Learning Deep Hierarchies of Representations

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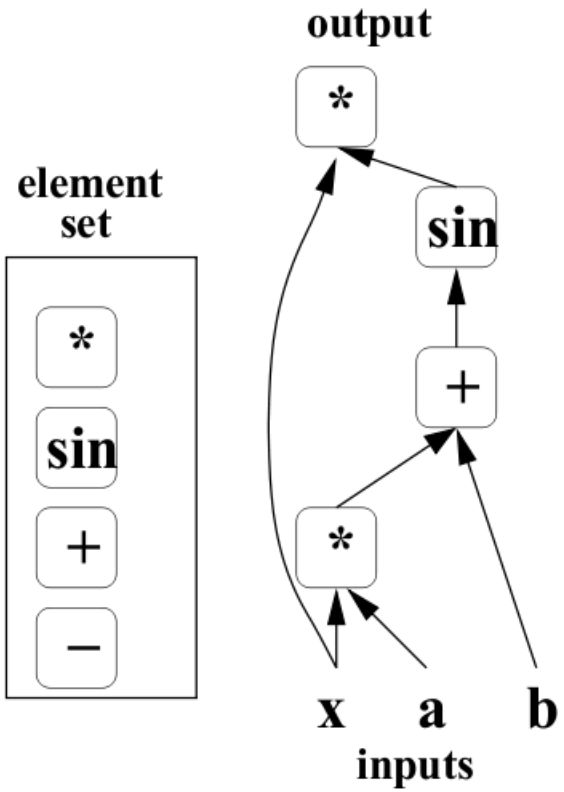
Interesting Experimental Results with Deep Architectures

- 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 or beating state-of-the-art performance in NLP
- Beating deep neural nets without unsupervised component
- Learn visual features similar to V1 and V2 neurons

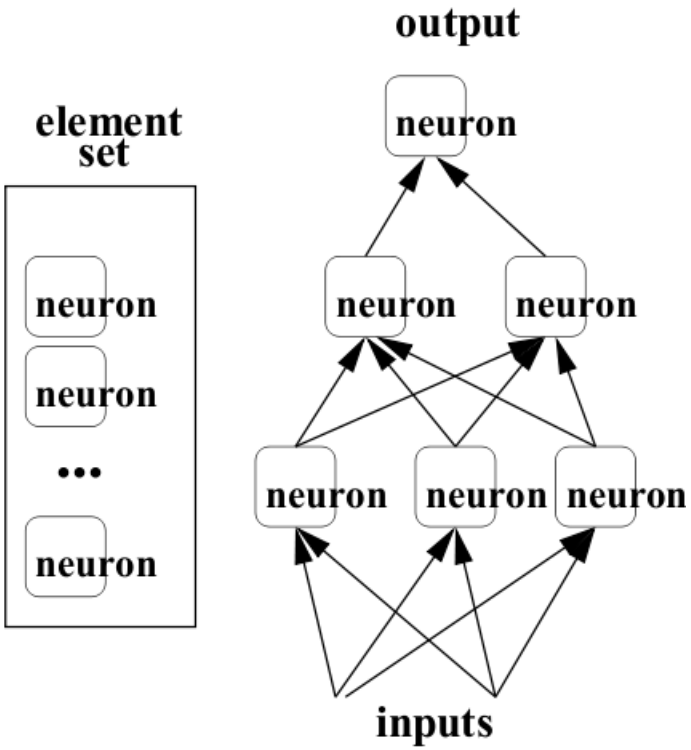
Deep Motivations

- Brains have a deep architecture
- Humans organize their ideas hierarchically, through composition of simpler ideas
- Unsufficiently deep architectures can be exponentially inefficient
- Distributed (possibly sparse) representations 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

Architecture Depth



Depth = 4



Depth = 3

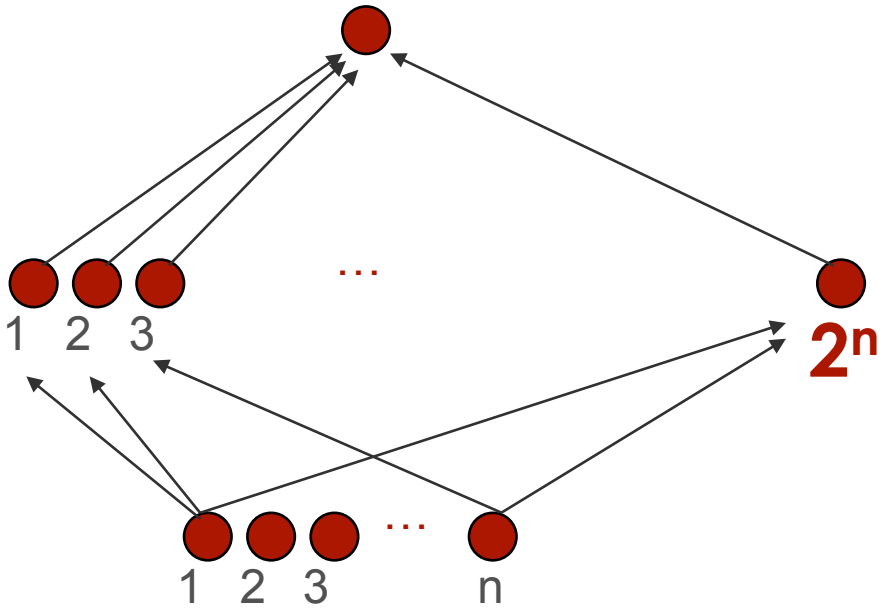
Deep Architectures are More Expressive

Theoretical arguments:

2 layers of { Logic gates / Formal neurons / RBF units } = universal approximator

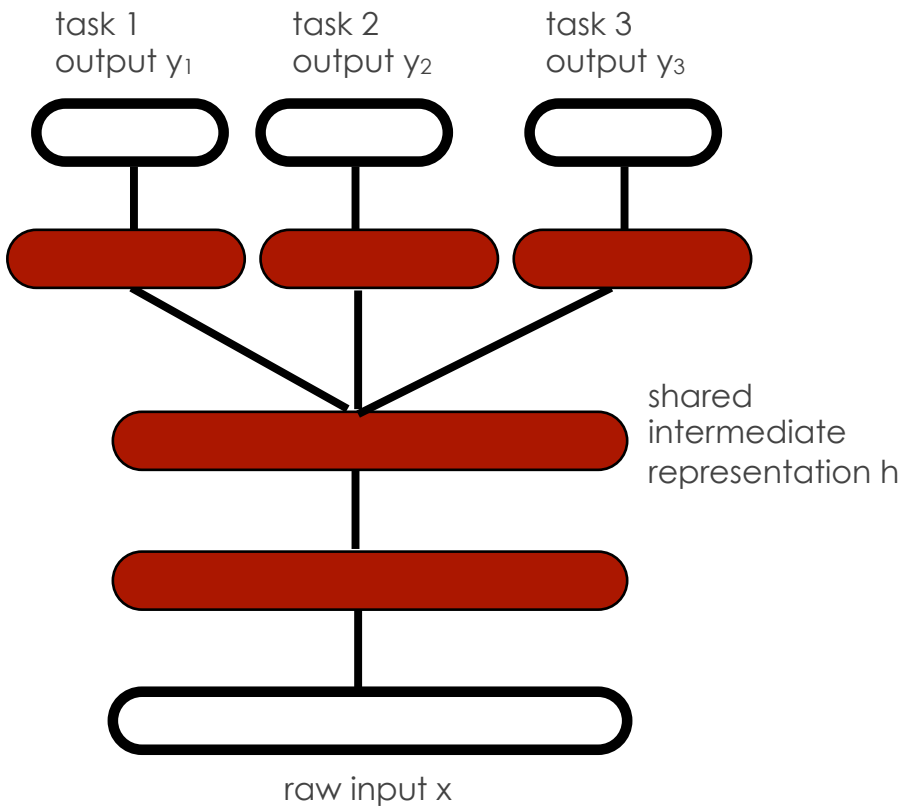
Theorems for all 3:
(Hastad et al 86 & 91, Bengio et al 2007)

