Tutorial:
Learning Deep Architectures

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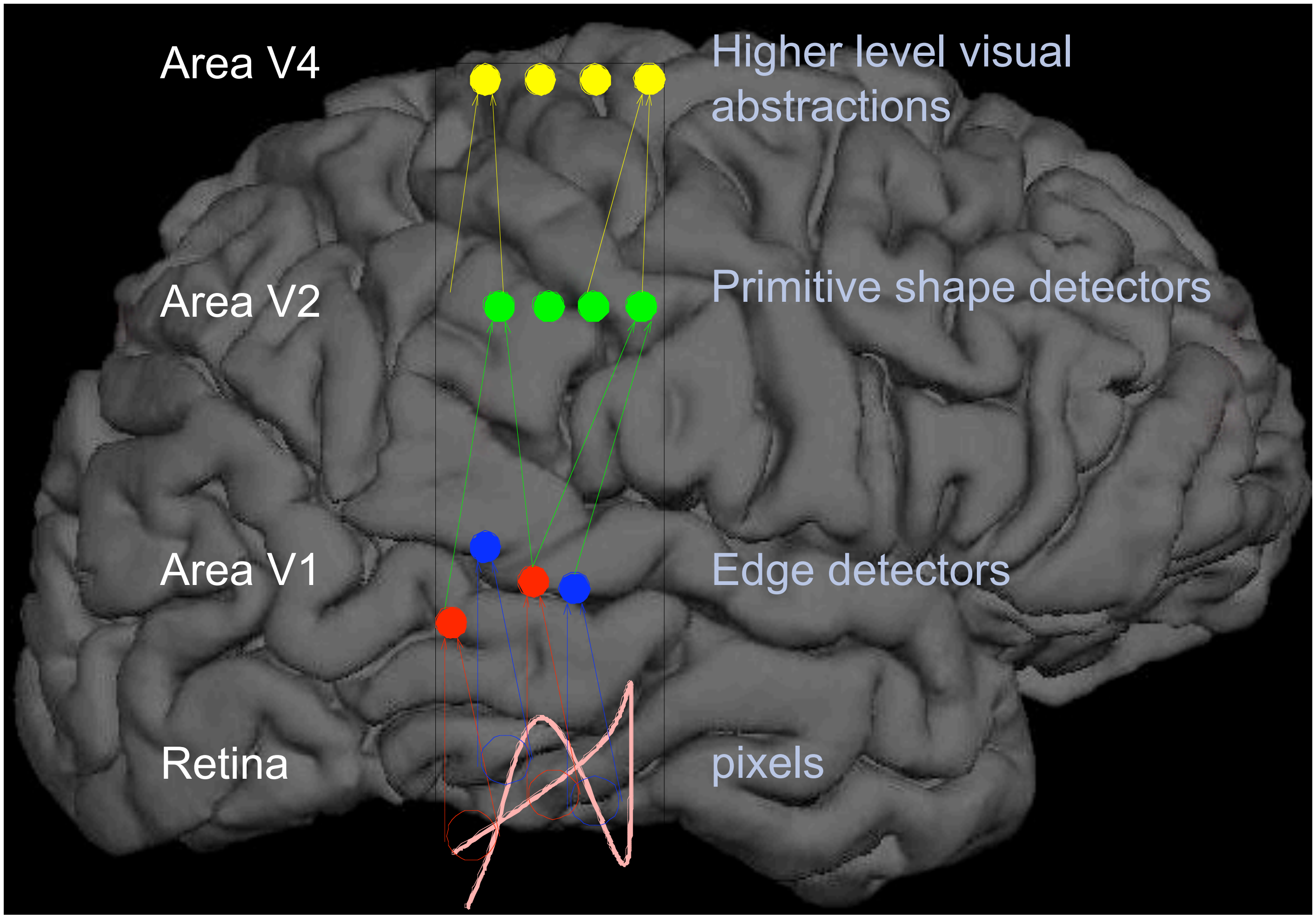
Deep Motivations

- 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
- Intermediate representations allow sharing statistical strength

