On the Difficulty of Training Deep Architectures

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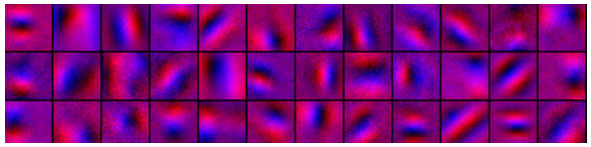
Deep Architectures Work Well

- 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

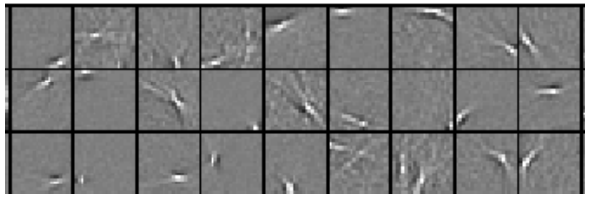
WHY?

V1 and V2-like Filters Learned

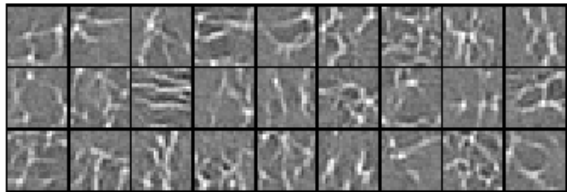
Slow features 1st layer



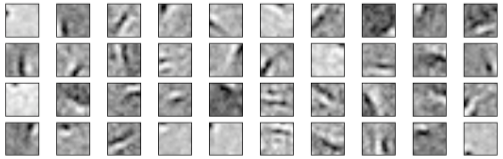
RBM 1st layer



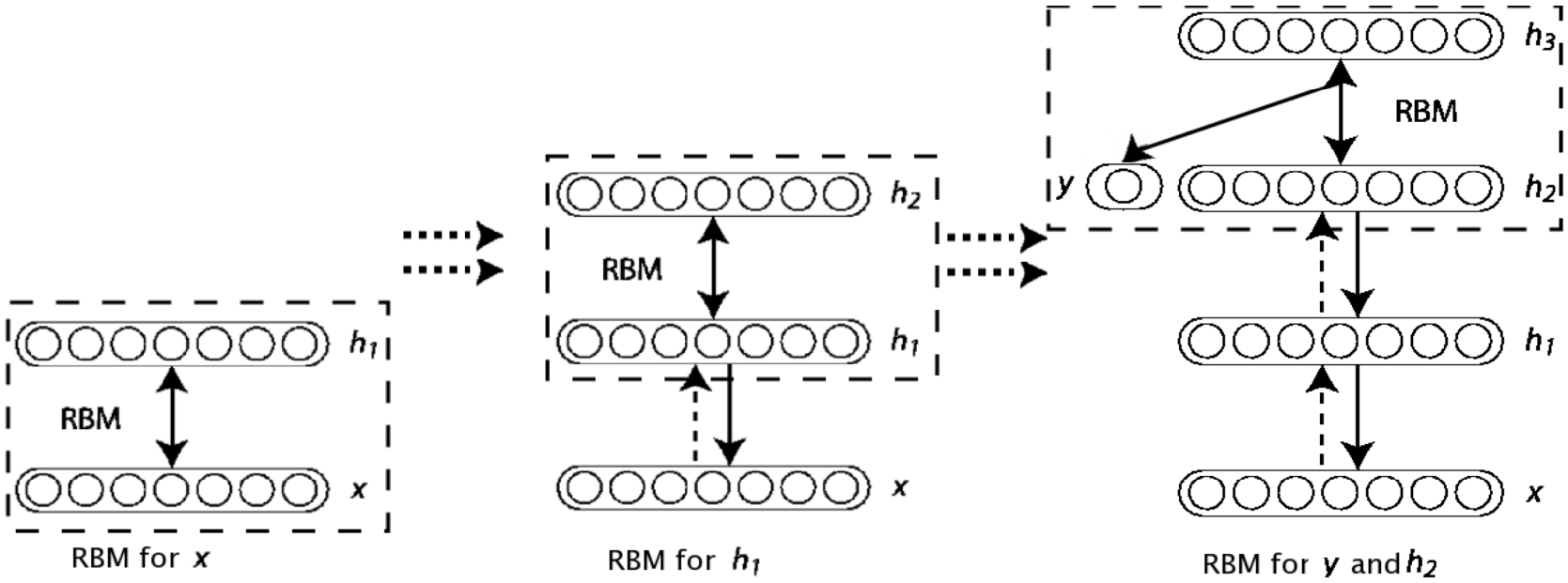
DBN 2nd layer



Denoising auto-encoder 1st layer



