Learning Deep Architectures

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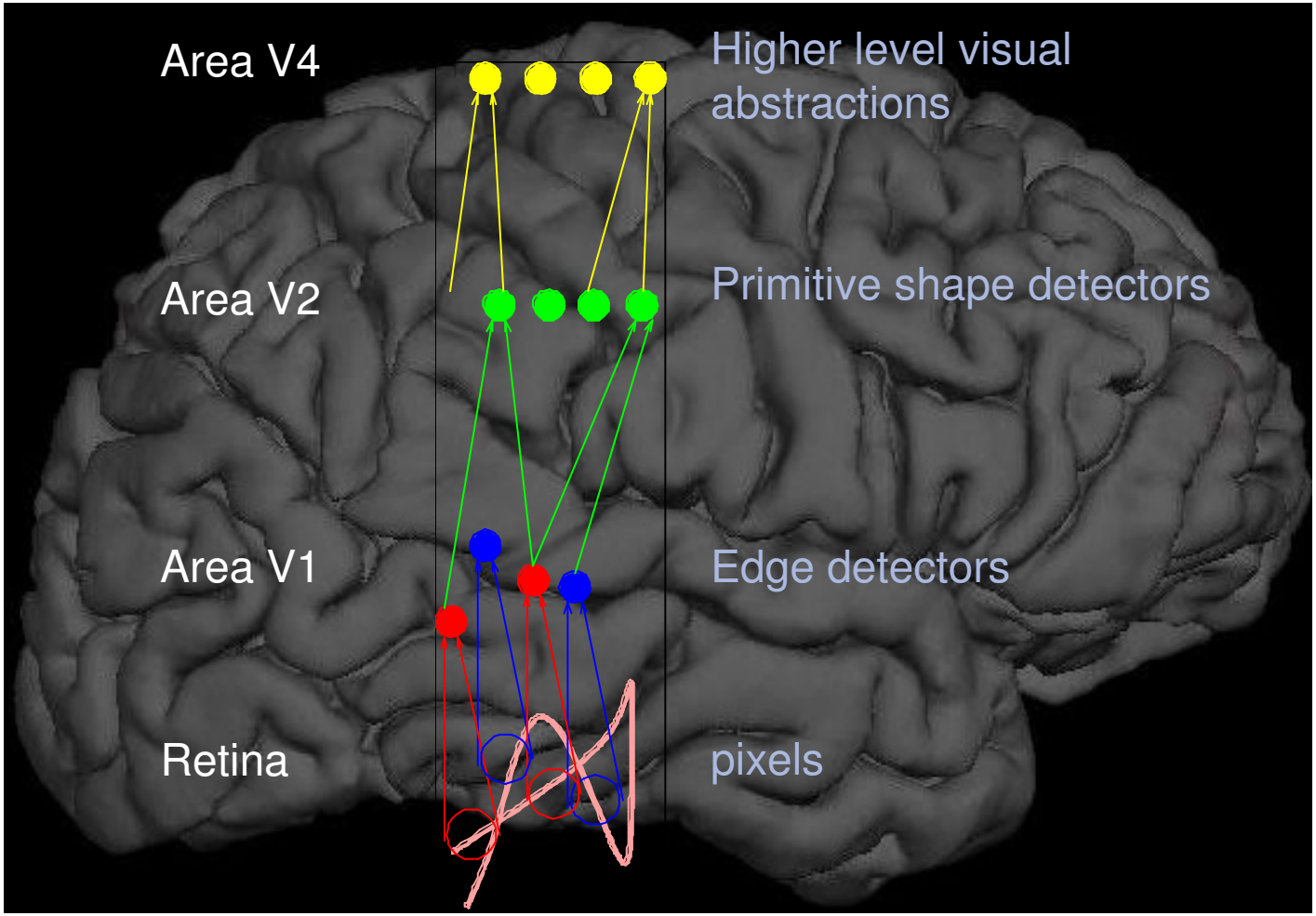
Deep Motivations

- 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, exponentially more efficient than 1-of-N enumeration latent variable values
- Multiple levels of latent variables allow combinatorial sharing of statistical strength