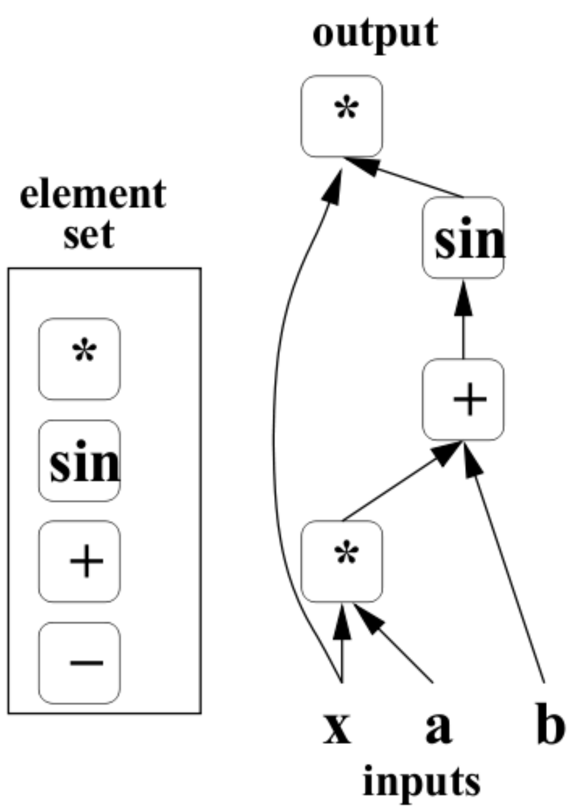
Deep Architecture in the Brain



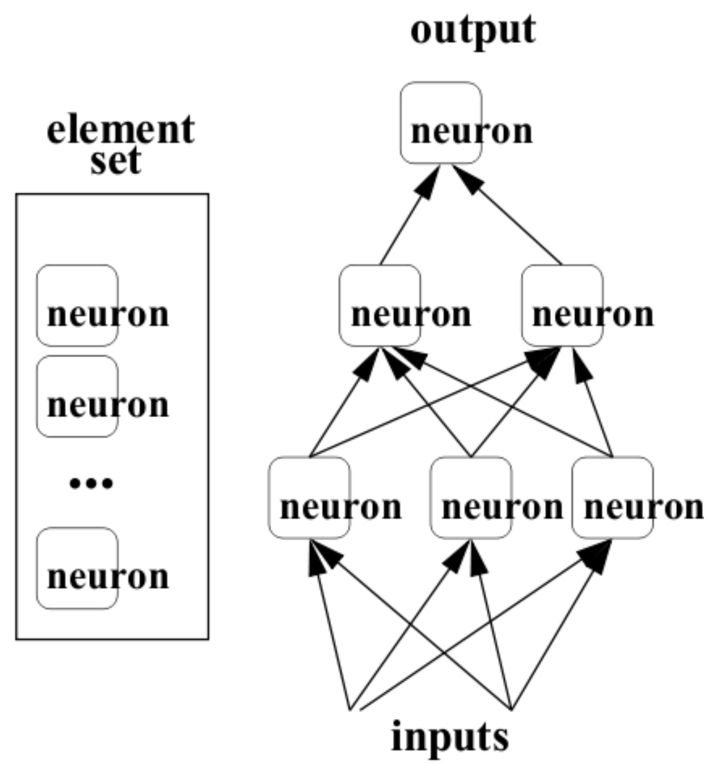
Deep Architecture in our Mind

- 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

Architecture Depth



Depth = 4

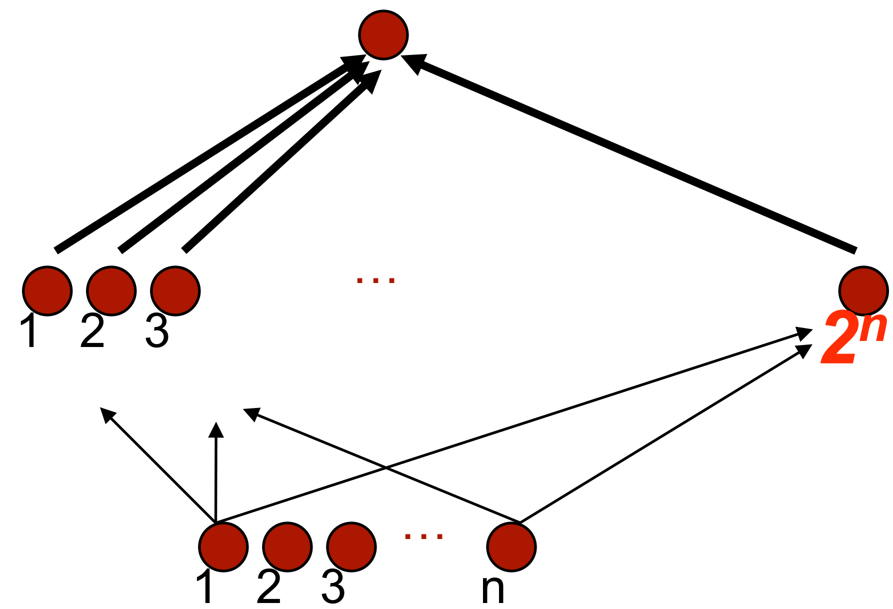


Depth = 3

Good News, Bad News

Theoretical arguments: deep architectures can be

2 layers of { logic gates / formal neurons / RBF units } = universal approximator



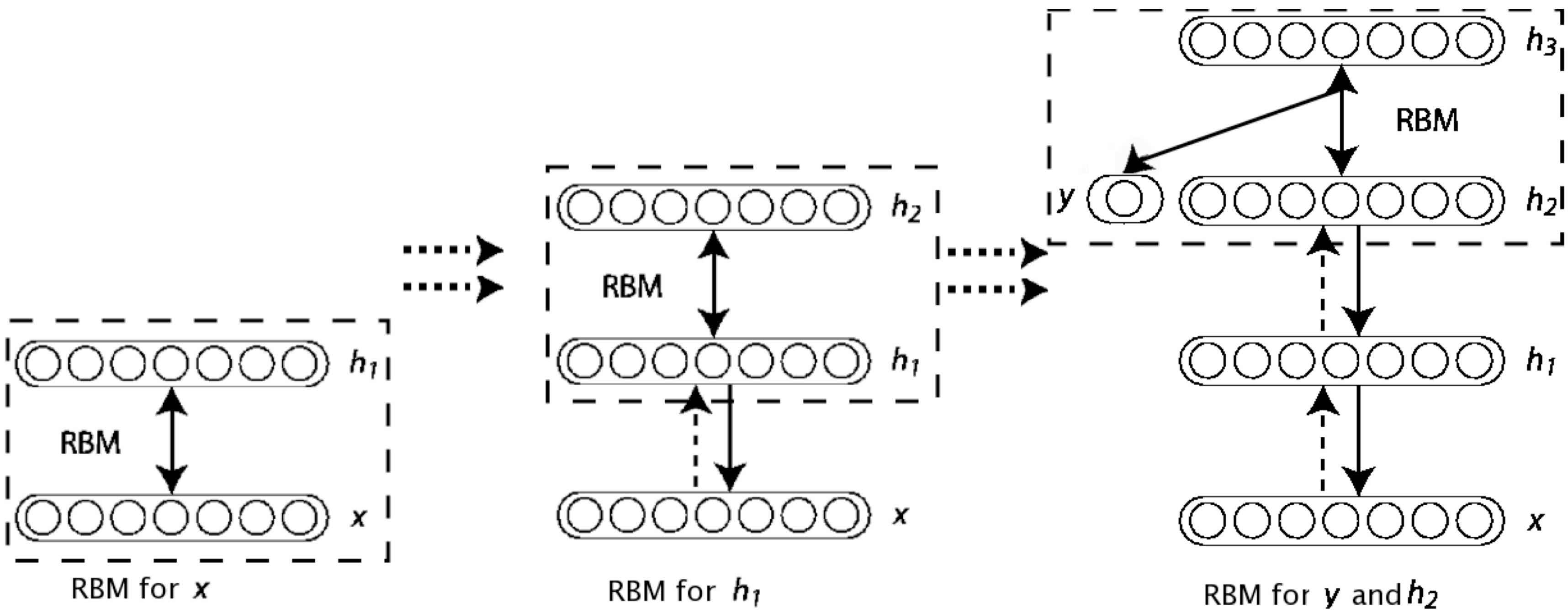
Theorems for all 3:
(Hastad et al 86 & 91, Bengio et al 2007)