Greedy Layer-Wise Pre-Training

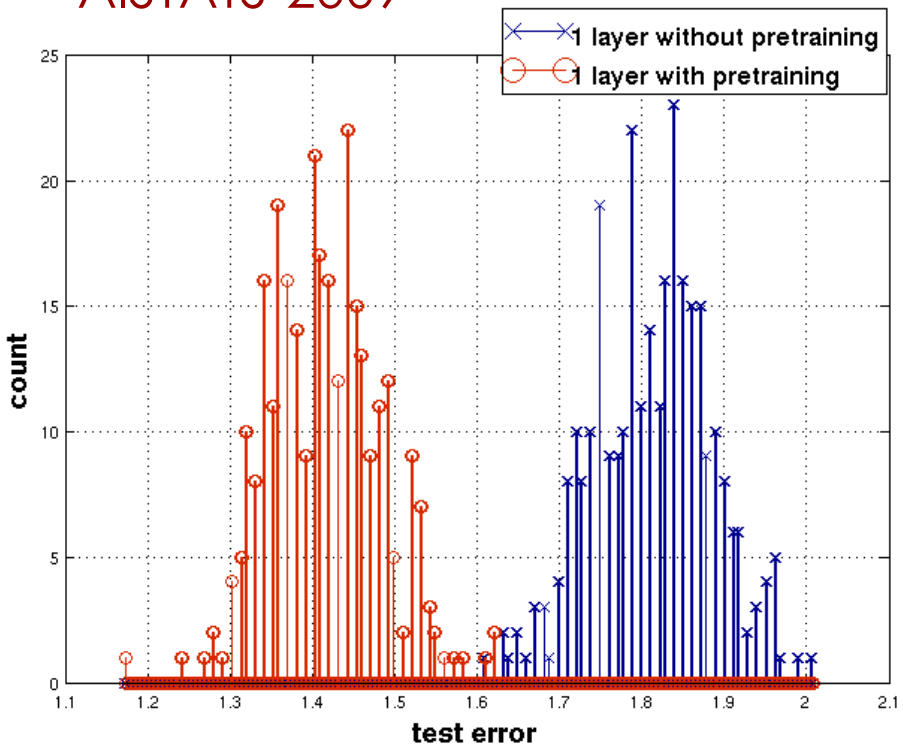


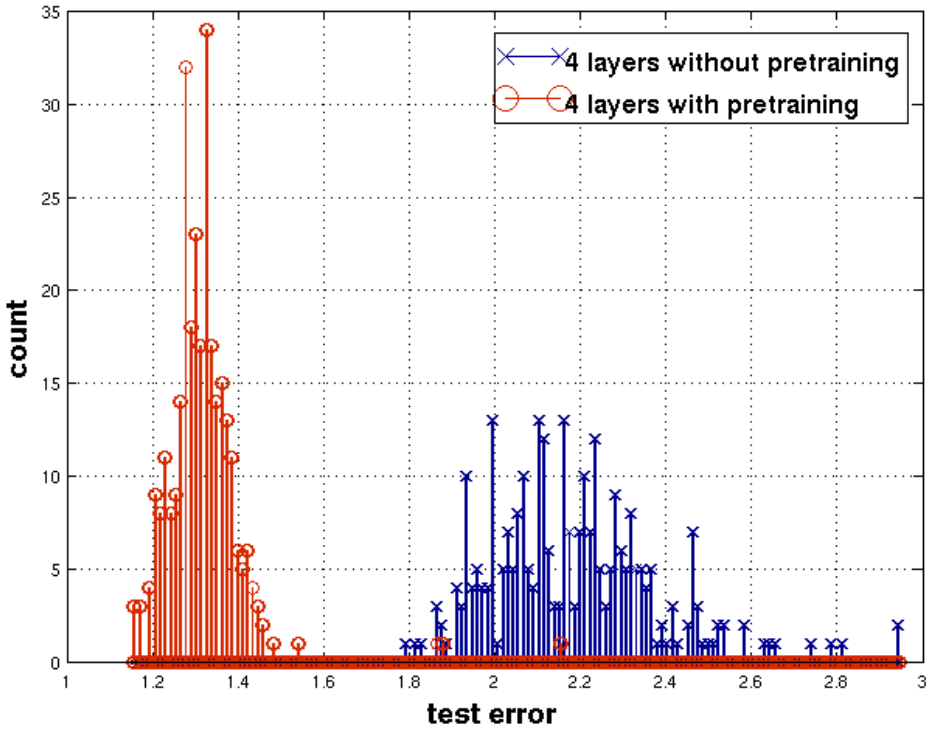
Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)

→ Supervised deep neural network

Effect of Unsupervised Pre-training

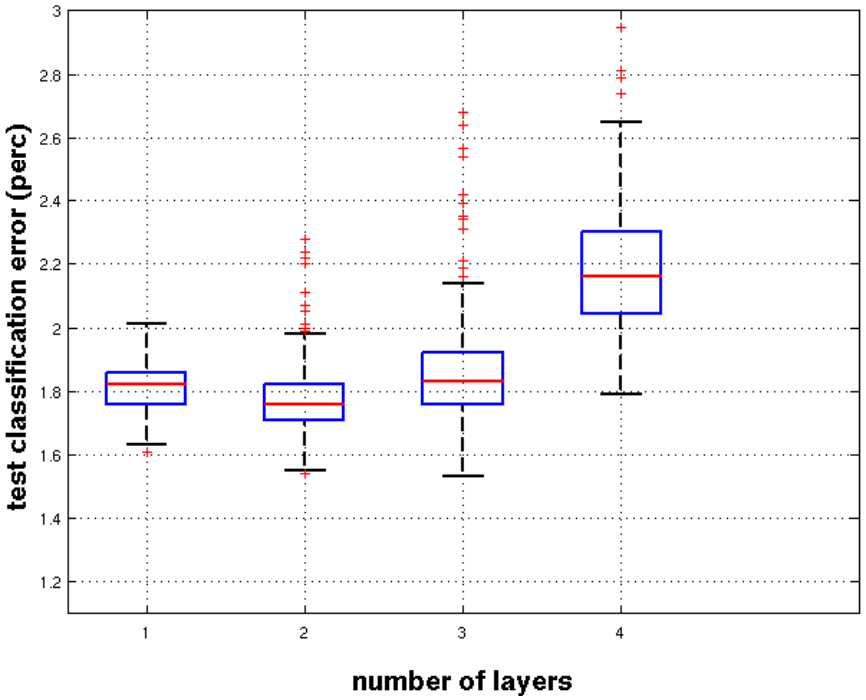
AISTATS'2009



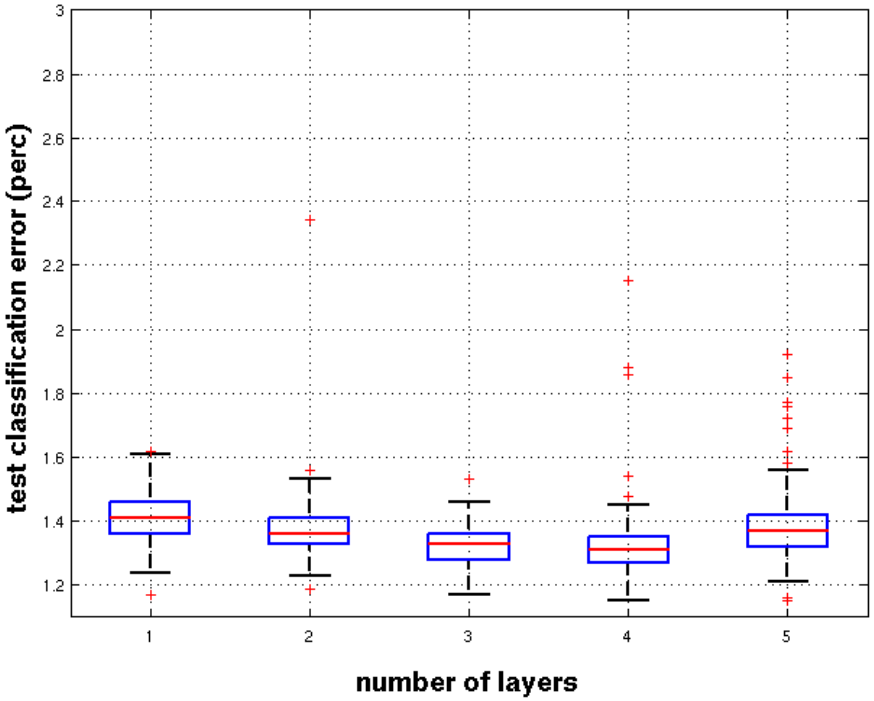


Effect of Depth

w/o pre-training



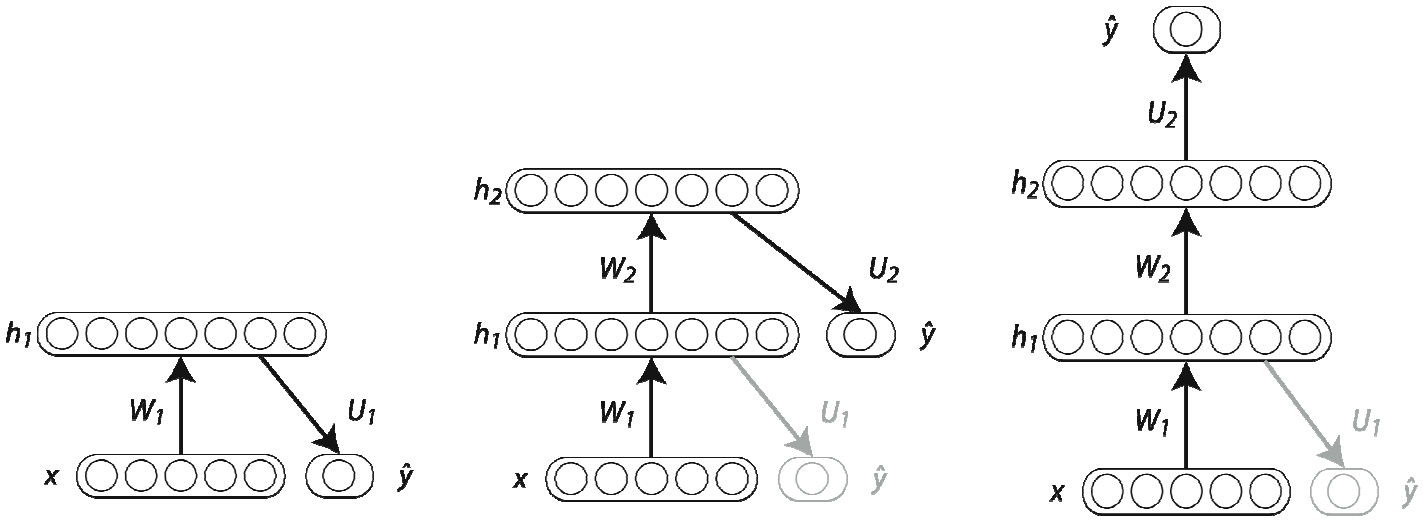
with pre-training



Why are Classifiers Obtained from Unsupervised Pre-Training Working so Well?