Functions compactly represented with k layers may require exponential size with k-1 layers



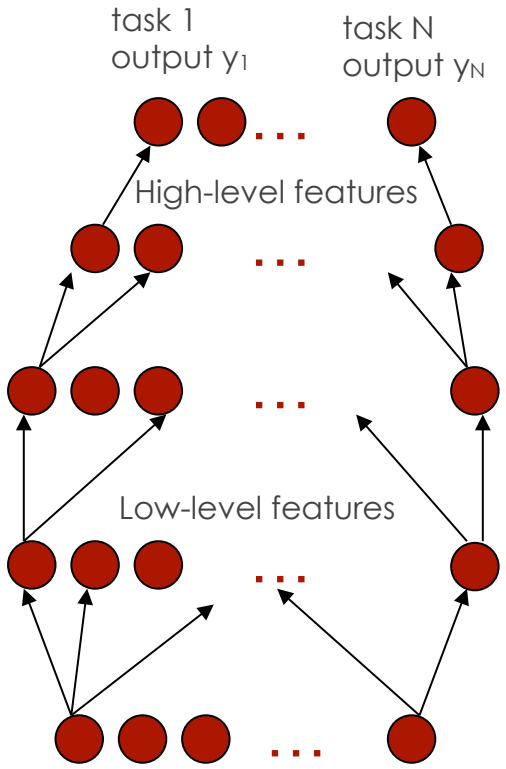
Deep Architectures and Sharing Statistical Strength, Multi-Task Learning

- 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

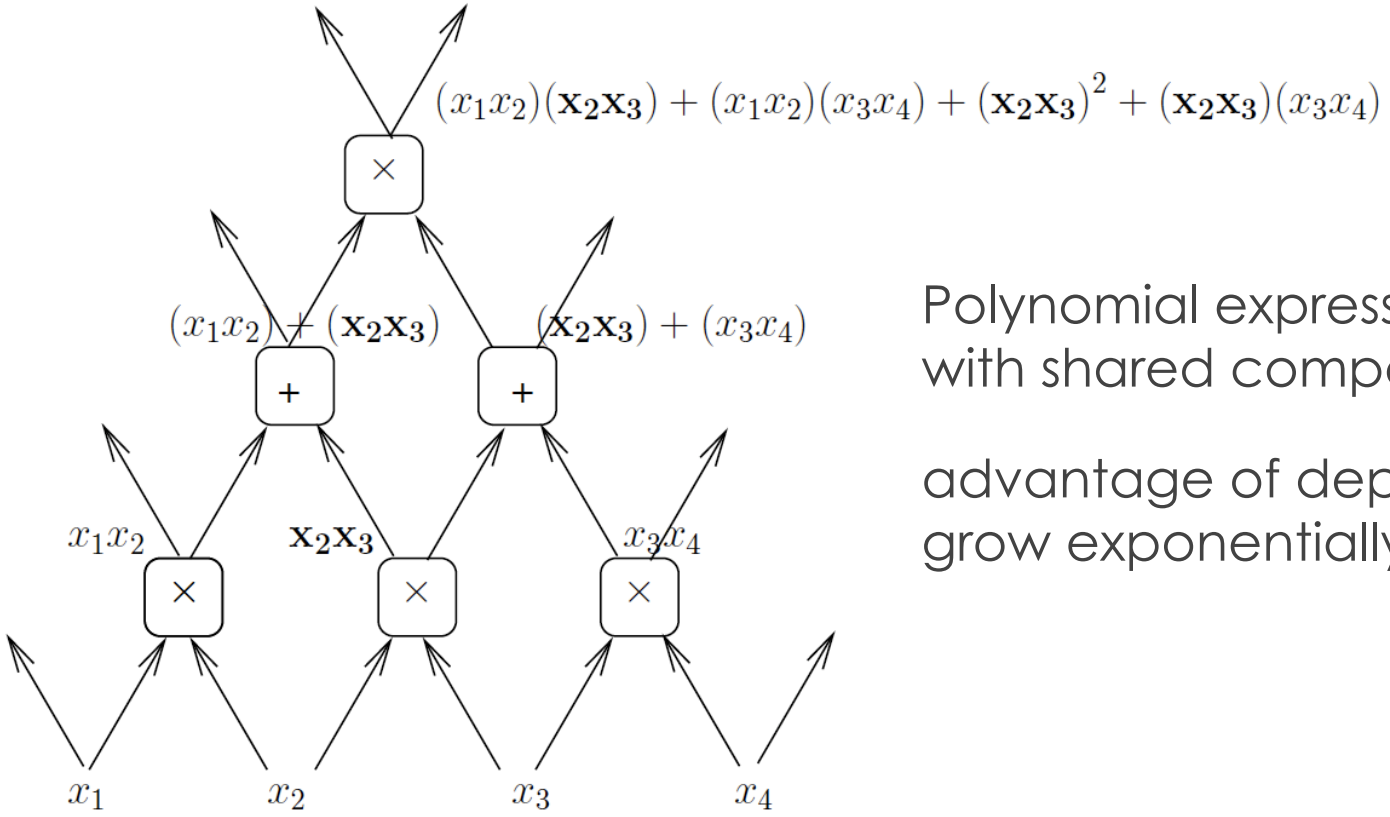


Feature and Sub-Feature Sharing

- 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



Sharing Components in a Deep Architecture



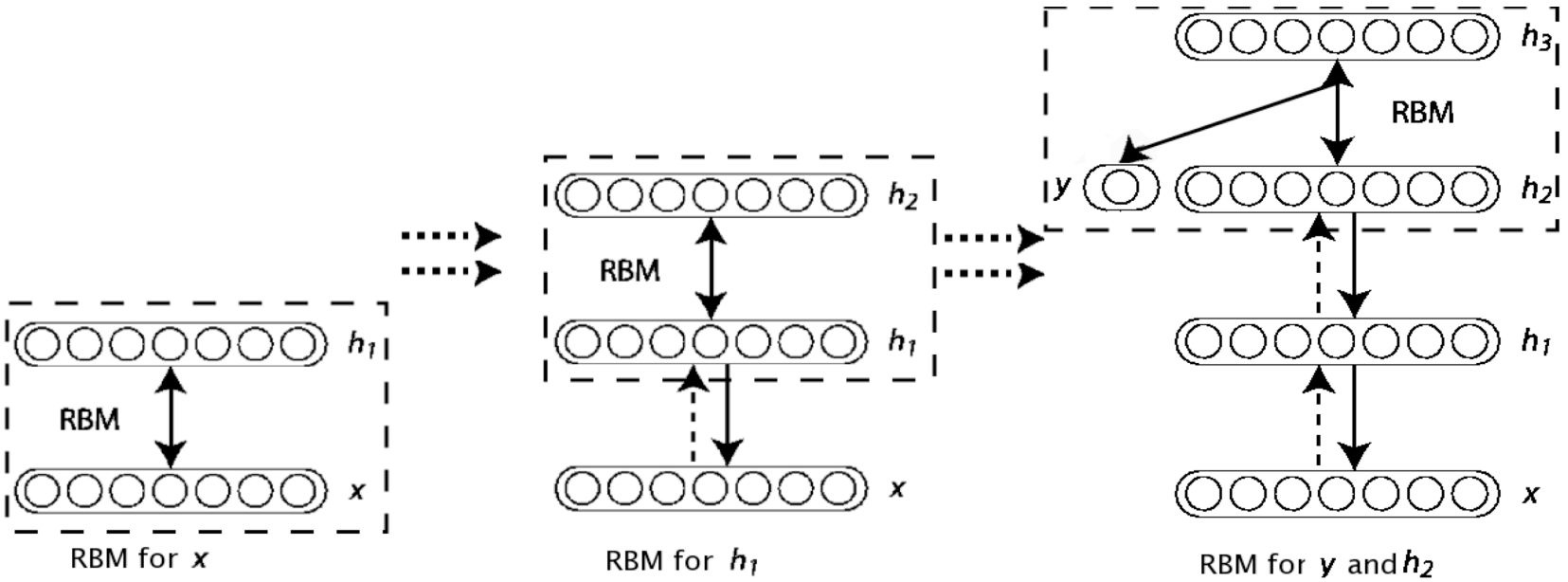
Polynomial expressed with shared components:

advantage of depth may grow exponentially

The Deep Breakthrough

- Before 2006, training deep architectures was unsuccessful, except for convolutional neural nets
- Hinton, Osindero & Teh « A Fast Learning Algorithm for Deep Belief Nets », *Neural Computation*, 2006
- Bengio, Lamblin, Popovici, Larochelle « Greedy Layer-Wise Training of Deep Networks », *NIPS'2006*
- Ranzato, Poultney, Chopra, LeCun « Efficient Learning of Sparse Representations with an Energy-Based Model », *NIPS'2006*