Deep Architecture in the Brain



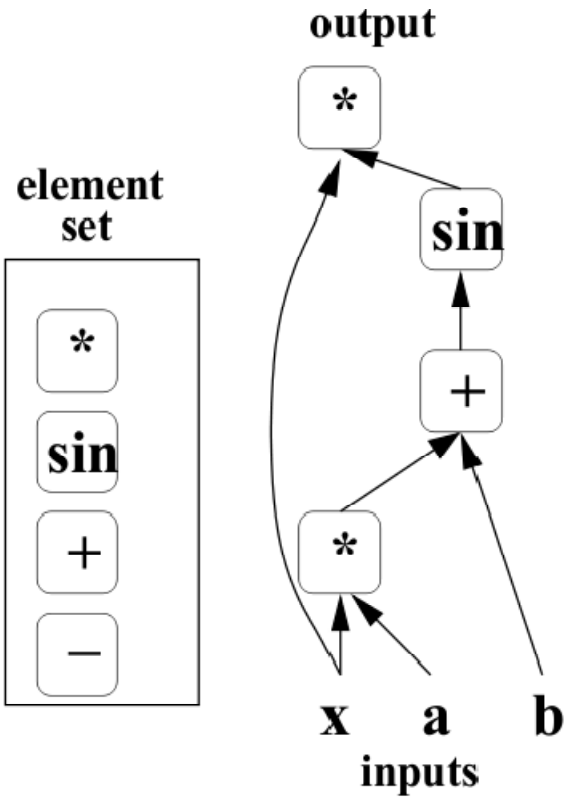
Deep Architecture in our Mind

- 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

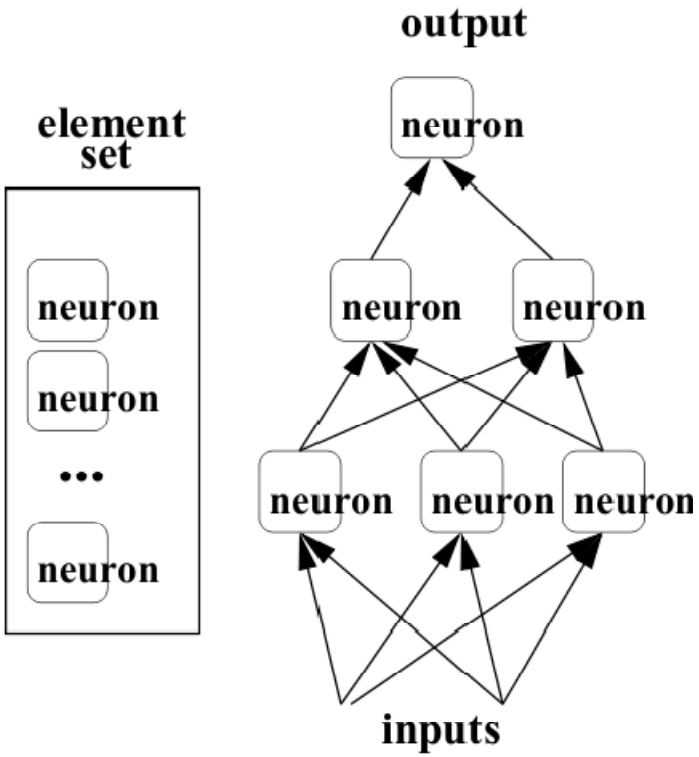
It would be nice to learn / discover these concepts

(knowledge engineering failed because of poor introspection?)

Architecture Depth



Depth = 4



Depth = 3

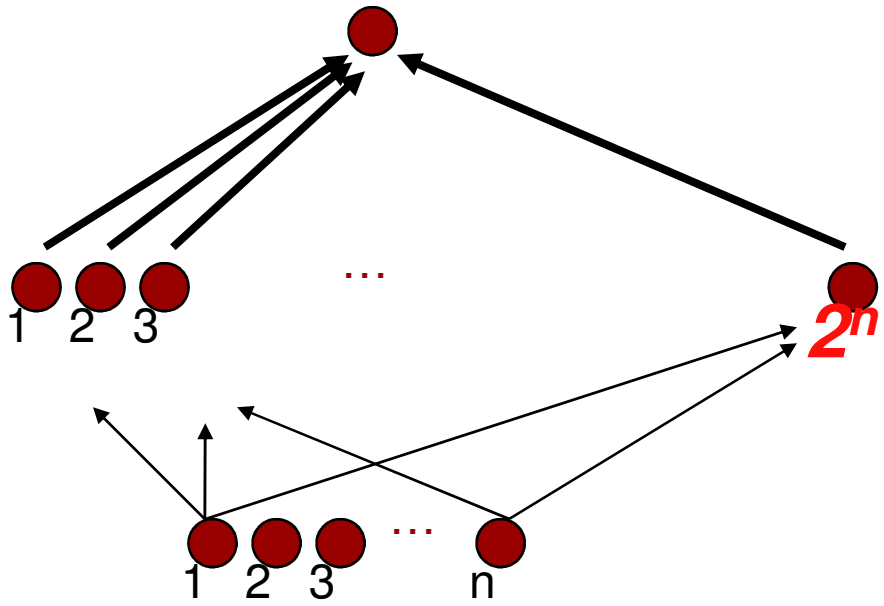
Good News, Bad News

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)