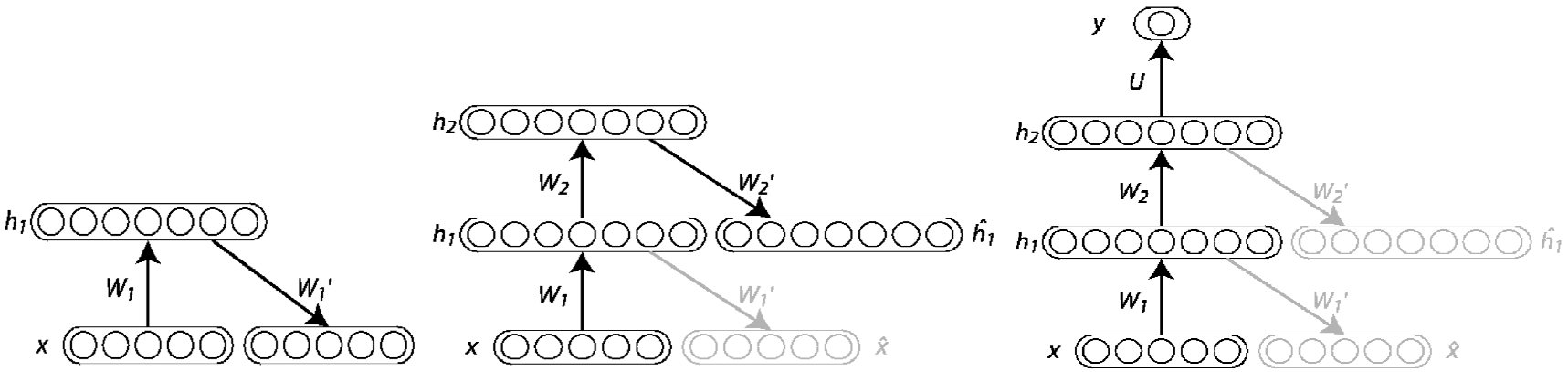
- General principles?
- Would these principles work for other single-level algorithms?
- Explanatory hypotheses?

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:

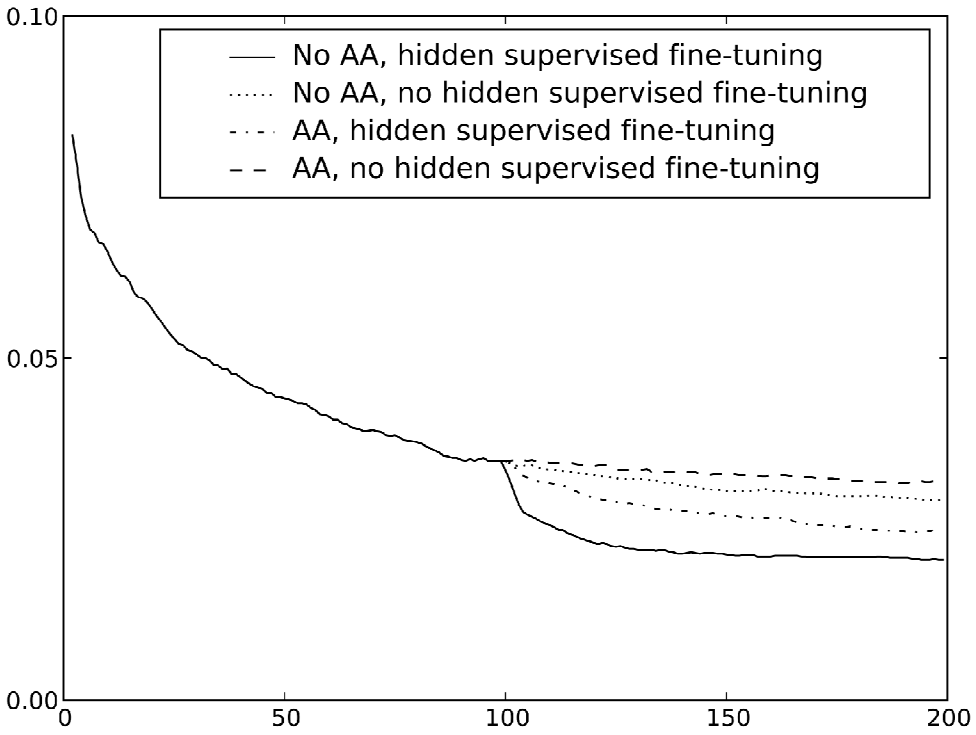
- CD-k = 2 k terms
- reconstruction error ~ 1 term

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

(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 alltogether?
- 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

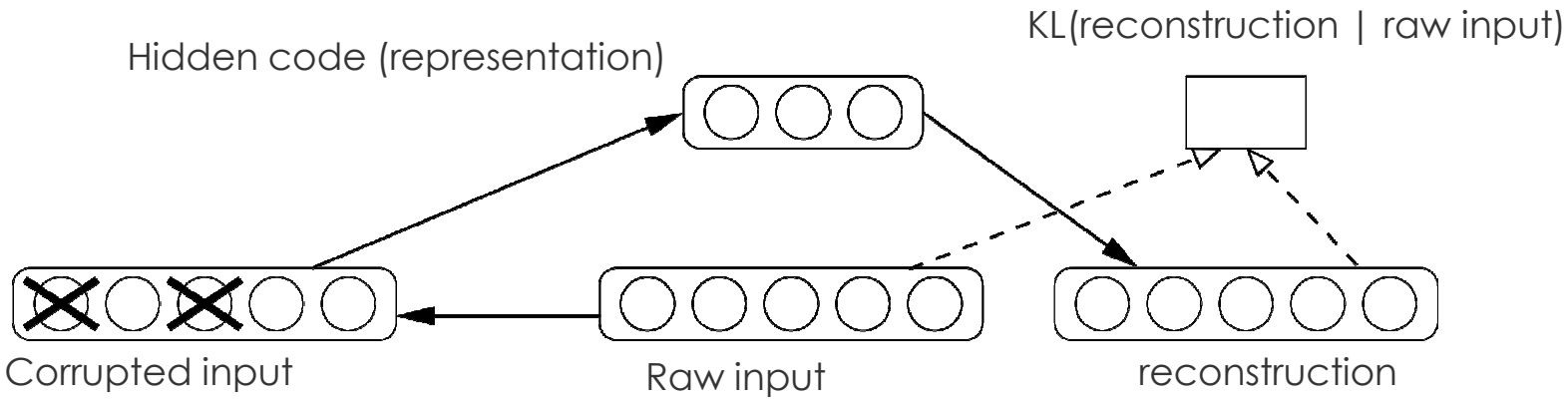
(Ranzato et al, 2007; Ranzato et al 2008)