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

The Deep Breakthrough

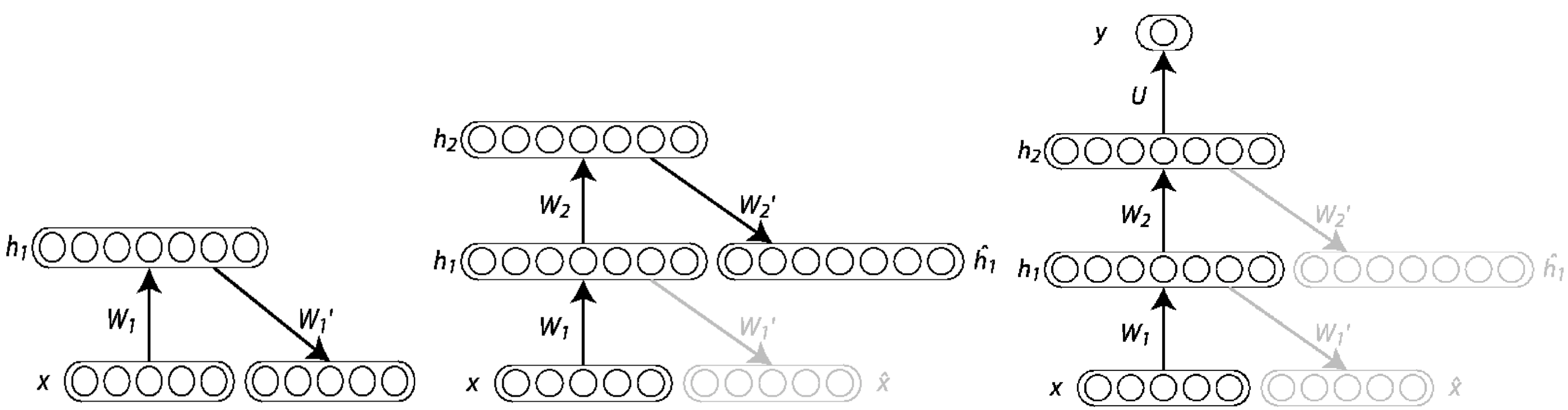
- Before 2006, training deep architectures was unsuccessful, except for convolutional neural nets
- Hinton, Osindero & Teh « A Fast Learning Algorithm for Deep Belief Nets », *Neural Computation*, 2006
- Bengio, Lamblin, Popovici, Larochelle « Greedy Layer-Wise Training of Deep Networks », *NIPS'2006*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

Greedy Layer-Wise Pre-Training

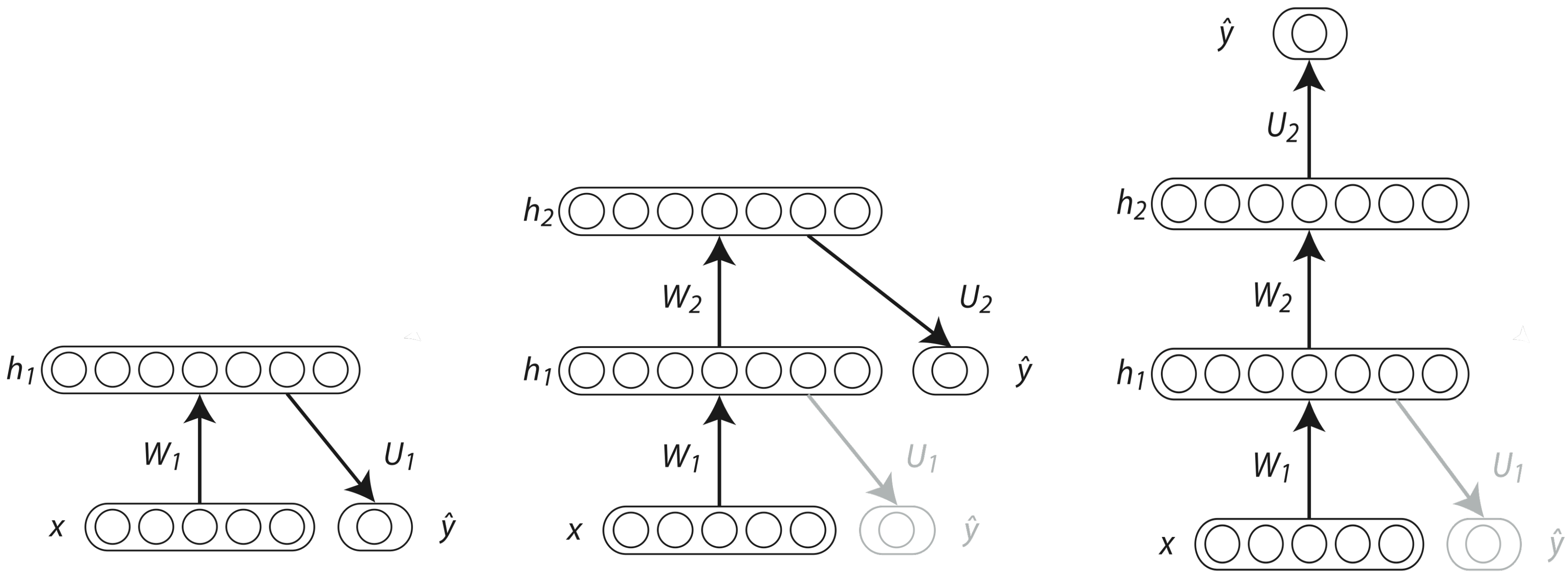


Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)