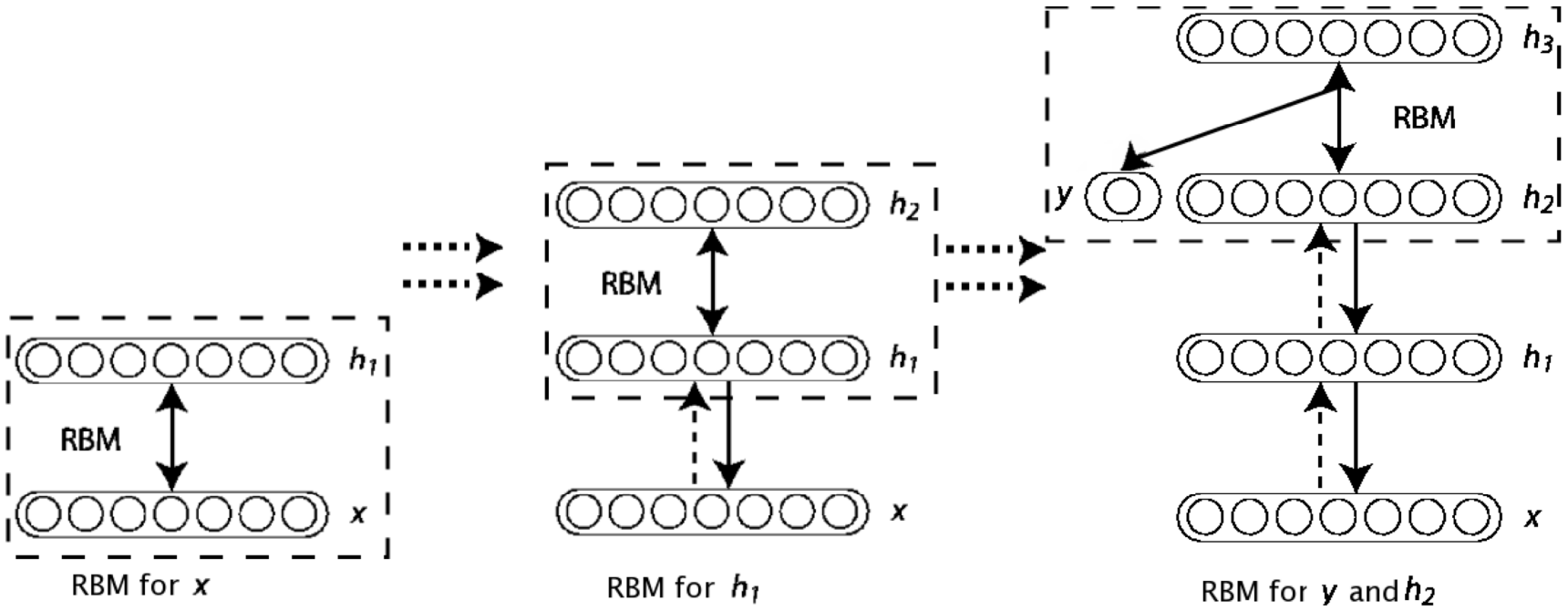
Functions representable compactly with k layers may require exponential size with k-1 layers



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*

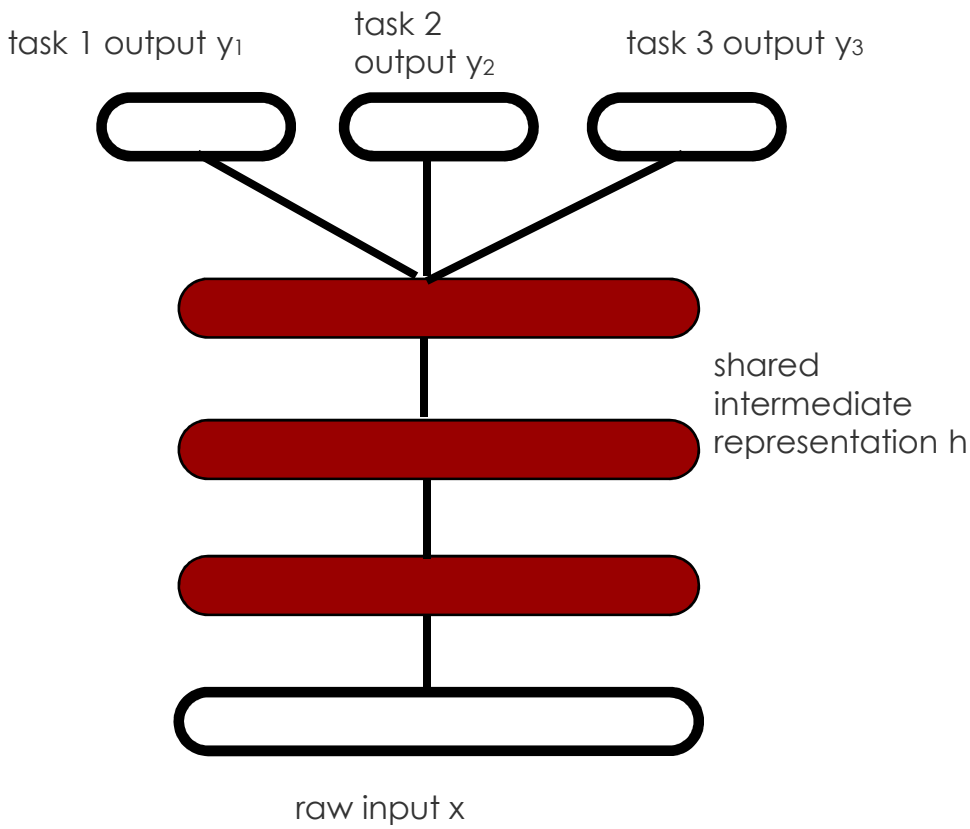
Greedy Layer-Wise Pre-Training



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

Deep Architectures and Sharing Statistical Strength, Multi-Task Learning

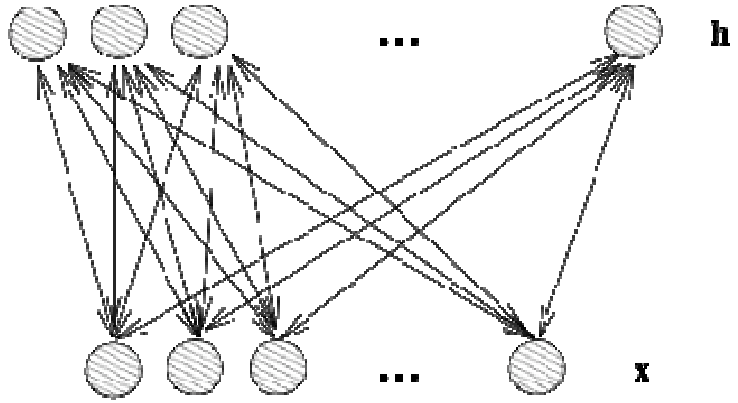
- Generalizing better to new tasks is crucial to approach AI
- Deep architectures learn good intermediate representations that can be shared across tasks
- A good representation is one that makes sense for many tasks



Restricted Boltzmann Machines

- The most popular building block for deep architectures
- Bipartite undirected graphical model.