- 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

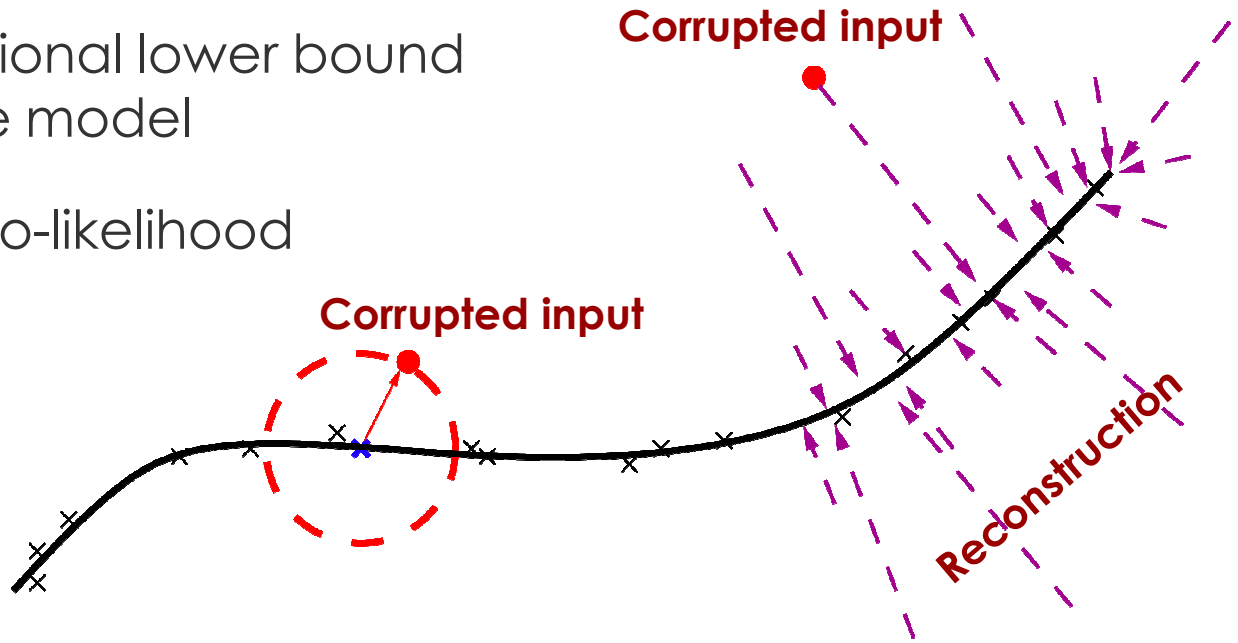
(Vincent et al, ICML 2008)

- Corrupt the input
- Reconstruct the uncorrupted input



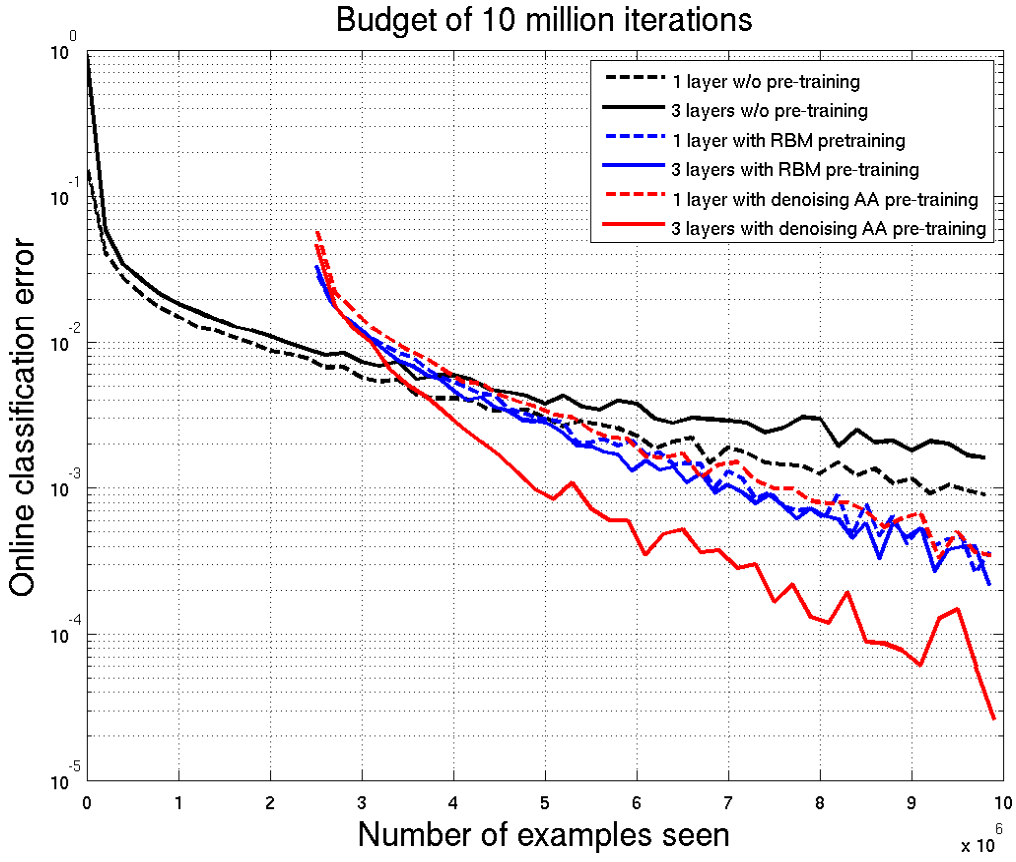
Denoising Auto-Encoder

- 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 usupervised pre-training



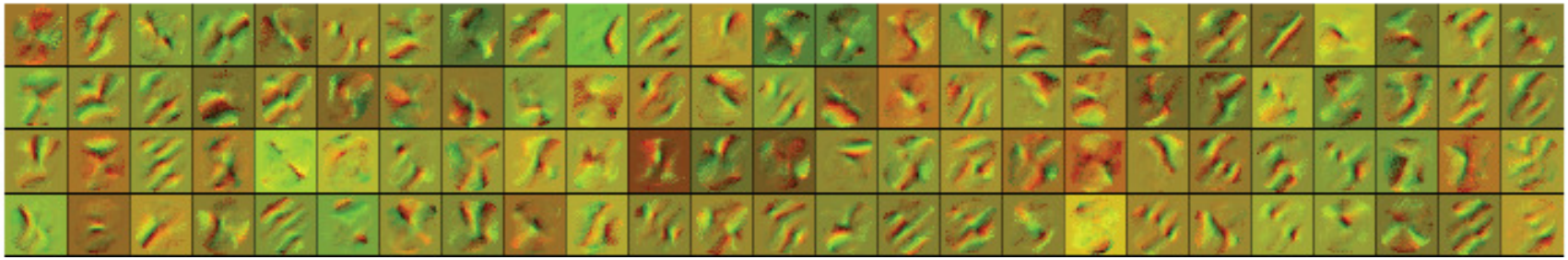
Infinite MNIST

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 ~ **I**, can be done in O(nfeat)



Pre-training Dataset	Number of pretraining iterations ($\times 10^4$)					
	0	1	2	3	4	5
MIXED-movies	1.56	1.32	1.42	1.34	1.35	1.28
MNIST-movies	1.56	1.32	1.33	1.32	1.27	1.30

