Weston & Collobert, ICML 2008) similar/dissimilar examples provide layer-local unsupervised criterion (Hadsell et al, CVPR 2006)

- Margin hinge loss: learned representations of similar examples should be more similar than of non-similar pairs

- Global supervised + layer-local unsupervised gradients

- Successfully tested in semi-supervised setting

- Trained up to 15-layer deep networks!

- No comparison yet with RBMs and auto-encoder variants
Slow Features & Temporal Constancy

- Similar pairs = successive inputs in a sequence (e.g. video)
- Try to make code covariance ~ 1, can be done in O(nfeat)
Why is Unsupervised Pre-Training Working So Well? Hypotheses:

- **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/o pre-training
Pre-Training Lower Layers More Critical

What matters is not just the marginal distribution over initial weight values (Histogram init.)
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.
Critical Impact of Early Updates

![Graph showing variance of output with and without pretraining]
Learning Dynamics of Deep Nets
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
What Optimization Tricks?

- Humans somehow find a good solution to an intractable non-convex optimization problem

**How?**

- **Guiding** the optimization near good solutions
- **Guiding** / giving hints to intermediate layers
Continuation Methods

- Target objective
- Final solution
- Track local minima
- Easy to find minimum

Heavily smoothed objective = surrogate criterion
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?
Guiding the Stochastic Optimization of Representations

- Train lower levels first (DBNs)
- Start with more noise / larger learning rate (babies vs adults)
- Slow features / multiple time scales
- Cross-modal mutual information
- Curriculum / shaping
Curriculum Learning

- Guided learning helps training humans and animals

- Start from simpler examples / easier tasks  
  (Piaget 1952, Skinner 1958)

- Cognition Journal: (Elman 1993) vs (Rohde & Plaut 1999), (Krueger & Dayan 2009)
Curriculum Learning as Continuation

1. Easiest
2. Lower level abstractions
3. Most difficult examples
   - Easiest
   - Lower level abstractions
   - Most difficult examples
   - Higher level abstractions

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

First: easier, basic shapes

Second = target: more varied geometric shapes
Shape Recognition Results
Language Modeling Results

- Gradually increase the vocabulary size (dips)
- Train on Wikipedia with sentences containing only words in vocabulary
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
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

- Unsupervised pre-training greatly helps deep architectures
- Unsupervised pre-training of classifiers acts like a strange regularizer with improved optimization of online error
- Inference approximations and learning dynamics at least as important as the model
- Early examples have greater influence: critical period?
- Guiding learning dynamics seems important:
  - Local hints to each layer
  - Curriculum / shaping = continuation?
Some Open Problems

- Why is it difficult to train deep architectures?
- What is important in the learning dynamics?
- How to improve joint training and sampling of all layers?
- Other ways to guide training of intermediate representations?
- How to design curricula / select examples?
- More complex models to handle spatial structure of images, occlusion, temporal structure, stereo, multiple modalities, etc.
Thank you for your attention!

- Questions?
- Comments?