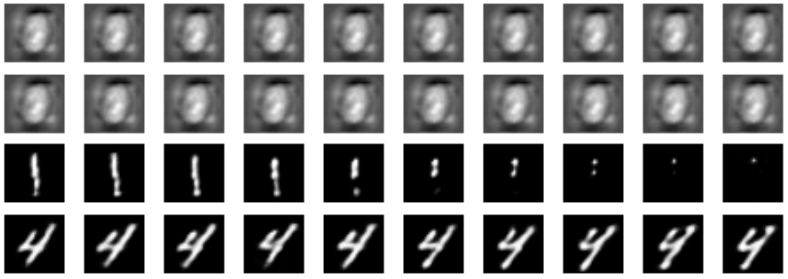
x=observed, h=hidden



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

- P(h | x) and P(x | h) factorize:
  - Easy inference
  - Convenient Gibbs sampling x→h→x→h…
- In practice, Gibbs sampling does not always mix well…

RBM trained by CD on MNIST



Chains from random state

Chains from real digit

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: 'positive phase' and 'negative phase'

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

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

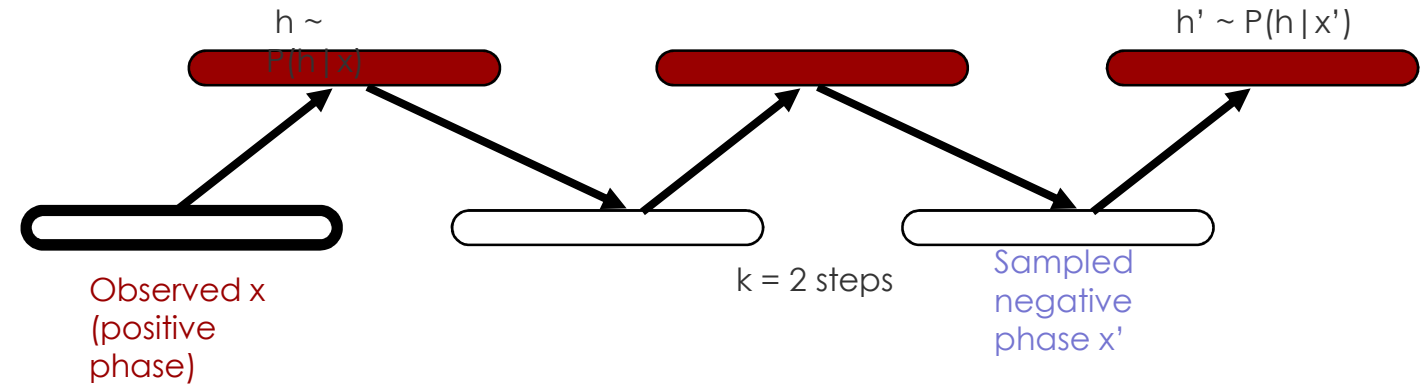
- In RBMs, easy to sample or sum over h | x:
- Difficult part: sampling from P(x), typically with a Markov chain

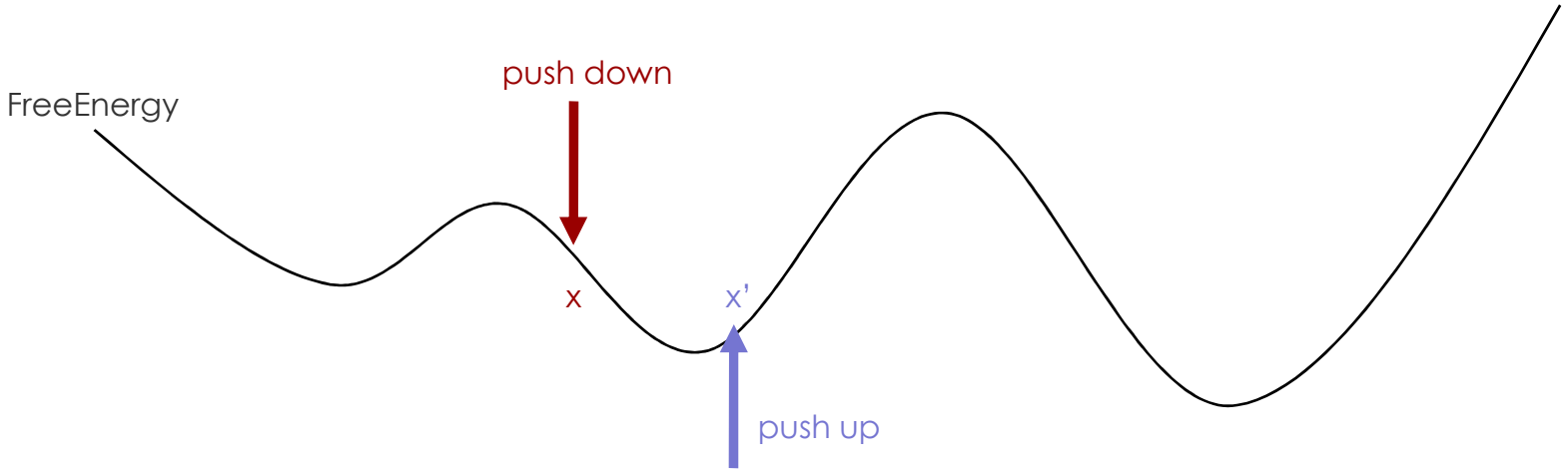
Training RBMs

- 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)
- Tempered MCMC: use higher temperature to escape modes