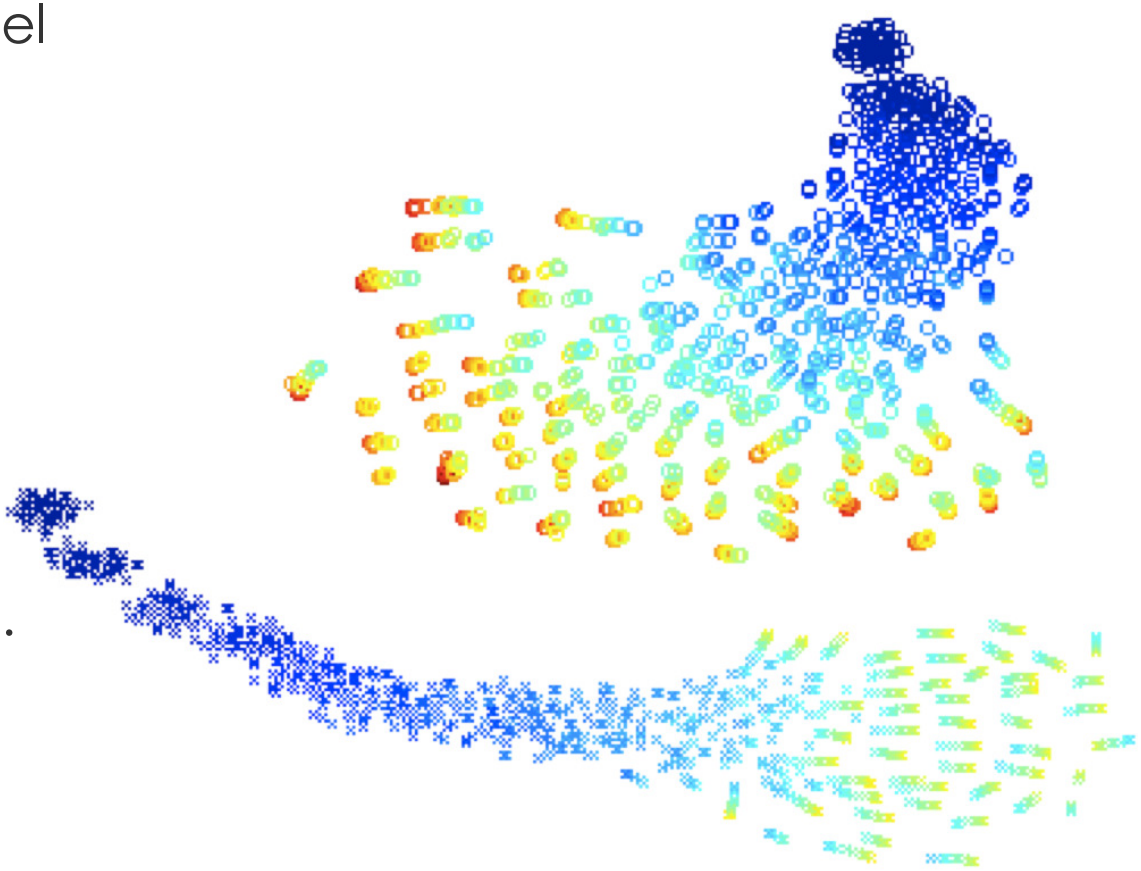
Why is Unsupervised Pre-Training Working So Well? Hypotheses:

- 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

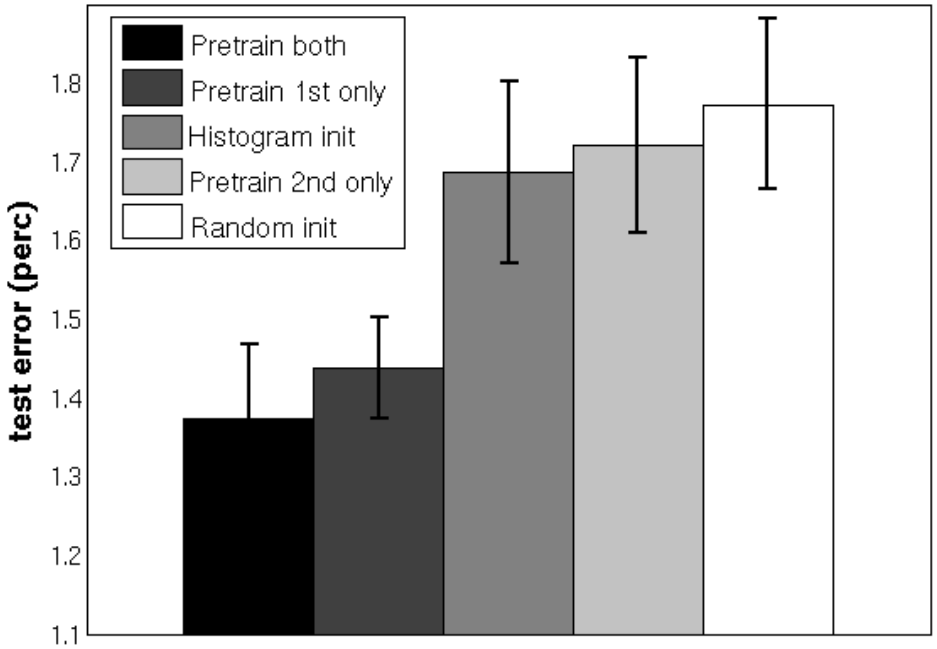
Learning Trajectories in Function Space

- 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



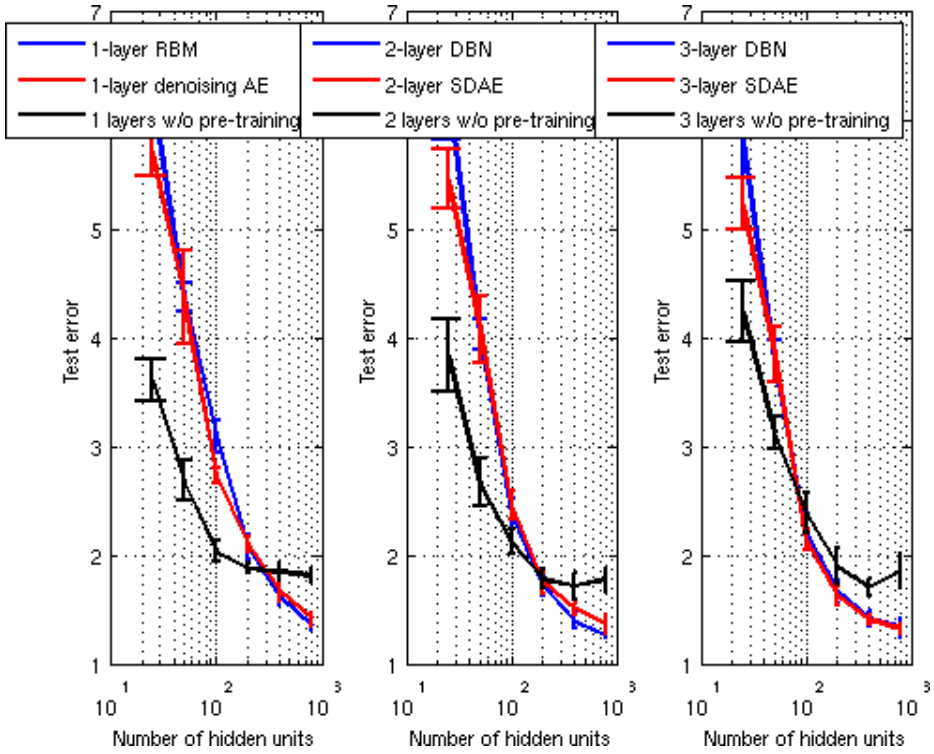
Pre-Training Lower Layers More Critical

What matters is not just the marginal distribution over initial weight values (Histogram init.)