Greedy Layer-Wise Pre-Training



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

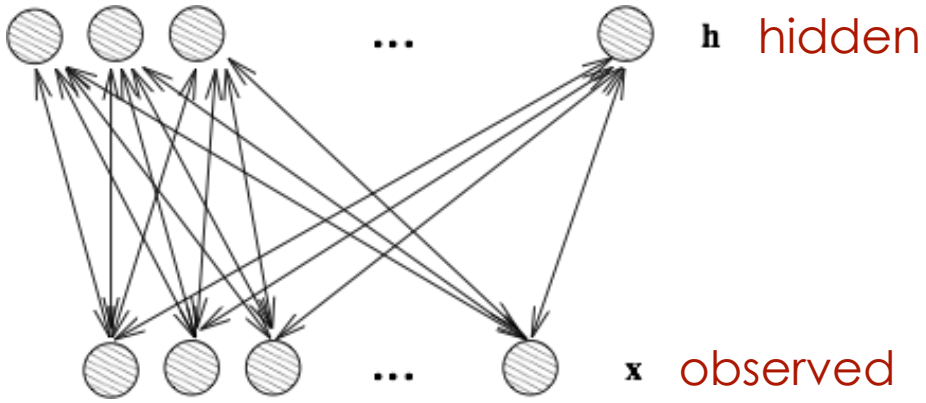
Greedy Layer-Wise Unsupervised Pre-Training Algorithm

- Train unsupervised feature extractor (e.g. RBM, auto-encoder) mapping input x to representation h_1, capturing main factors of variation in x (models $P(x)$)
- Taking $h_1(x)$ as an input, train a second unsupervised feature extractor, obtaining representation h_2 of x
- Etc. to level k gives h_k
- Plug a supervised classifier $P(Y \mid h_k(x))$ on top, taking h_k as input
- Fine-tune parameters of whole system $P(Y \mid x)$ wrt supervised objective

Restricted Boltzman Machine

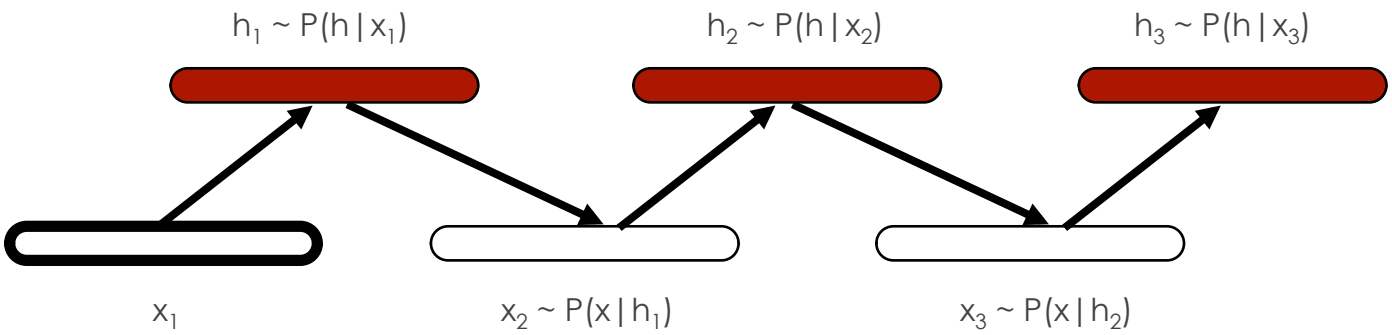
- The most popular building block for deep architectures
  (Smolensky 86, Hinton 2002)

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



- Bipartite undirected graphical model
- *h~P(h | x)*, or *(P(h$_i$=1 | x))* are representations of x

Gibbs Sampling in RBMs



P(h | x) and P(x | h) factorize

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

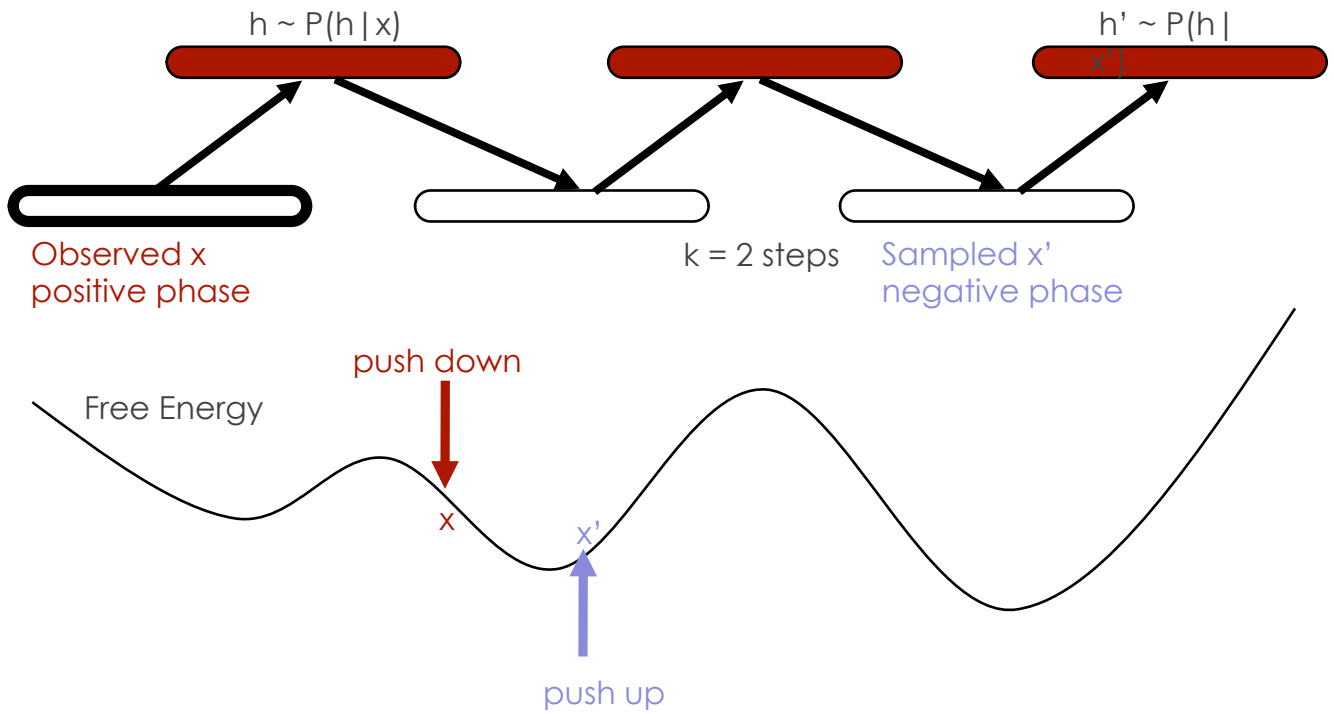
- Easy inference
- Convenient Gibbs sampling
  x→h→x→h…