Contrastive Divergence

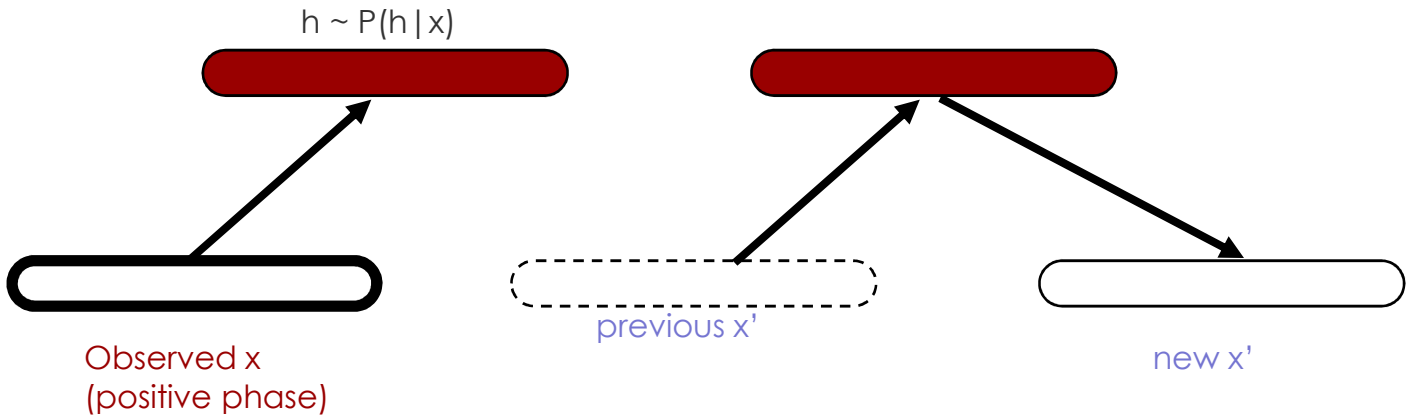
- Contrastive Divergence (CD-k): start negative phase block Gibbs chain at observed x, run k Gibbs steps (Hinton 2002)





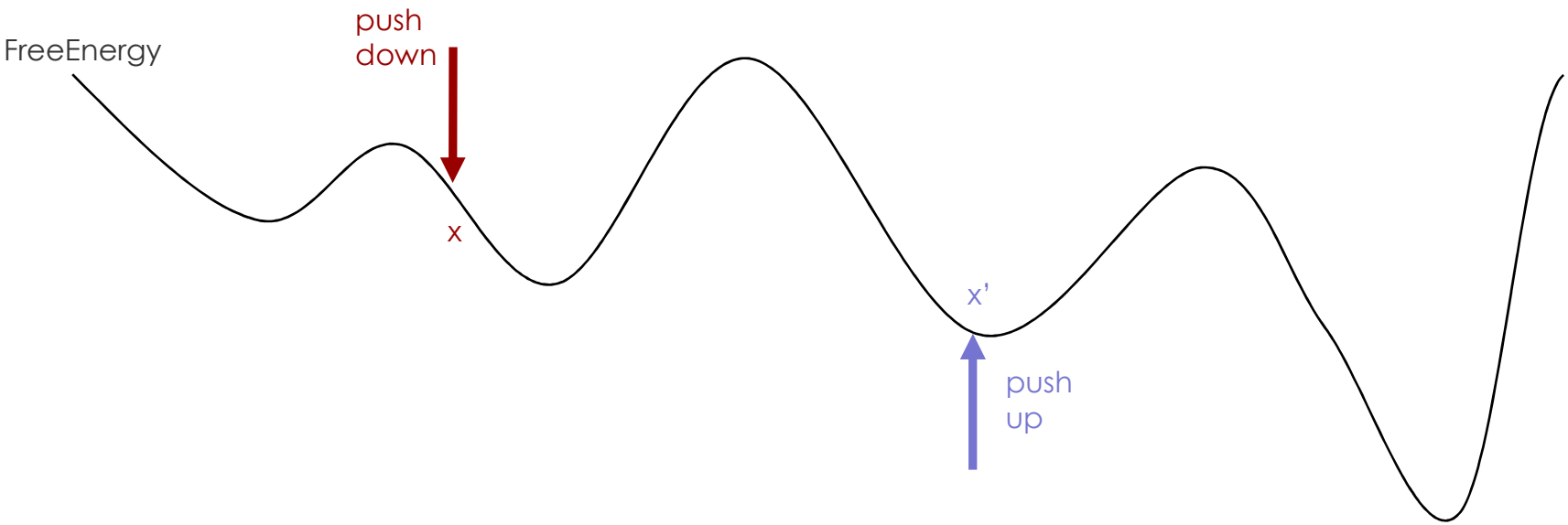
Persistent CD

- 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.