Stacking Auto-Encoders



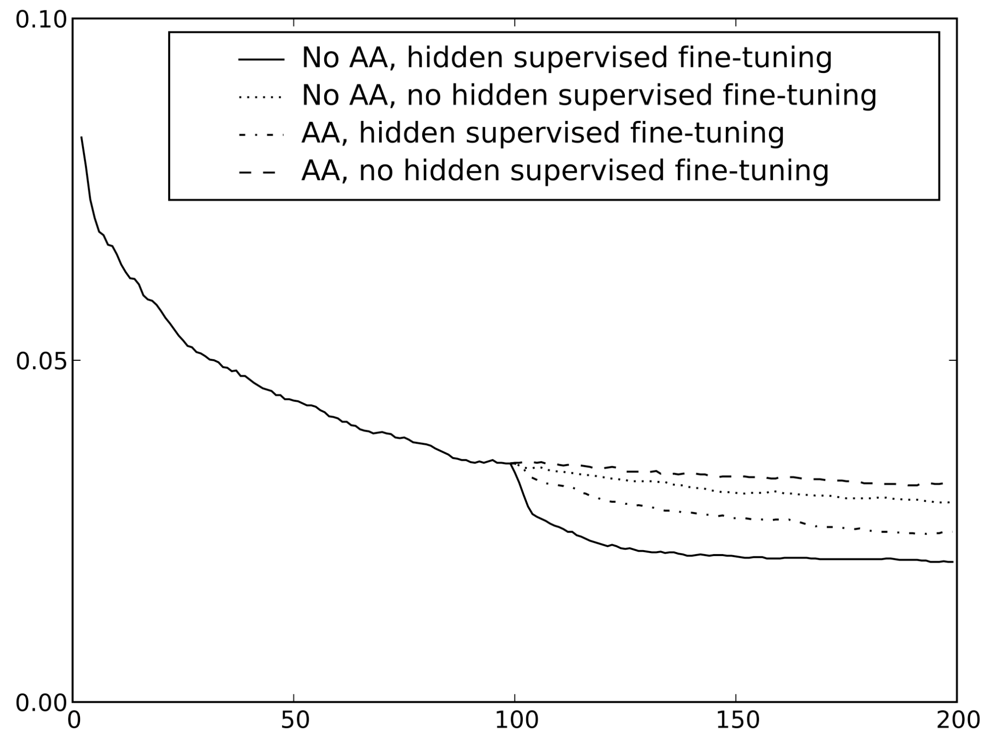
Greedy Layerwise Supervised Training



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

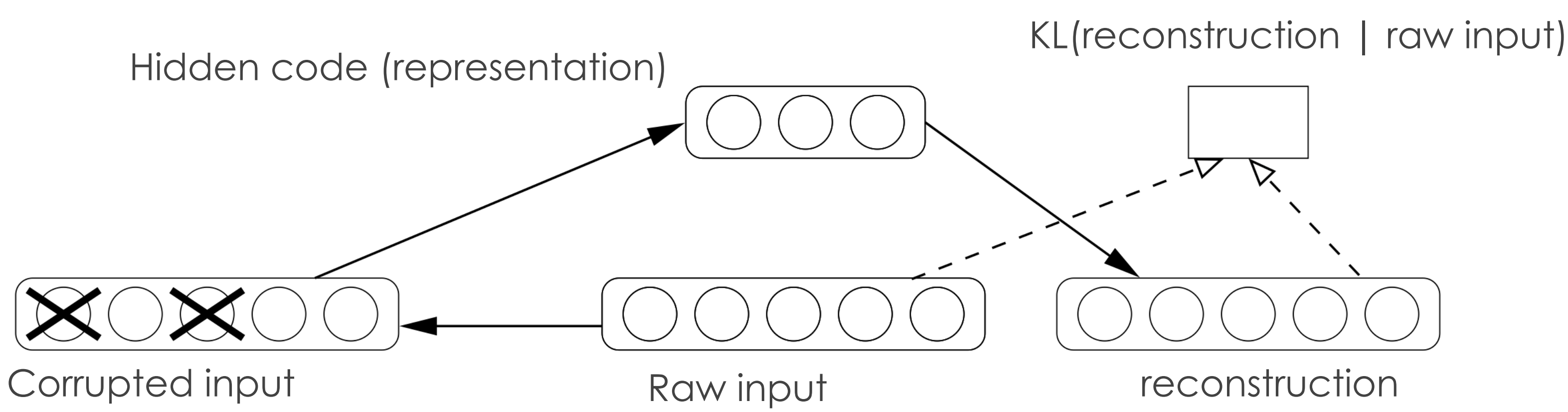
Supervised Fine-Tuning is Important

- 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



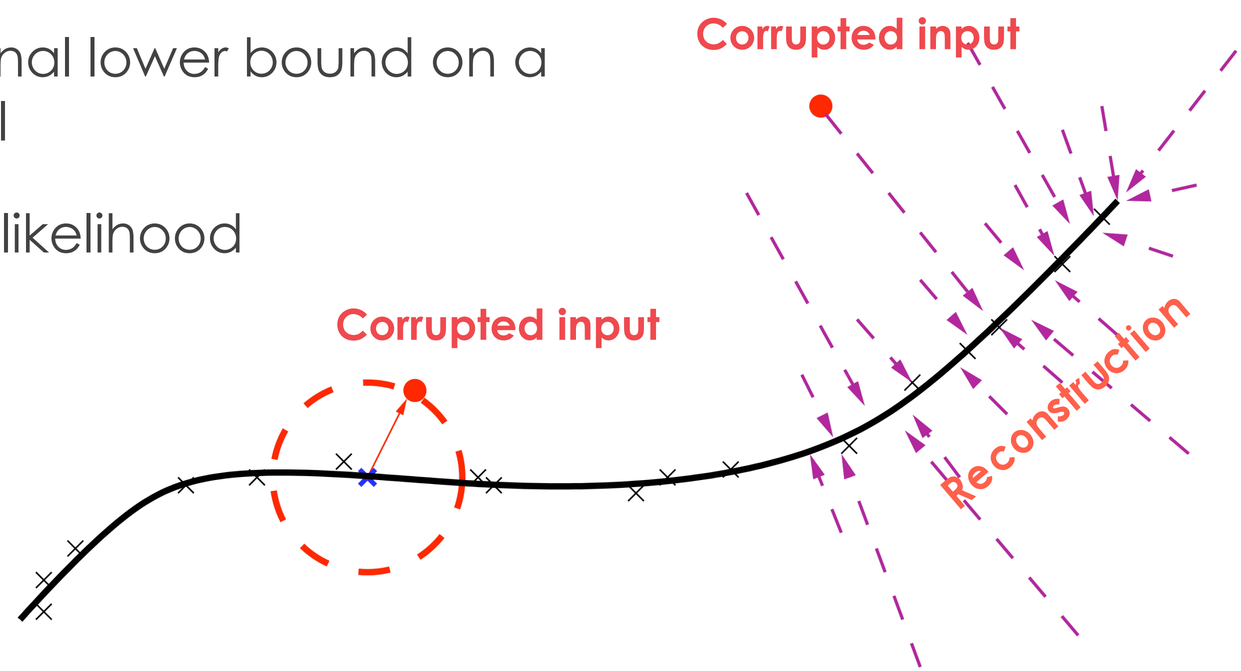
Denoising Auto-Encoder

- Corrupt the input