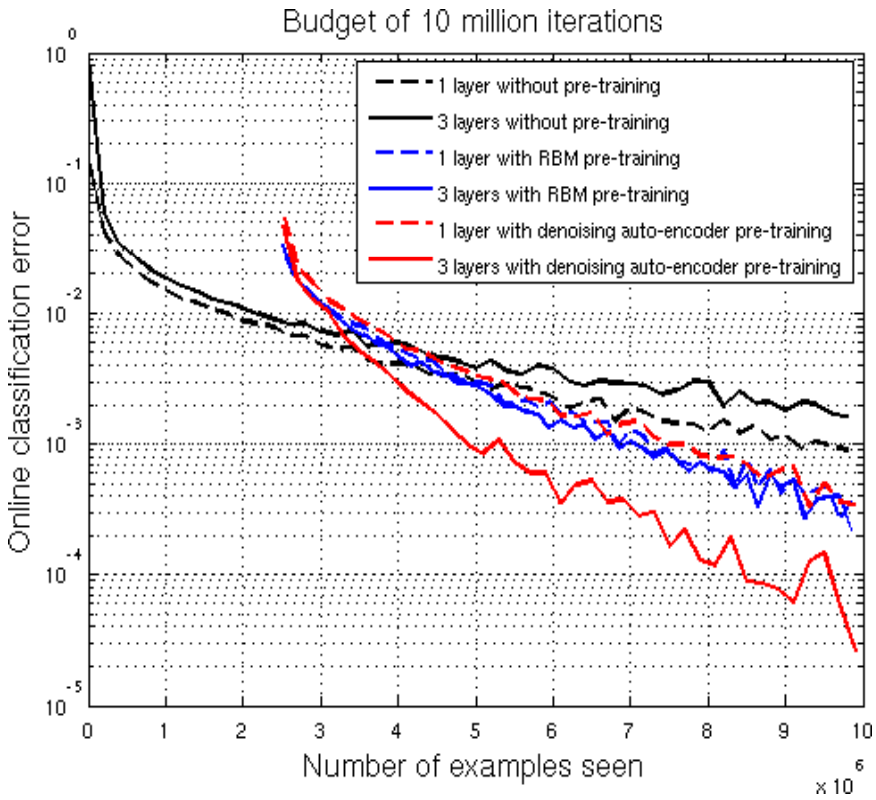
Unsupervised Learning as Regularizer

- 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

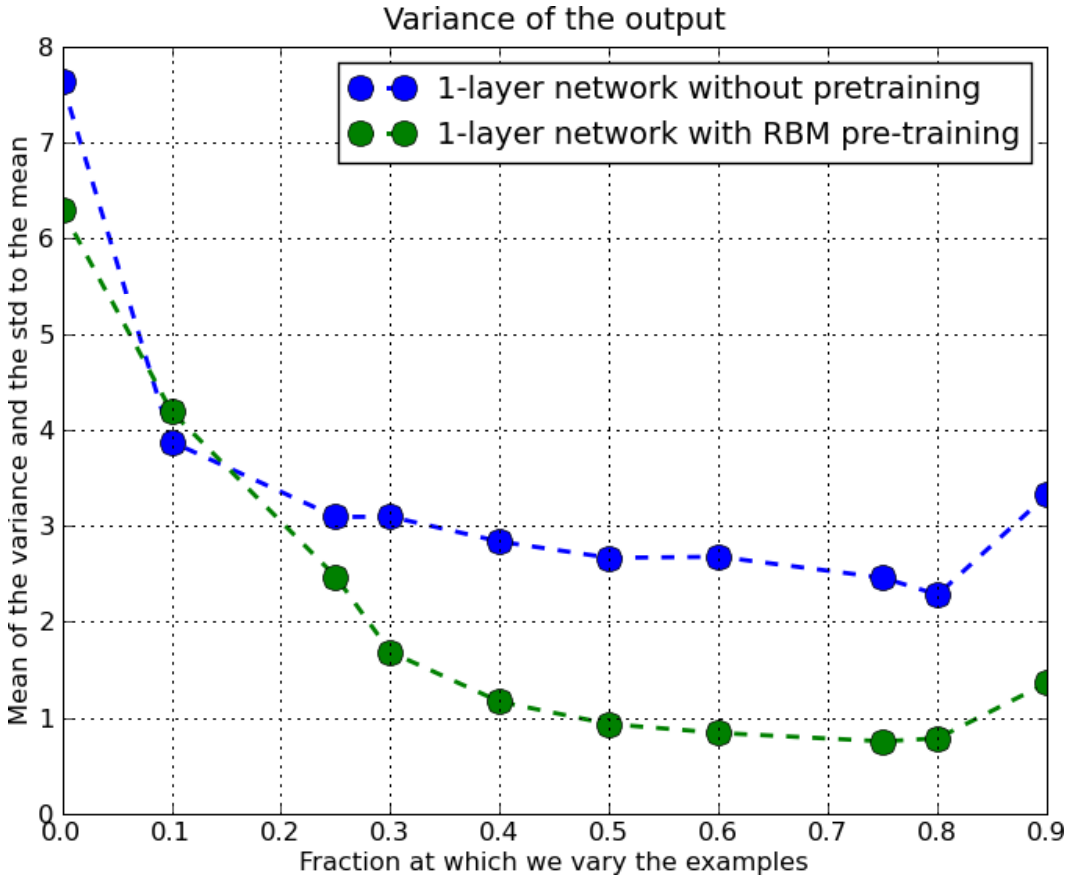


Better Optimization of Online Error

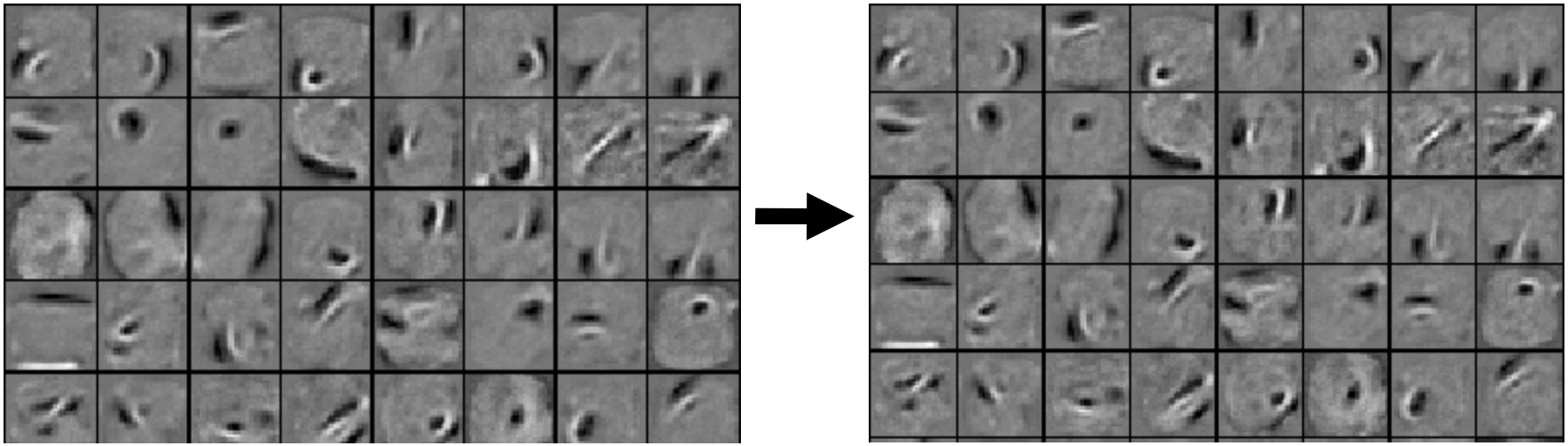
- Both training and online error are smaller with unsupervised pre-training
- As # samples → ∞
  training err. = online err. = generalization err.
- Without unsup. pre-training: can't exploit capacity to capture complexity in target function from training data