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 ICML workshop talks)
Tempered MCMC:	use higher temperature to escape modes

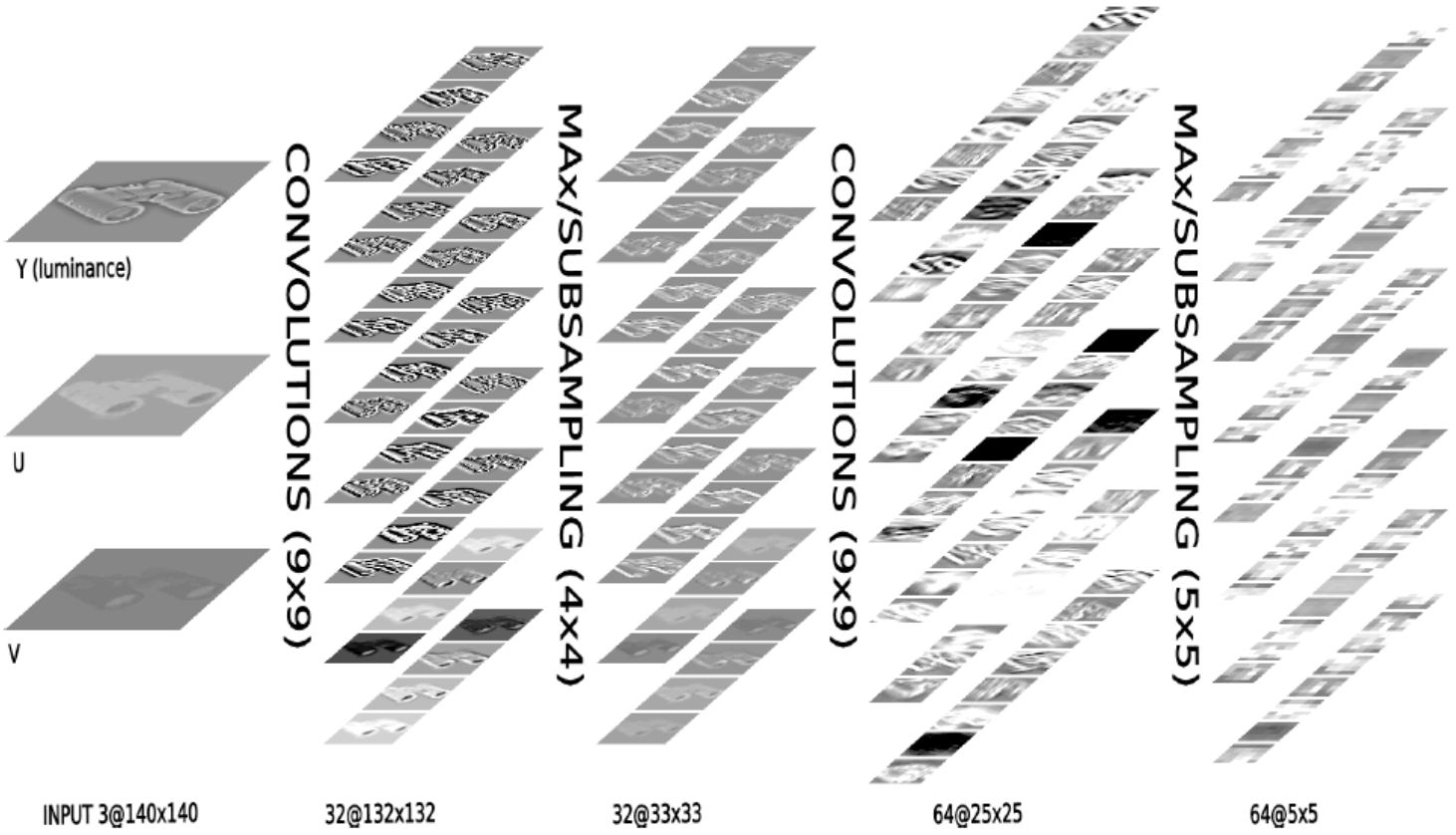
Contrastive Divergence

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



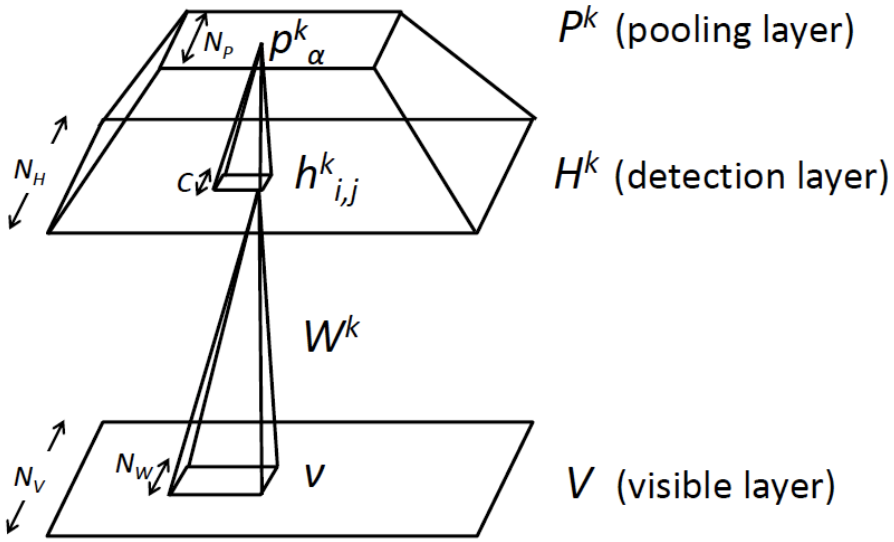
Deep Convolutional Architectures

Mostly from Le Cun's (NYU) and Ng's (Stanford) groups:
state-of-the-art on MNIST digits, Caltech-101 objects, faces



Convolutional DBNs

(Lee et al, ICML'2009)

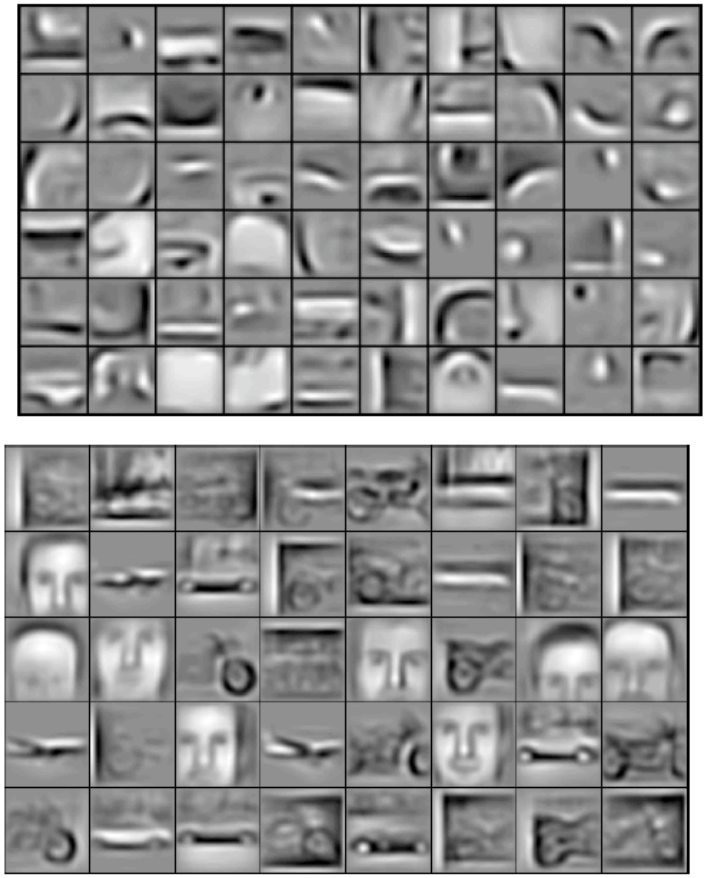


P^k (pooling layer)