- Reconstruct the uncorrupted input



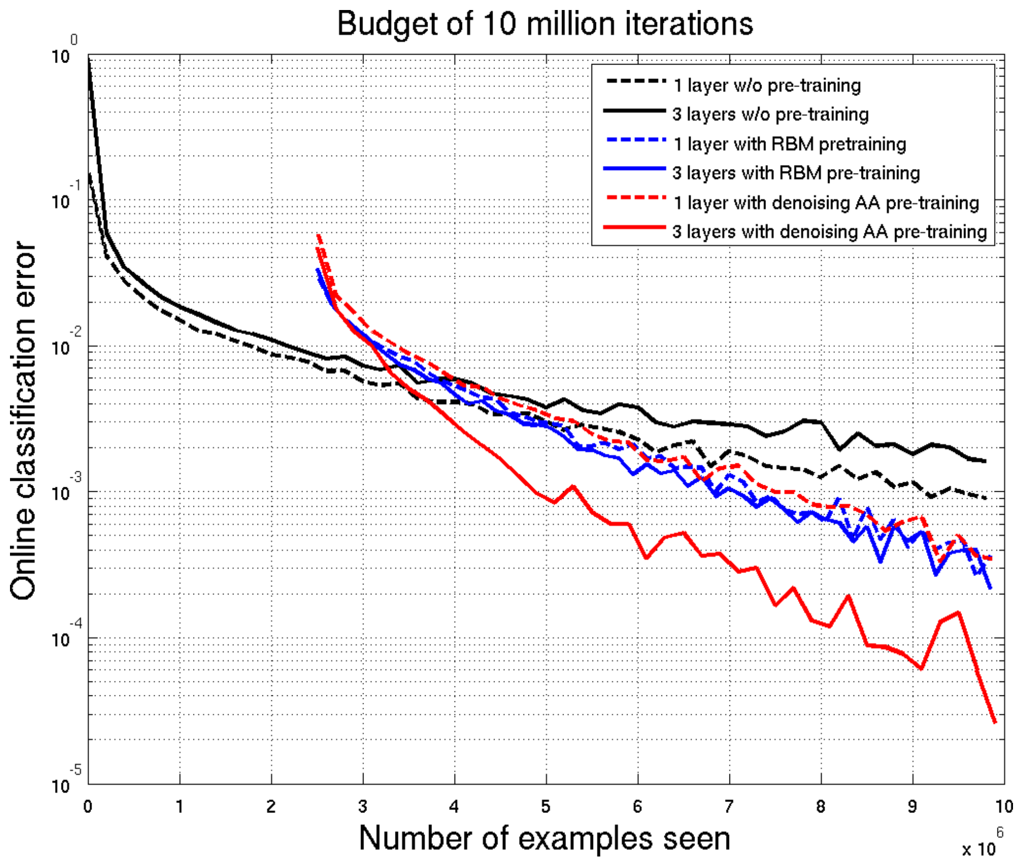
Denoising Auto-Encoder

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



Stacked Denoising Auto-Encoders

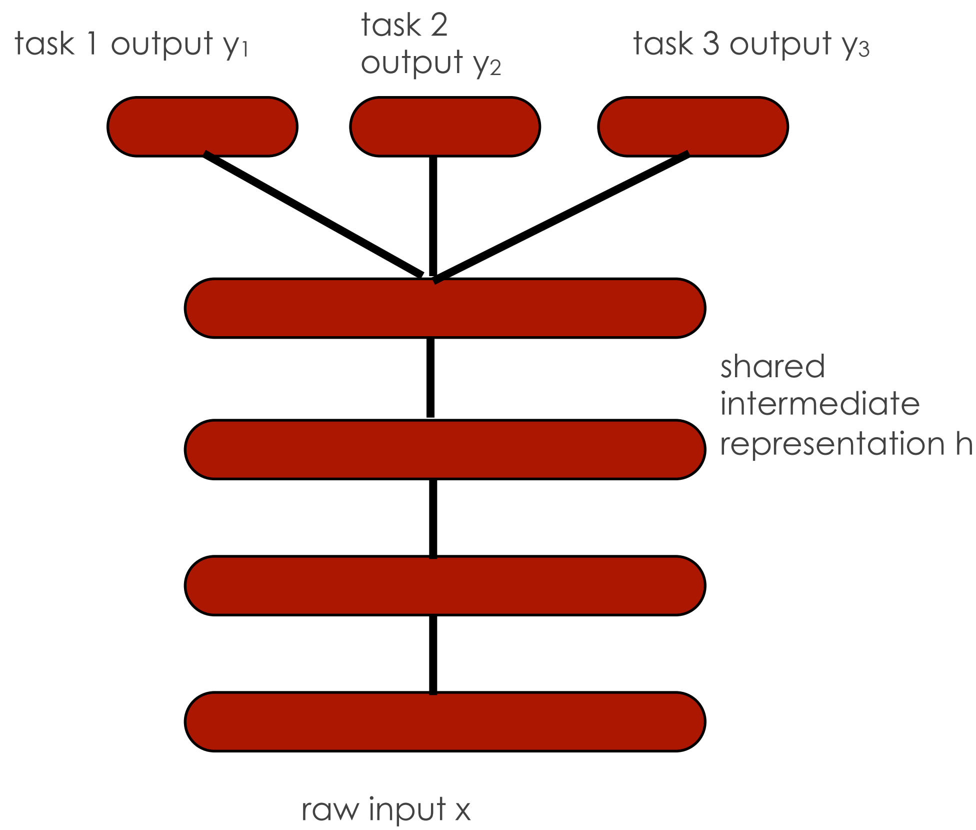
- No partition function, can measure training criterion
- Encoder & decoder: any parametrization
- Performs as well or better than stacking RBMs for usupervised pre-training