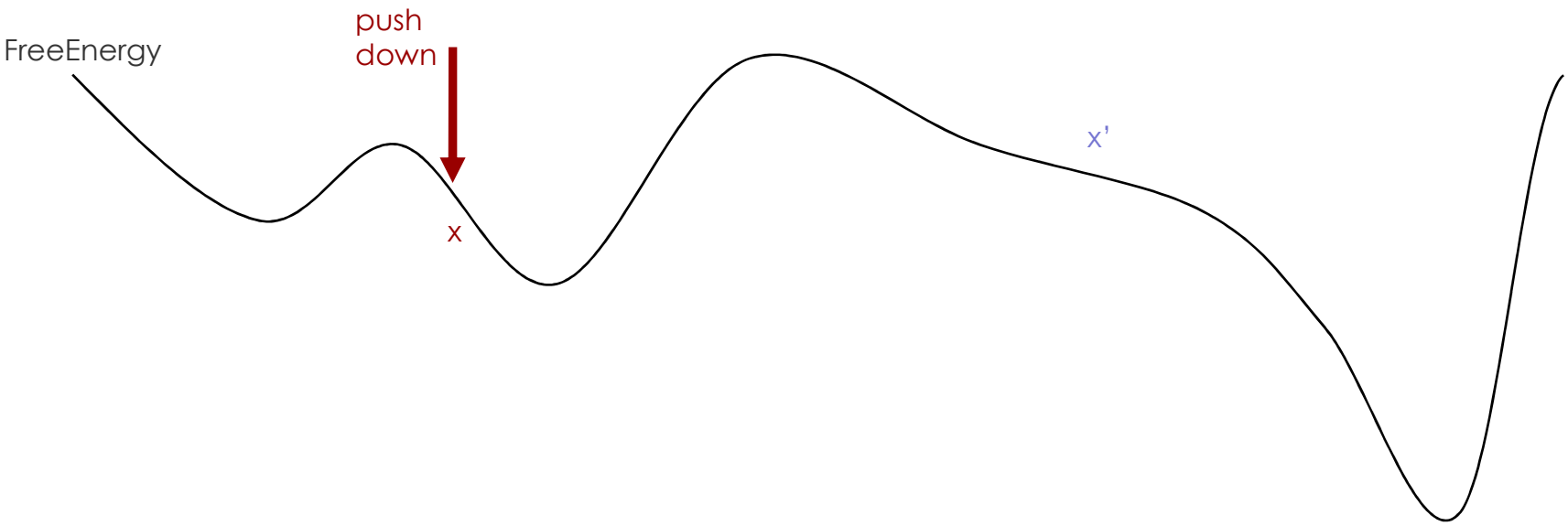
Persistent CD with large learning rate

- Negative phase samples quickly push up the energy of whereever they are and quickly move to another mode



Persistent CD with large step size

- Negative phase samples quickly push up the energy of whereever they are and quickly move to another mode



Persistent CD with large learning rate

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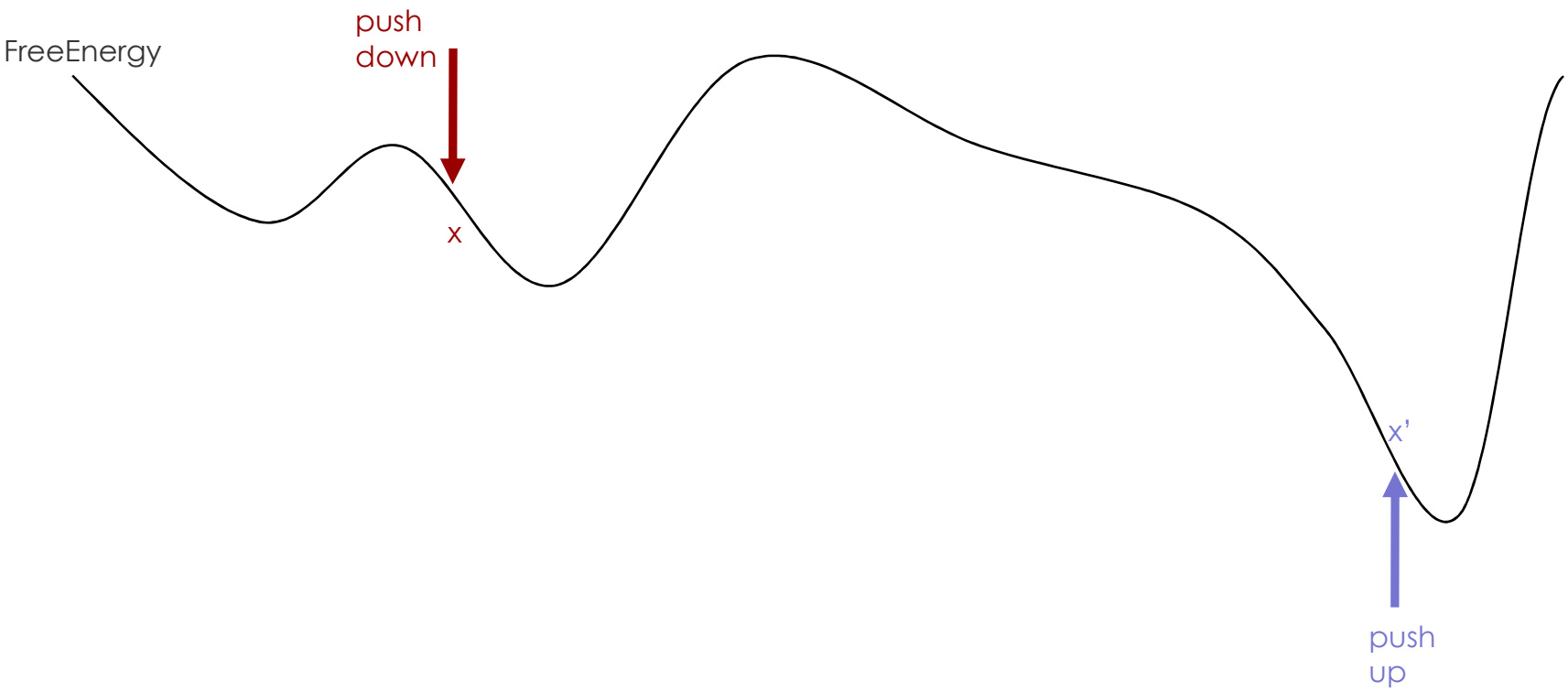
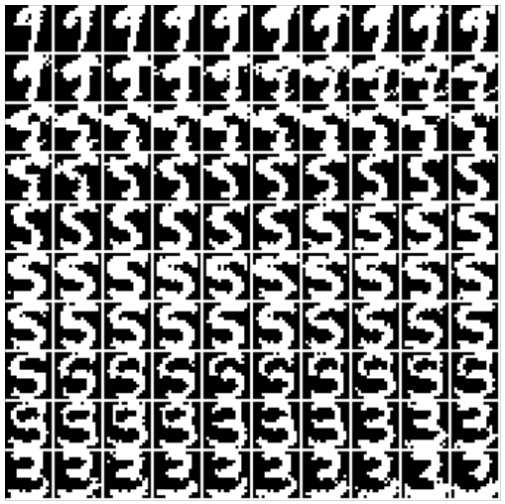
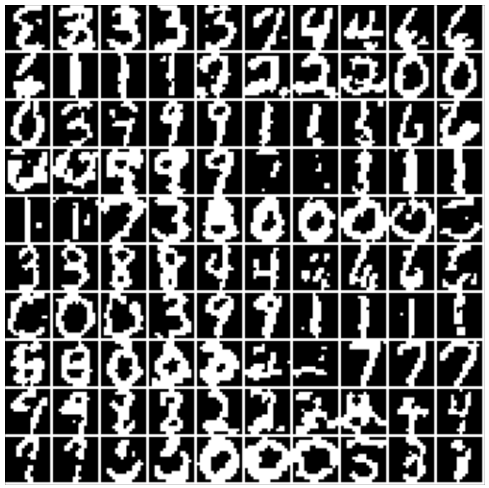