H^k (detection layer)

V (visible layer)

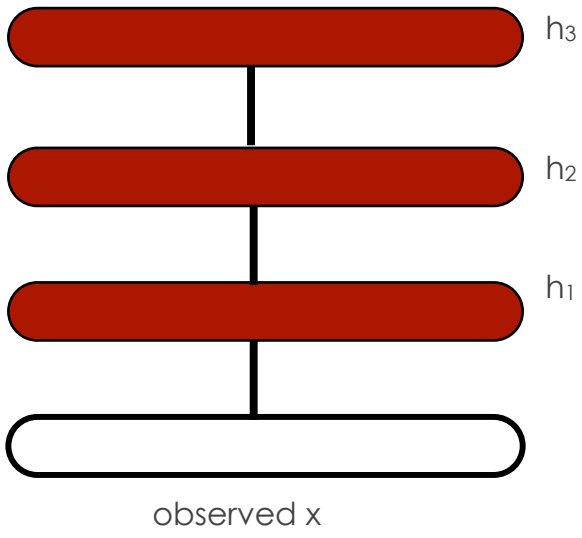
faces, cars, airplanes, motorbikes



Deep Boltzman Machines

(Salakhutdinov et al, AISTATS 2009, Lee et al, ICML 2009)

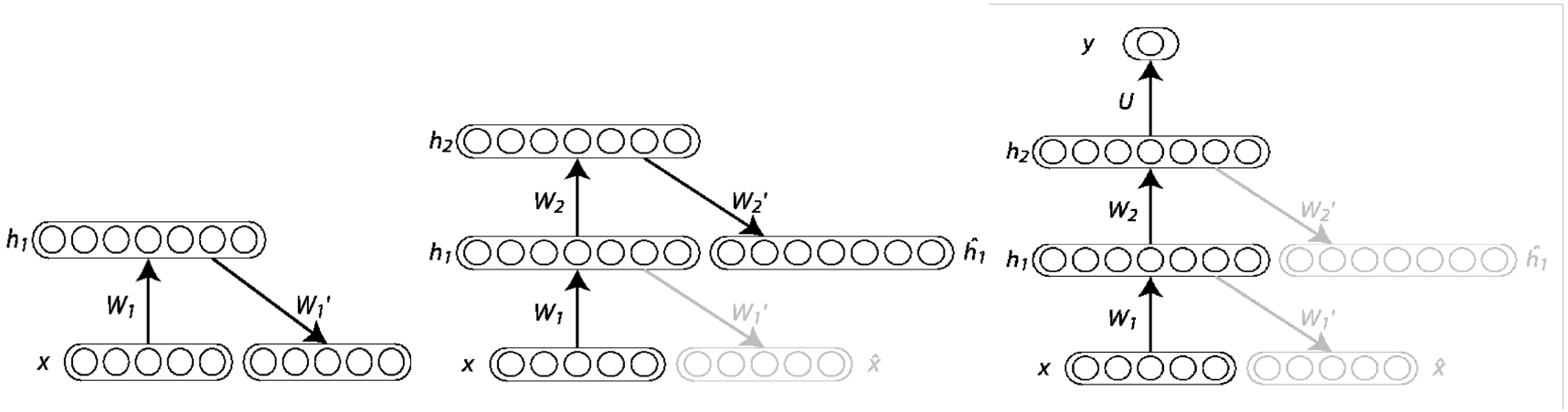
- Positive phase: variational approximation (mean-field)
- Negative phase: persistent chain
- **Can (must) initialize from stacked RBMs**
- Improved performance on MNIST from 1.2% to .95% error
- Can apply AIS with 2 hidden layers



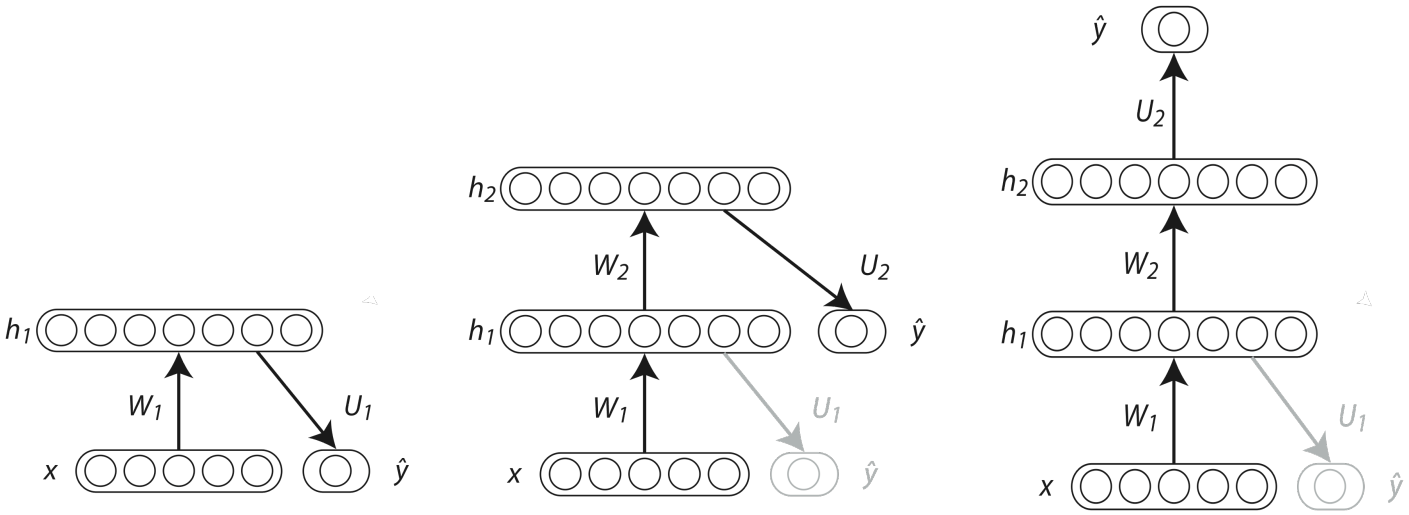
Why are Classifiers Obtained from DBNs Working so Well?

- General principles?
- Would these principles work for other single-level algorithms?
- Why does it work?