Infinite MNIST

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



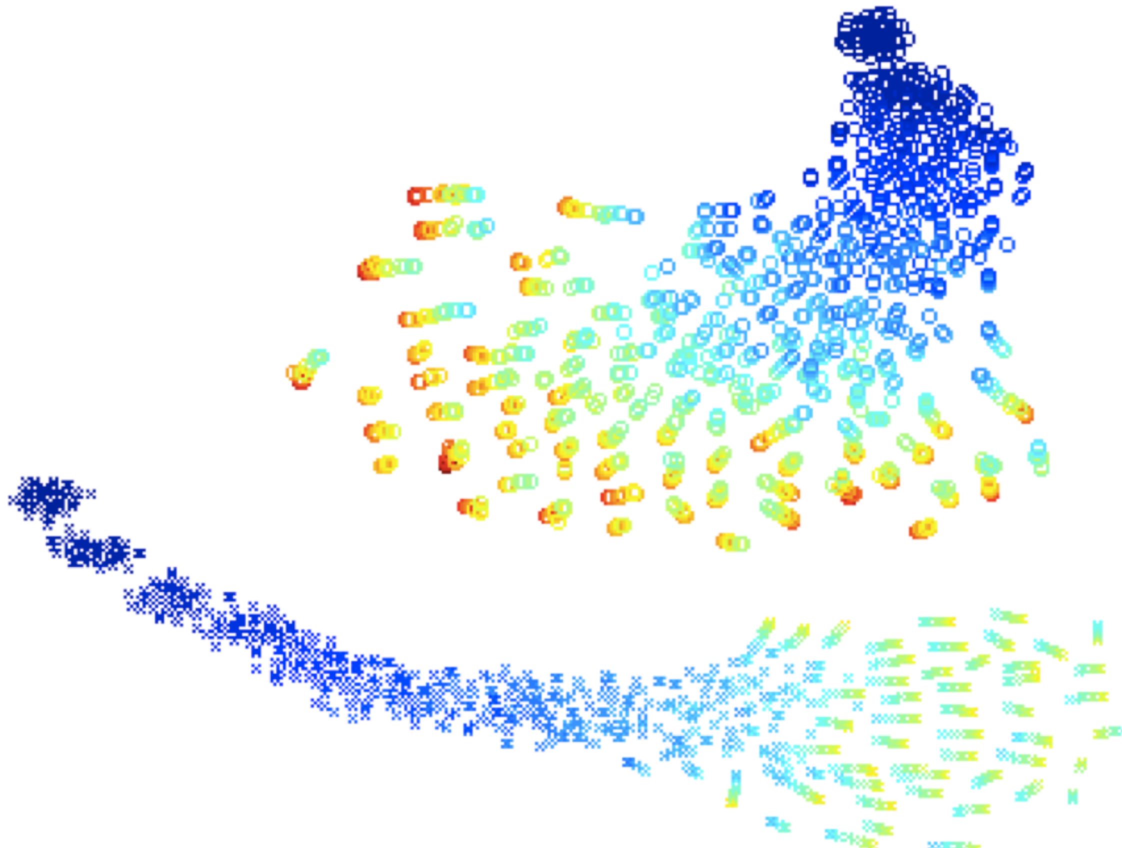
Why is Unsupervised Pre-Training Working So Well?

- 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
  - Easier to train each layer using a layer-local criterion