Fast Persistent CD and Herding

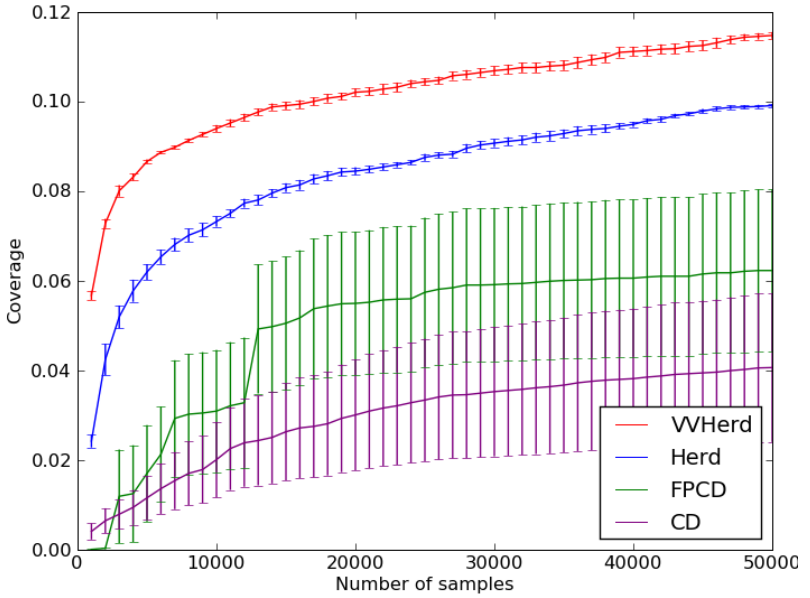
- Exploit **impressively faster mixing** achieved when parameters change quickly (large learning rate) while sampling
- Fast PCD: two sets of weights, one with a large learning rate only used for negative phase, quickly exploring modes
- Herding (see Max Welling's ICML, UAI and workshop talks): 0-temperature MRFs and RBMs, only use fast weights



FPCD



Herding



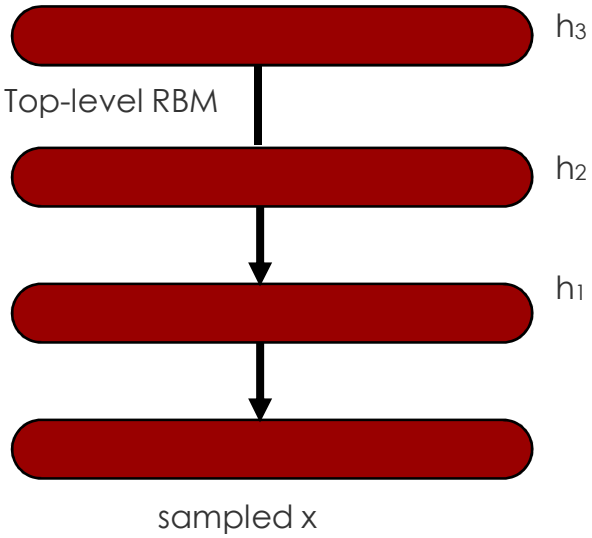
Tempered MCMC

- 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		
Training procedure	TMCMC	Gibbs (random start)	Gibbs (test start)
TMCMC	**215.45** $\pm$ 2.24	88.43 $\pm$ 2.75	60.04 $\pm$ 2.88
PCD	44.70 $\pm$ 2.51	-28.66 $\pm$ 3.28	-175.08 $\pm$ 2.99
CD	-2165 $\pm$ 0.53	-2154 $\pm$ 0.63	-842.76 $\pm$ 6.17

Deep Belief Networks

- Sampling:
  - Sample from top RBM
  - Sample from level k given k+1
- Easy approximate inference
- Training:
  - Variational bound justifies greedy layerwise training of RBMs
  - How to train all levels together?