Stacking Auto-Encoders



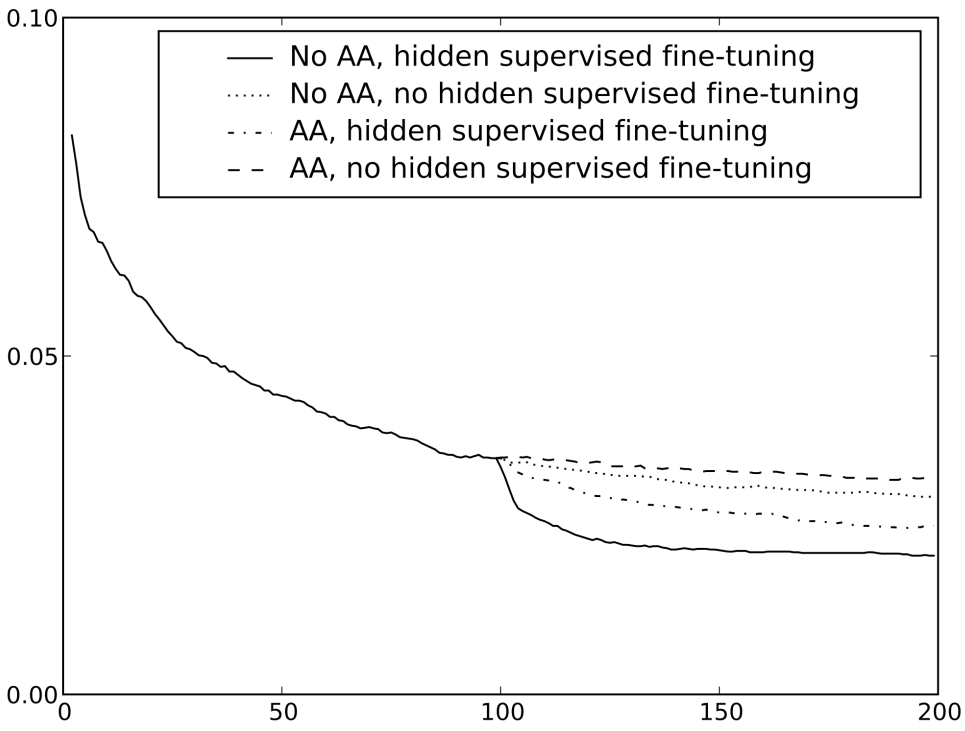
Greedy Layerwise Supervised Training



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

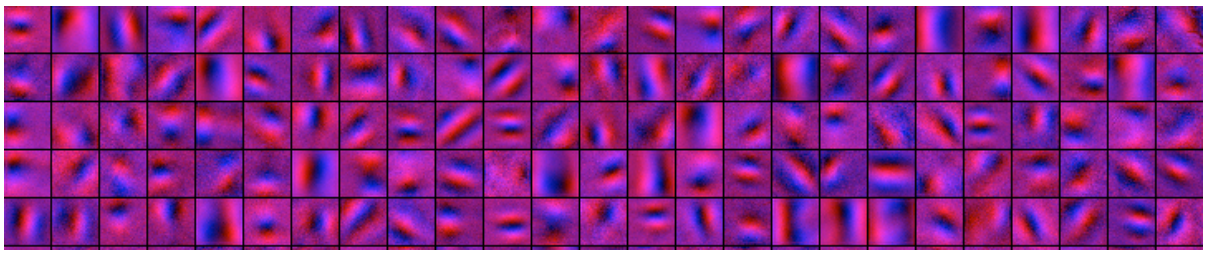


Level-Local Learning is Important

- Initializing each layer of an unsupervised deep Boltzmann machine helps a lot
- Initializing each layer of a supervised neural network as an RBM or auto-encoder helps a lot
- Helps most the layers further away from the target
- Jointly training all the levels of a deep architecture is difficult

Replacing RBMs by Other Layer-Local Unsupervised Learning

- Auto-encoders (Bengio et al, NIPS'2006)
- Sparse auto-encoders (Ranzato et al, NIPS'2006)
- Kernel PCA (Erhan 2008)
- Denoising auto-encoders (Vincent et al, ICML'2008)
- Unsupervised embedding (Weston et al, ICML'2008)
- Slow features (Mohabi et al, ICML'2009, Bergstra & Bengio NIPS'2009)



Sparse Auto-Encoders

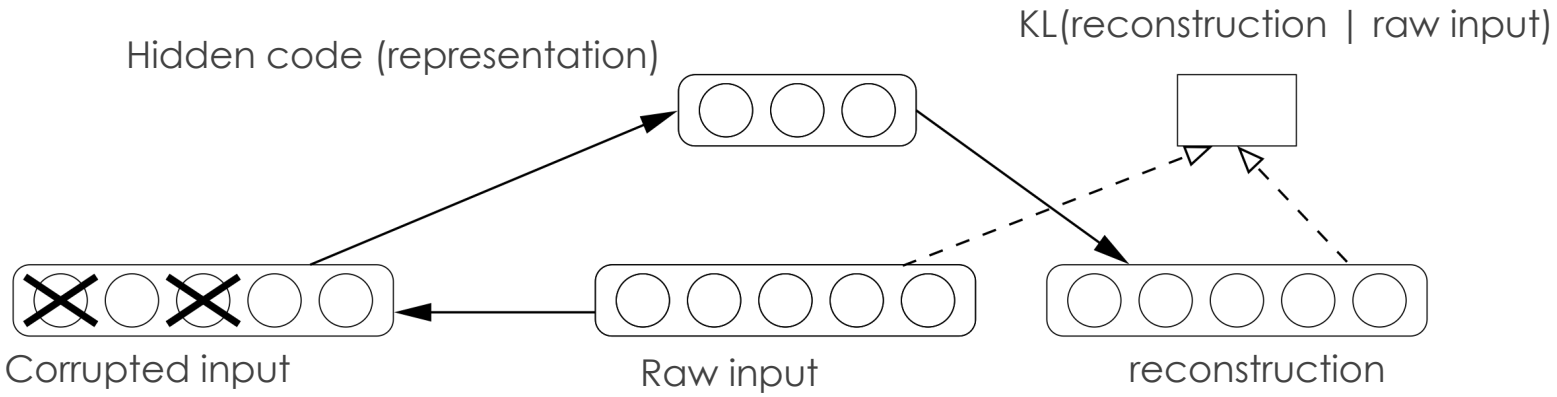
(Ranzato et al, 2007; Ranzato et al 2008)

- 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 obtained with a convolutional DBN (Lee et al, ICML'2009)

Denoising Auto-Encoder

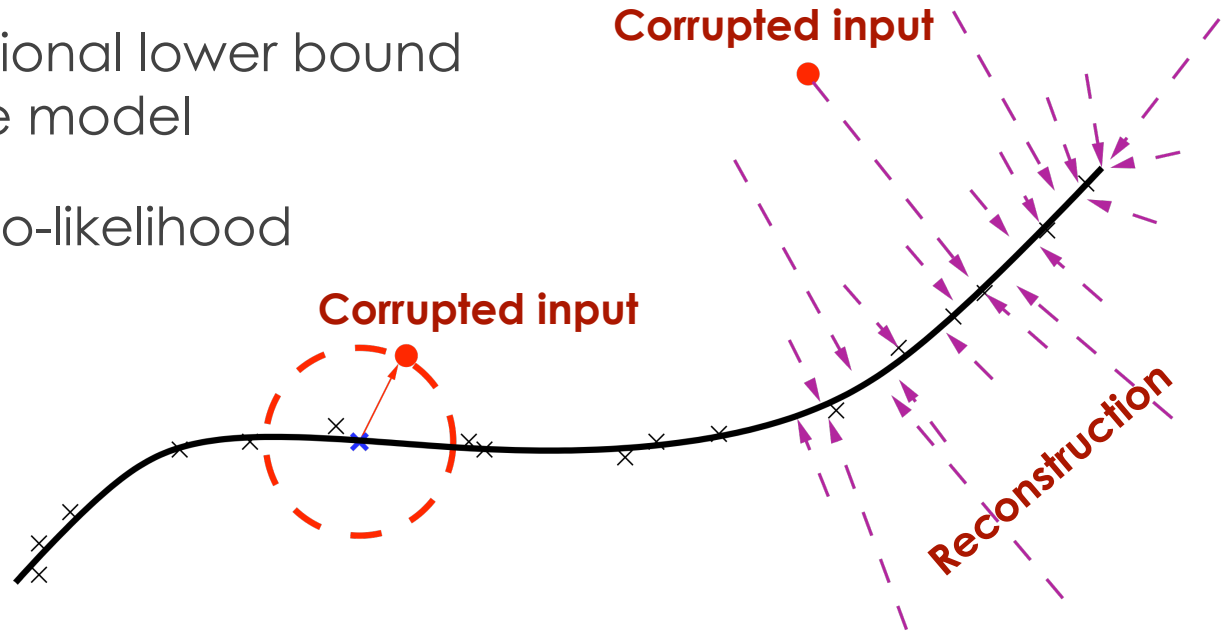
(Vincent et al, ICML 2008)