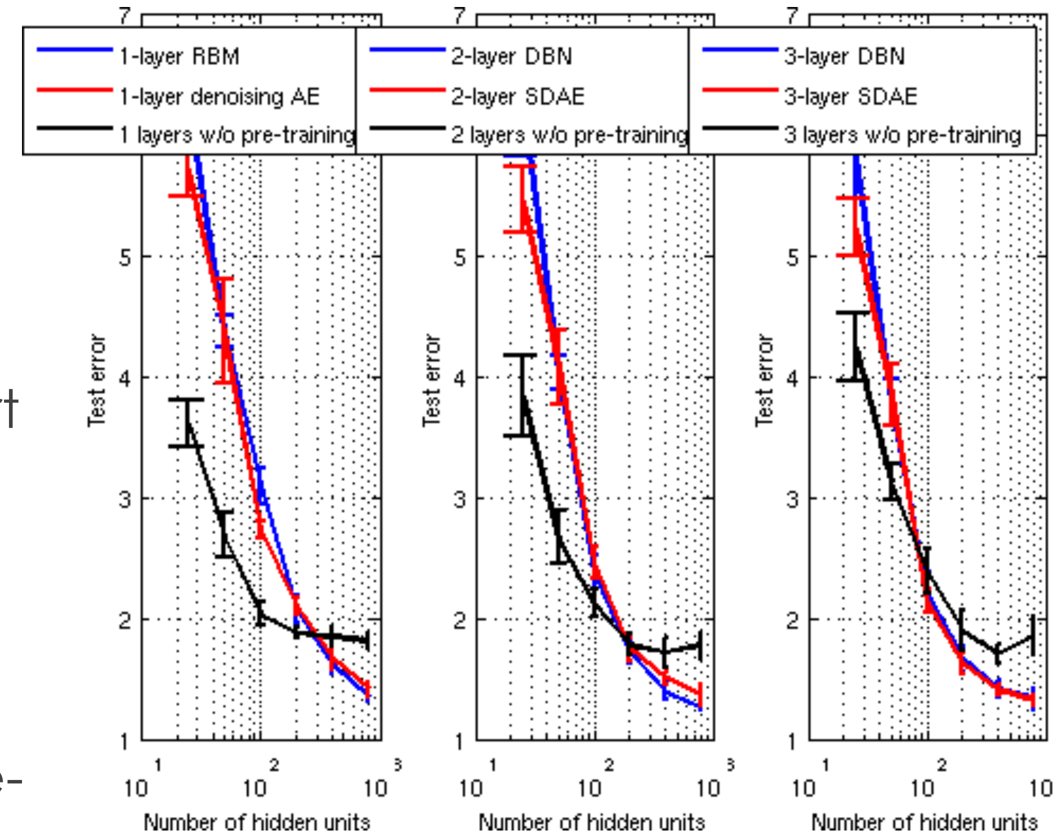
Learning Trajectories in Function Space

- 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



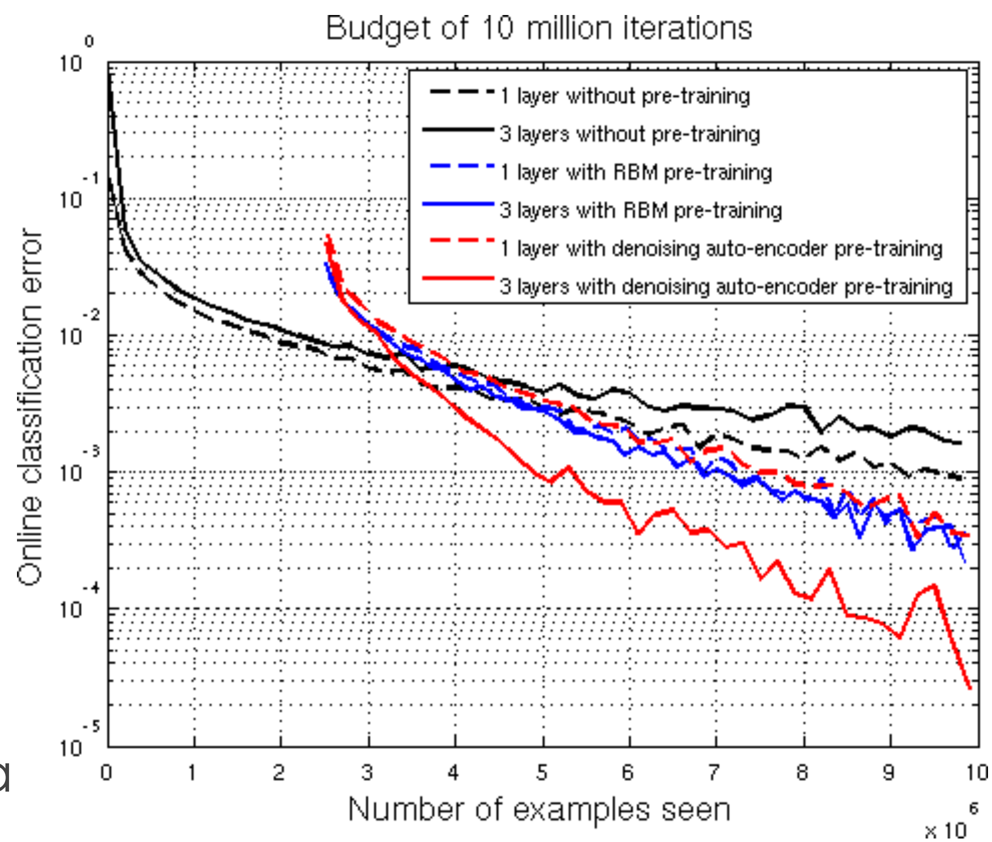
Unsupervised learning as regularizer

- 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

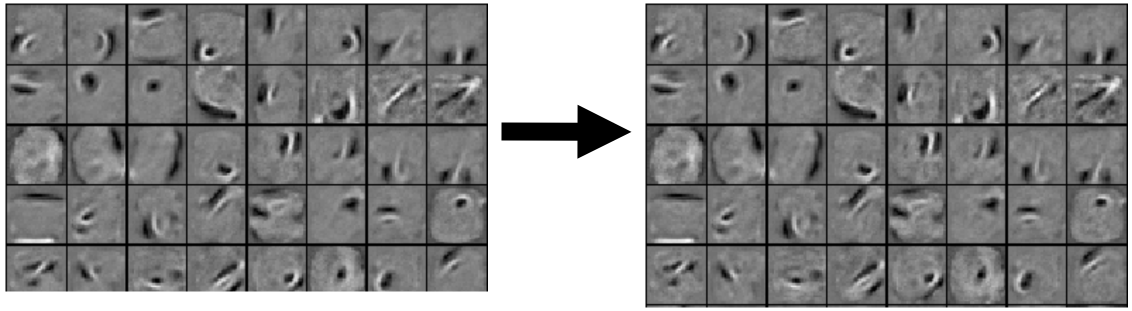


Better optimization of online error

- 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



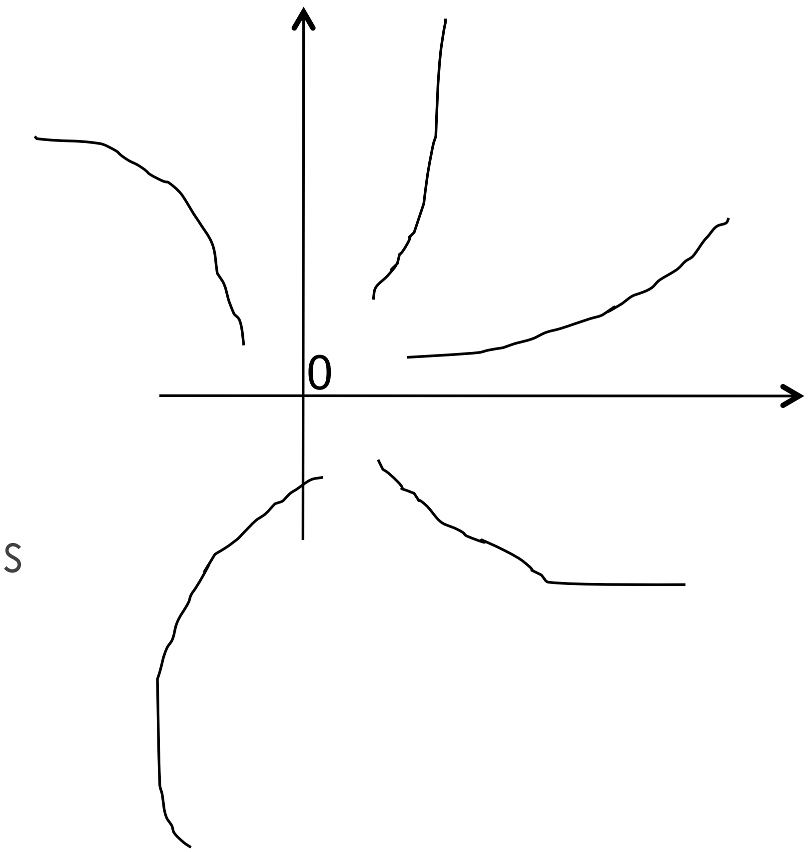
Before fine-tuning



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

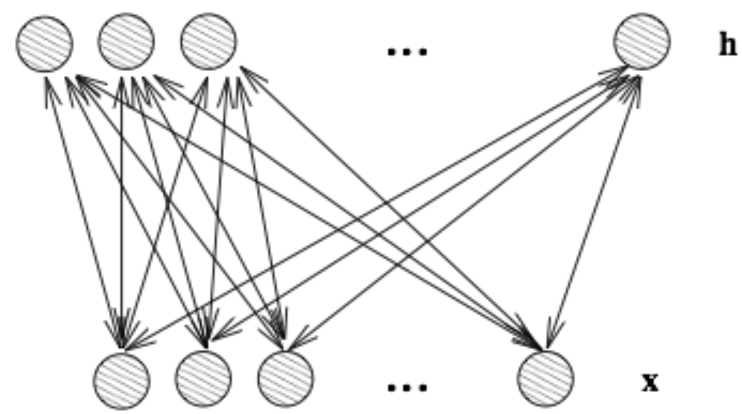


Restricted Boltzmann Machines

- The most popular building block for deep architectures
- Main advantage over auto-encoders: can sample from the model
- Bipartite undirected graphical model.

x=observed, h=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|x) and P(x|h) factorize:

Convenient Gibbs sampling x→h→x→h…

- In practice, Gibbs sampling does not always mix well

Boltzmann Machine Gradient

$$P(x) = \frac{1}{Z}\sum_h e^{-\mathrm{Energy}(x,h)} = \frac{1}{Z}e^{-\mathrm{FreeEnergy}(x)}$$

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

$$\frac{\partial \log P(x)}{\partial\theta} = -\frac{\partial \mathrm{FreeEnergy}(x)}{\partial\theta} + \sum_{\tilde{x}} P(\tilde{x})\frac{\partial \mathrm{FreeEnergy}(x)}{\partial\theta}$$