Critical Impact of Early Updates



Learning Dynamics of Deep Nets

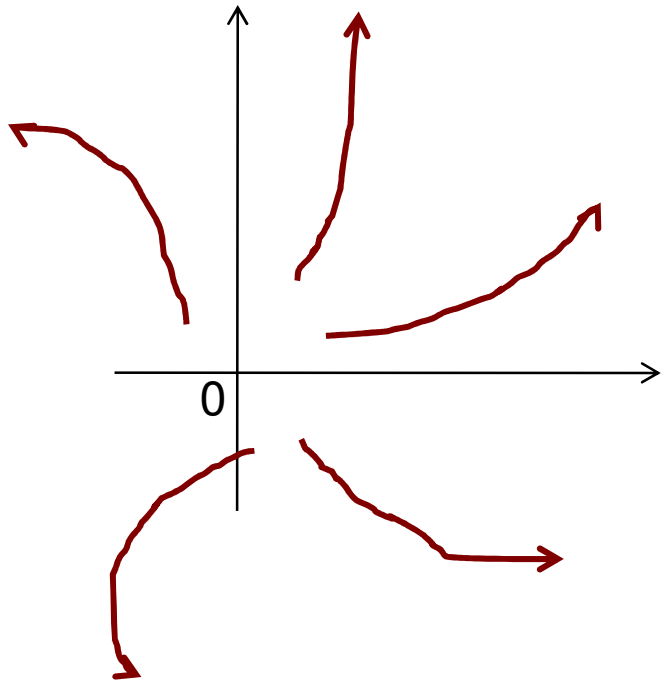


Before fine-tuning

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



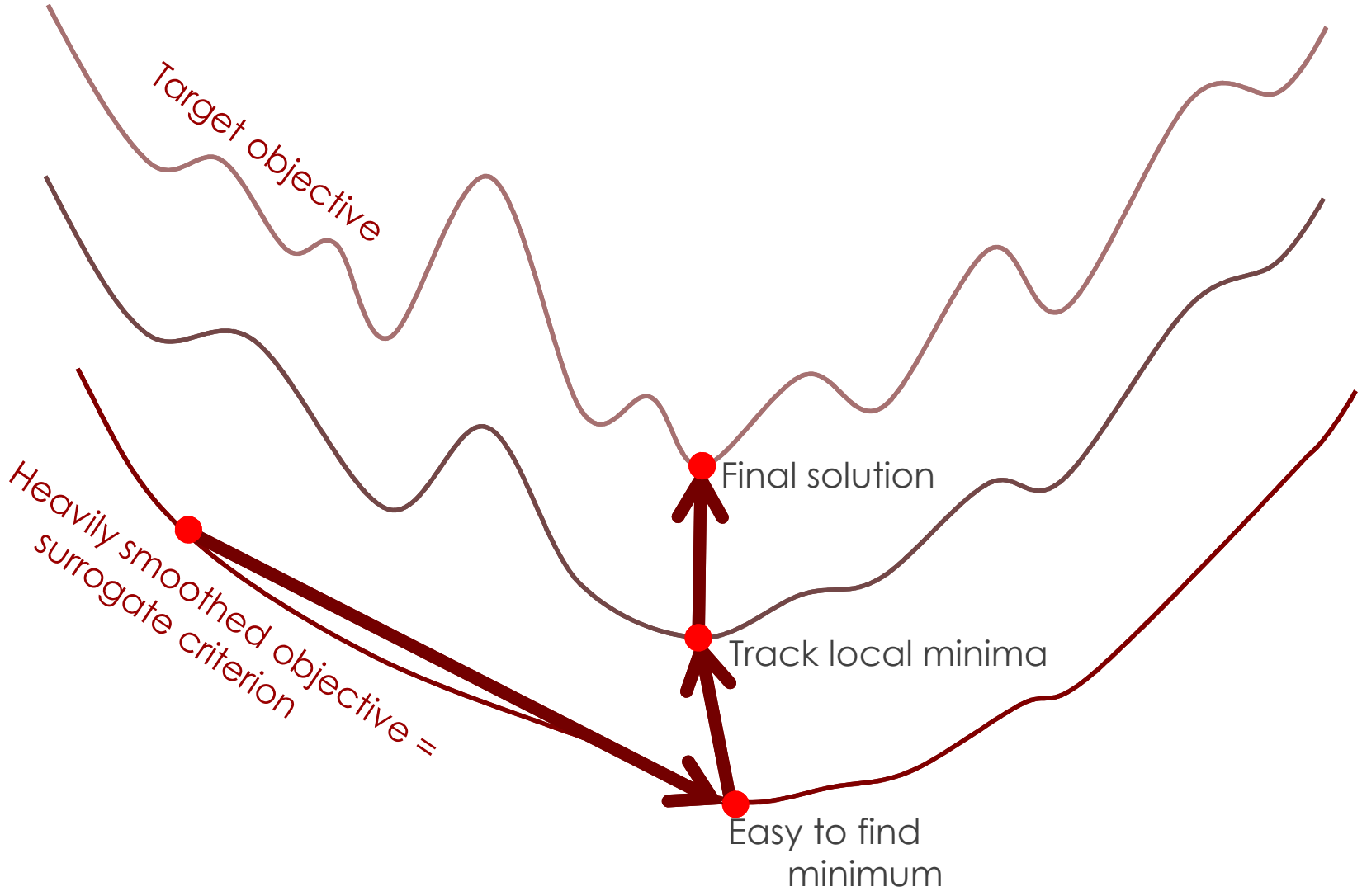
What Optimiztion Tricks?

- 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



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?

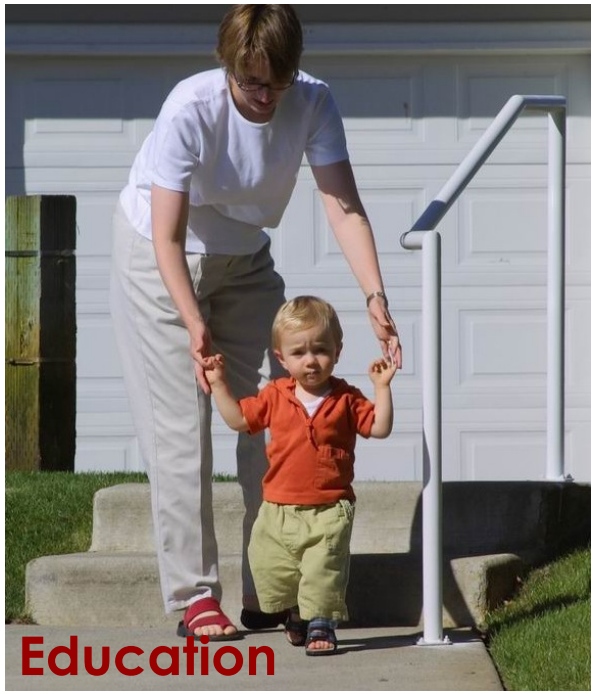
Guiding the Stochastic Optimization of Representations