- Corrupt the input
- Reconstruct the uncorrupted input



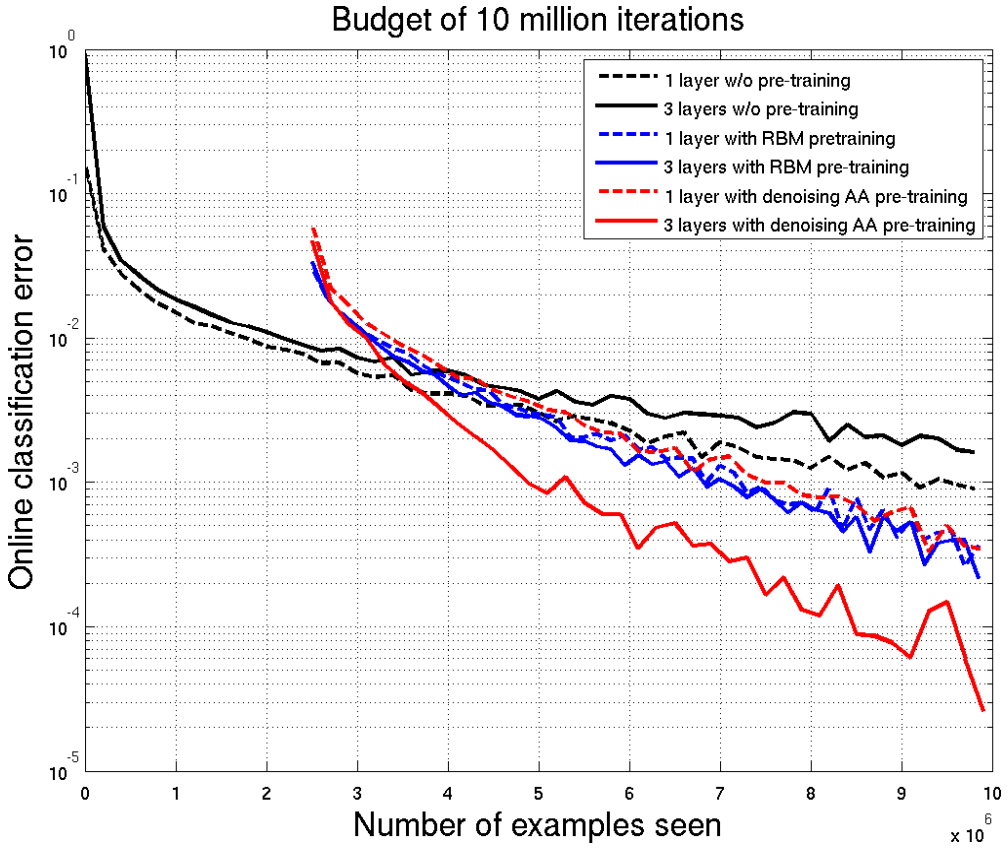
Denoising Auto-Encoder

- 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

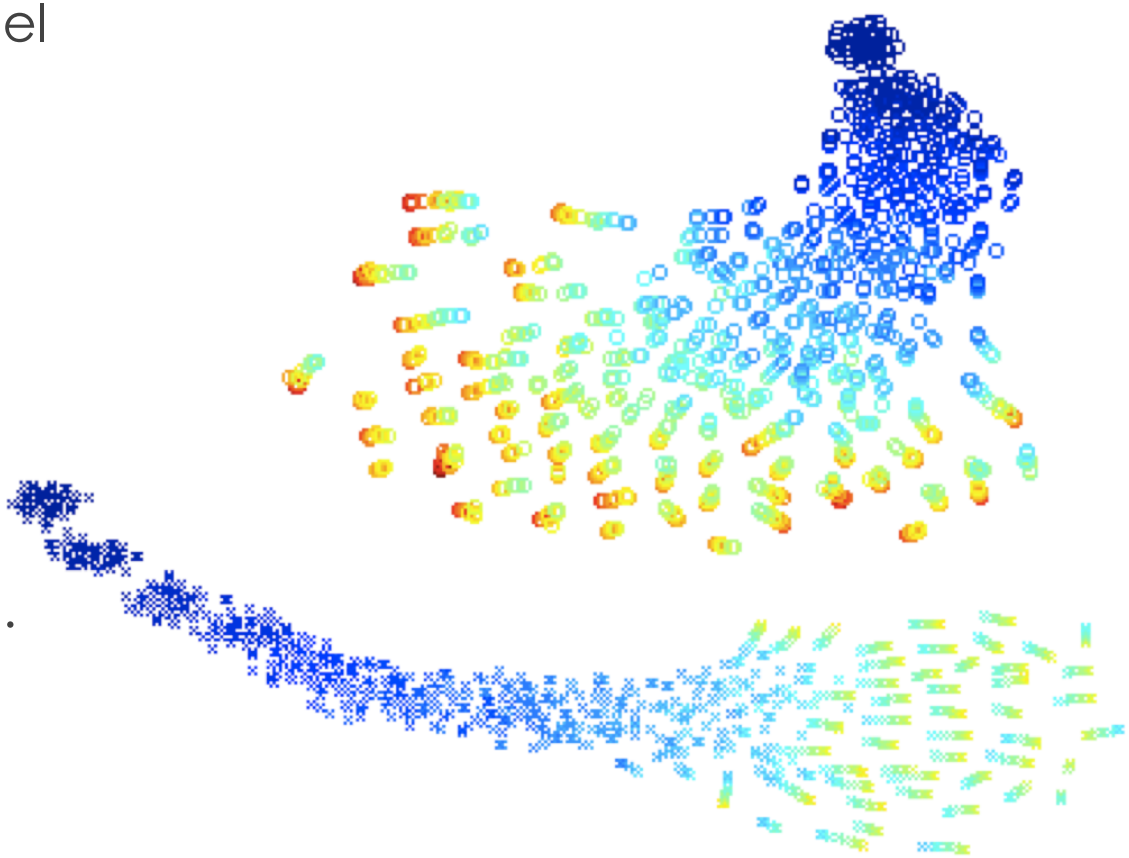
Why is Unsupervised Pre-Training Working So Well?