$$= -\sum_h P(h|x)\frac{\partial \mathrm{Energy}(x)}{\partial\theta} + \sum_{\tilde{x},\tilde{h}} P(\tilde{x},\tilde{h})\frac{\partial \mathrm{Energy}(x)}{\partial\theta}$$

- In RBMs, easy to sample or sum over h|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.

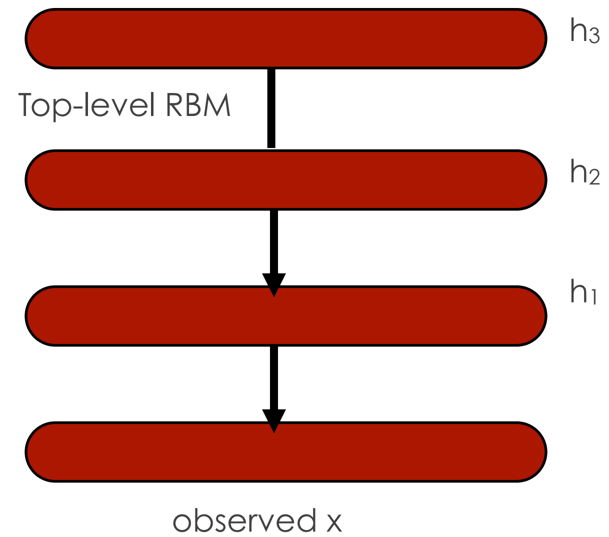
- Persistent CD (PCD): run negative Gibbs chain in background while weights slowly change

- 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)

Deep Belief Networks

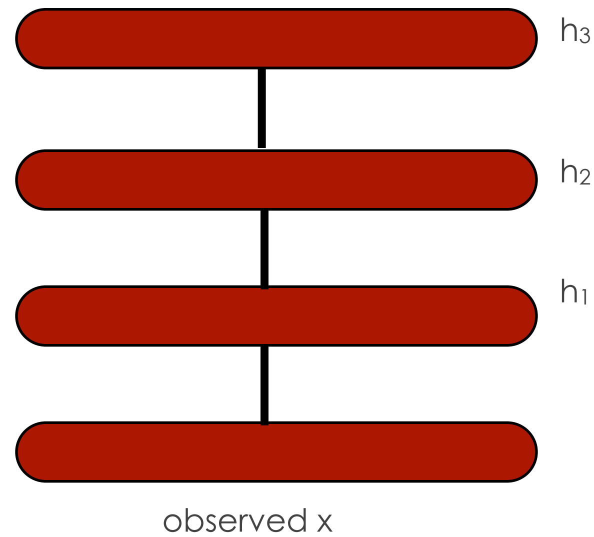
- Sampling:
  - Sample from top RBM
  - Sample from level k given k+1
- Estimating log-likelihood (not easy) (Salakhutdinov & Murray, ICML'2008, NIPS'2008)
- Training:
  - Variational bound justifies greedy layerwise training of RBMs
  - How to train all levels together?



Deep Boltzmann Machines

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

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



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

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 with Annealed Importance Sampling (AIS)
- Deep Belief Networks:
  - Extensions of AIS (Salakhutdinov et al 2008)

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?
- Getting rid of learning rates?

THANK YOU!

- Questions?
- Comments?