- 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

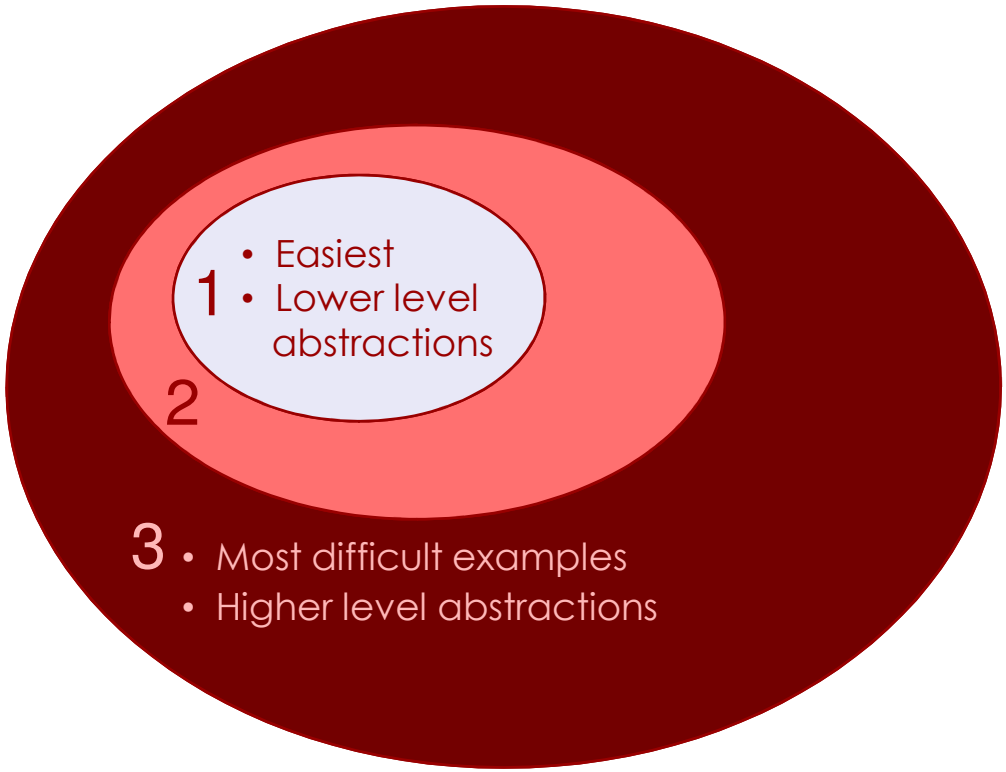
ICML'2009

- 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



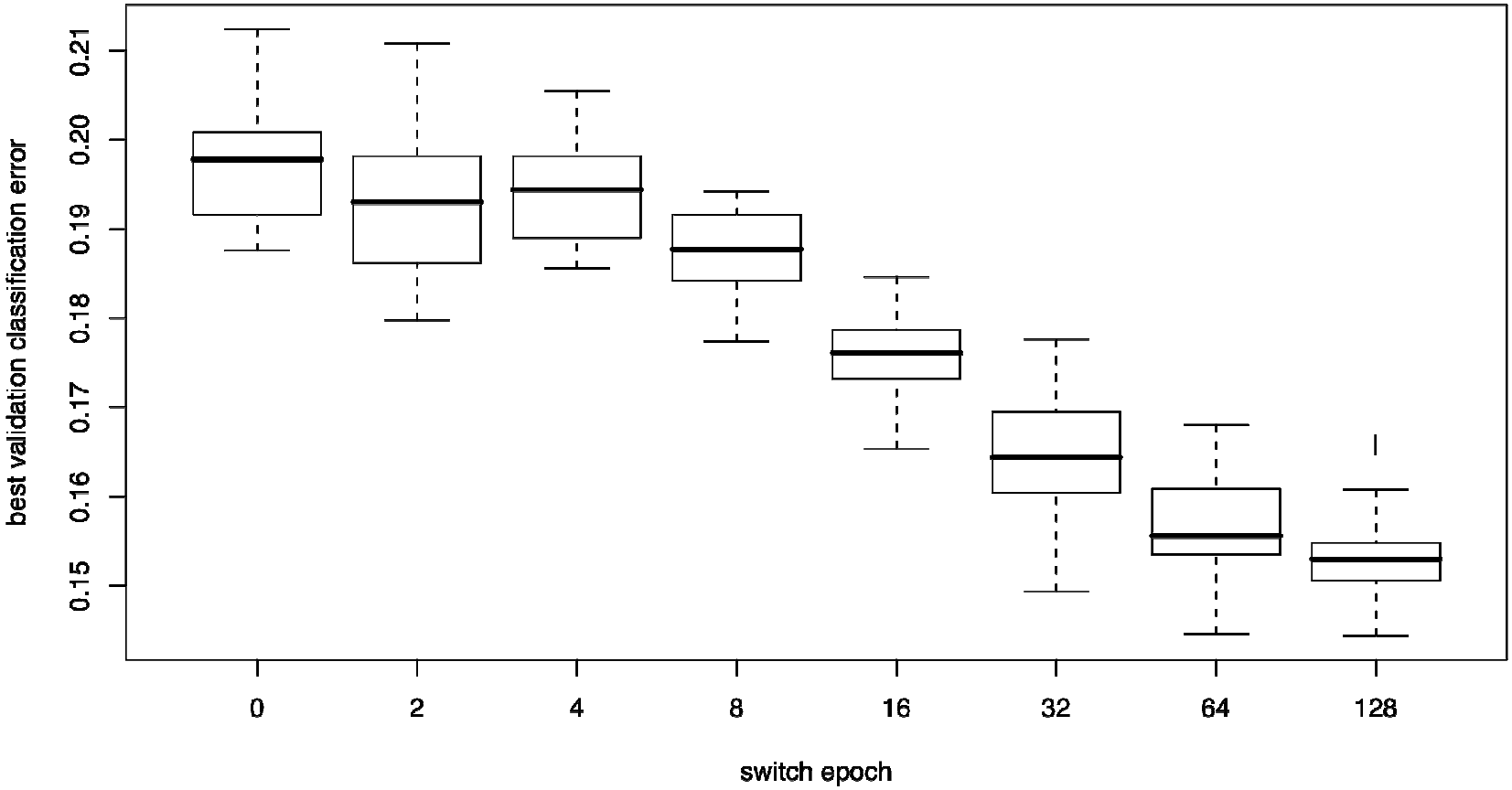
- Sequence of training distributions
- Initially peaking on easier / simpler ones
- Gradually give more weight to more difficult ones until reach target distribution

Shape Recognition

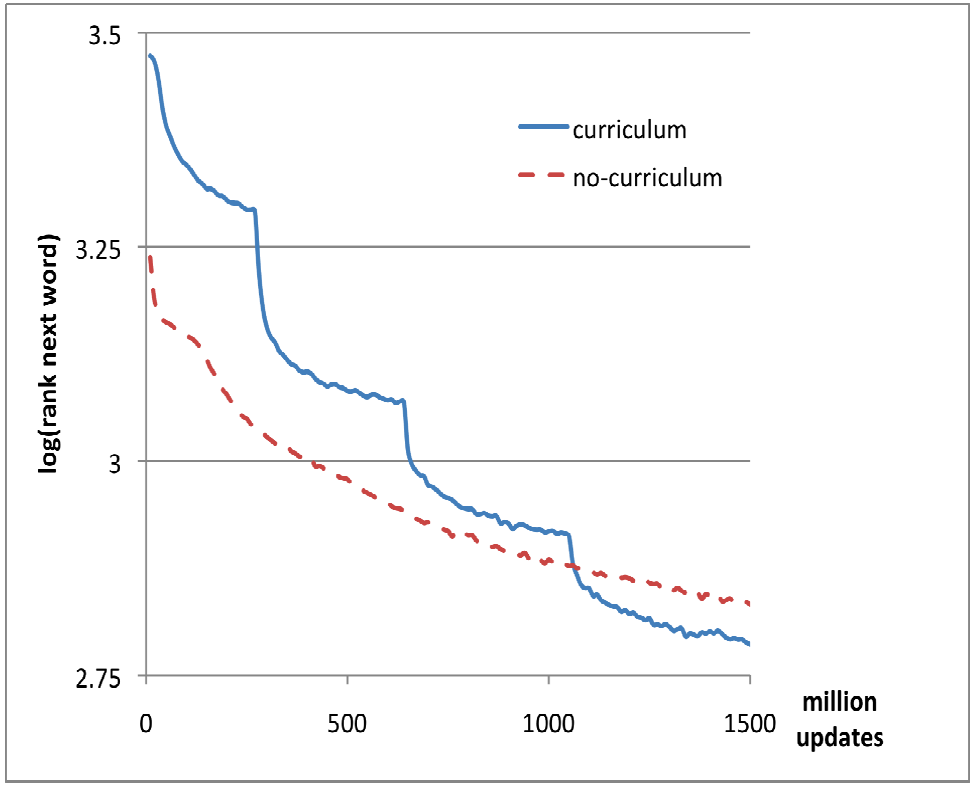
First: easier, basic shapes

Second = target: more varied geometric shapes

Shape Recognition Results



Language Modeling Results



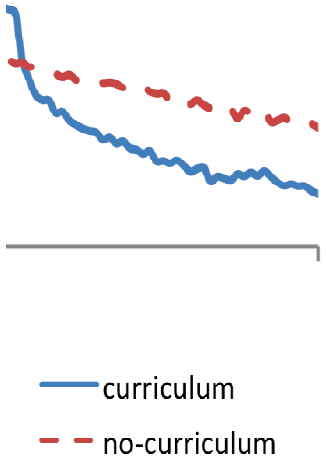
- Gradually increase the vocabulary size (dips)
- Train on Wikipedia with sentences containing only words in vocabulary

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?