- 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

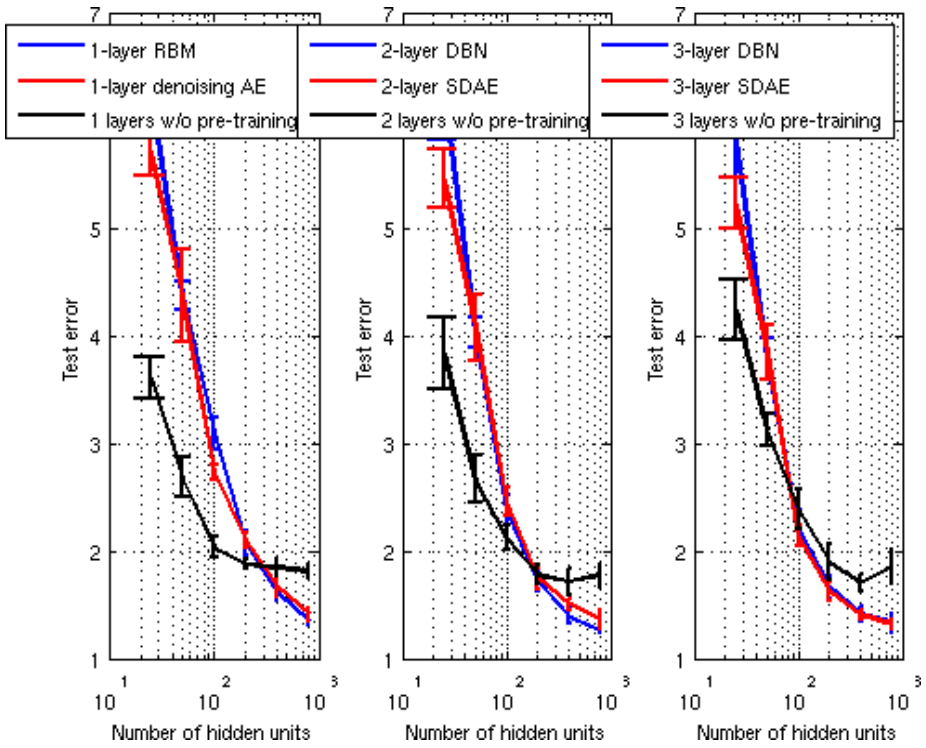
Learning Trajectories in Function Space

- 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/o pre-training



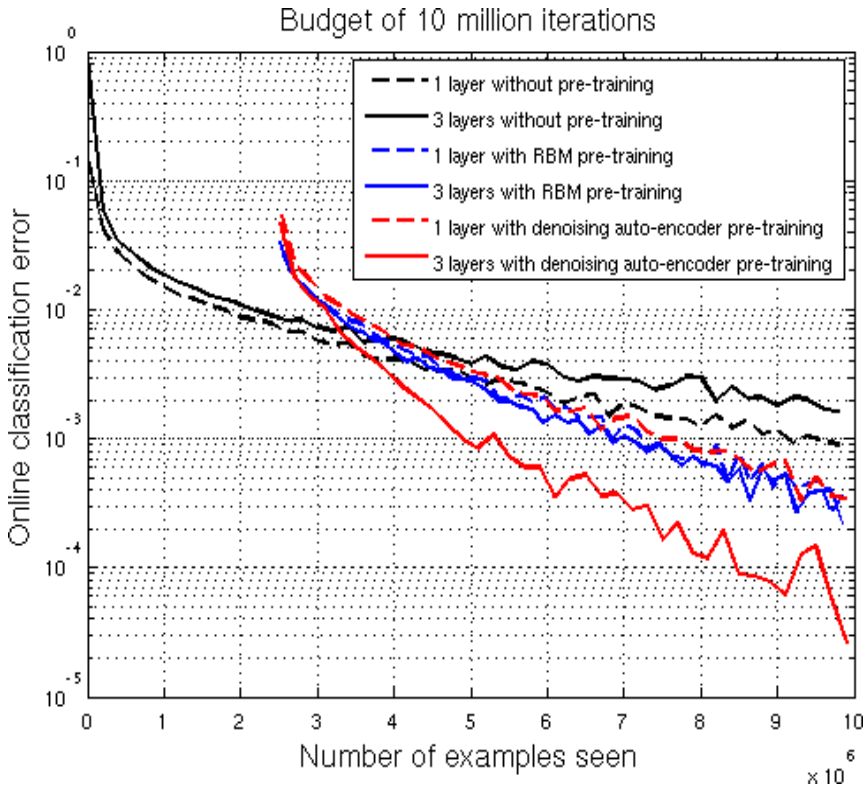
Unsupervised Learning as Regularizer

- 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

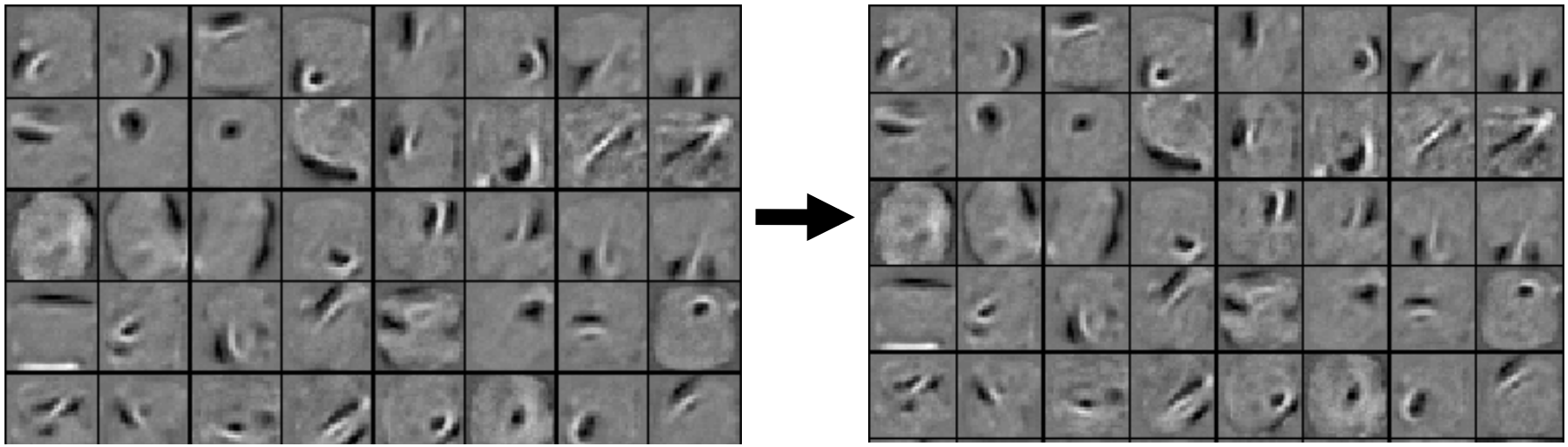


Better Optimization of Online Error

- Both training and online error are smaller with unsupervised pre-training
- As # samples → ∞ 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

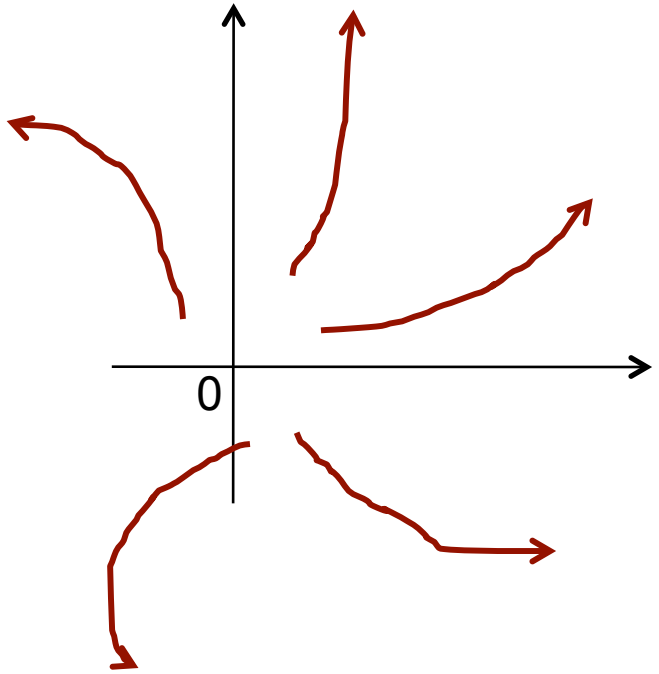


Before fine-tuning

After fine-tuning

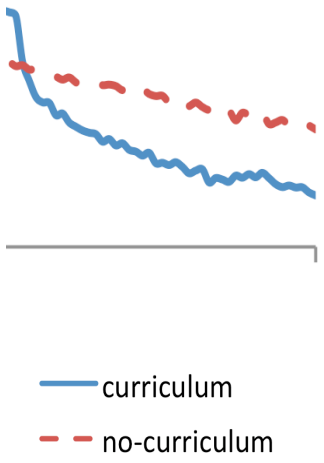
Learning Dynamics of Deep Nets

- 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



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



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 sometimes 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

Research Program

- Unsupervised pre-training is good but we want more
- Understand why gradient-based optimization of lower layers of deep supervised architecture gets stuck
- Is it the same reason that global coordination fails in deep Boltzmann machines?
- Is it related to problem with recurrent nets and dynamic Bayes net failing with long-term dependencies? Important to capture contextual effects in sequential data such as video and text.
- Applications to information retrieval:

Deep Representations for Information Retrieval

- Sparsity to help computational & representational efficiency
  - Combine semantic hashing idea (make representation gradually nearly binary) with sparse code penalty (reduced cost of measuring similarity between objects)
  - Allow effective number of non-zeros to vary per example (representational efficiency)
- Combining supervised (ranking) & unsupervised criteria **online**
  - Current training process with phases not practical with huge datasets = online
- Put different modalities (image, query) in the same space
  - May actually help each other during training
  - Learn a distributed representation of requests to generalize across rarely occuring requests

Thank you for your attention!

- Questions?
- Comments?