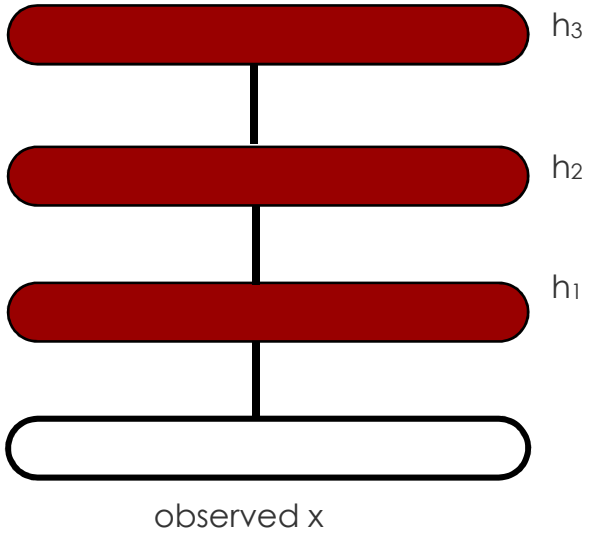


$$\log P(\mathbf{x}) \geq H_{Q(\mathbf{h}|\mathbf{x})} + \sum_{\mathbf{h}} Q(\mathbf{h}|\mathbf{x}) \left(\log P(\mathbf{h}) + \log P(\mathbf{x}|\mathbf{h})\right)$$

Deep Boltzmann Machines

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

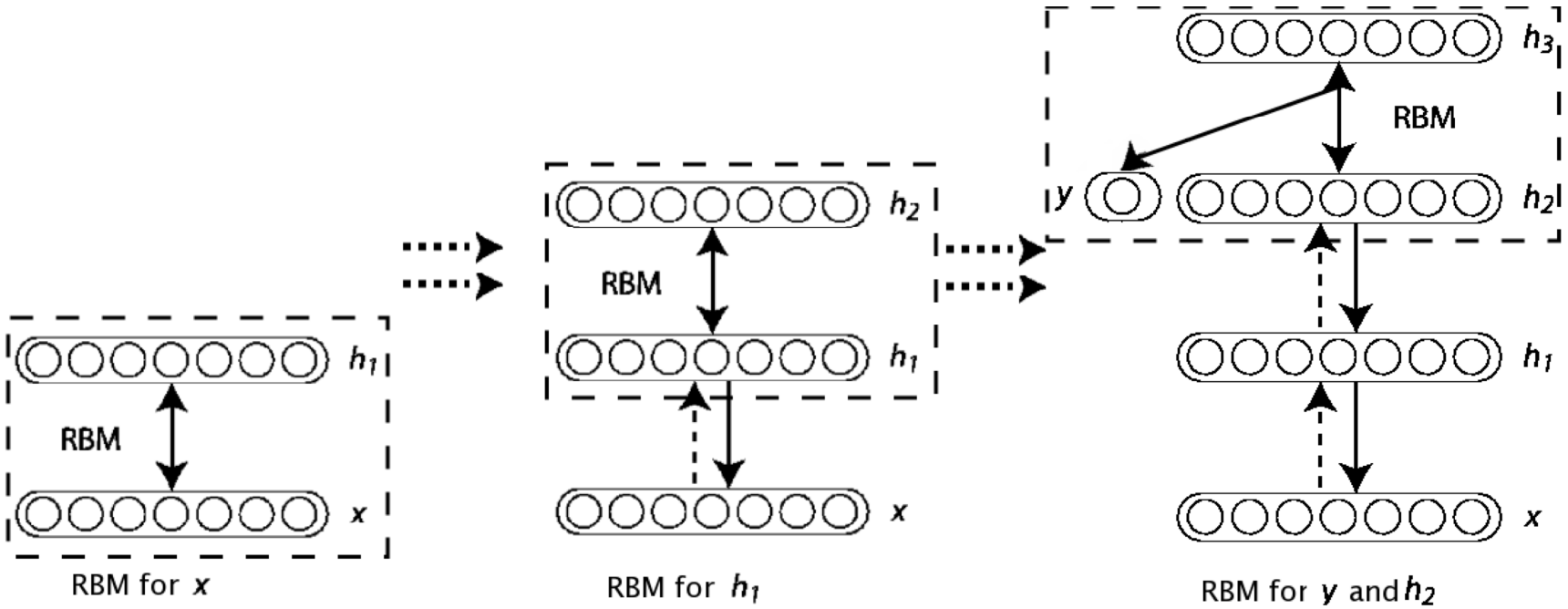
- Positive phase: variational approximation (mean-field)
- Negative phase: persistent chain
- Can (must) initialize from stacked RBMs
- Improved performance on MNIST from 1.2% to .95% error
- Can apply AIS with 2 hidden layers



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

Back to Greedy Layer-Wise Pre-Training

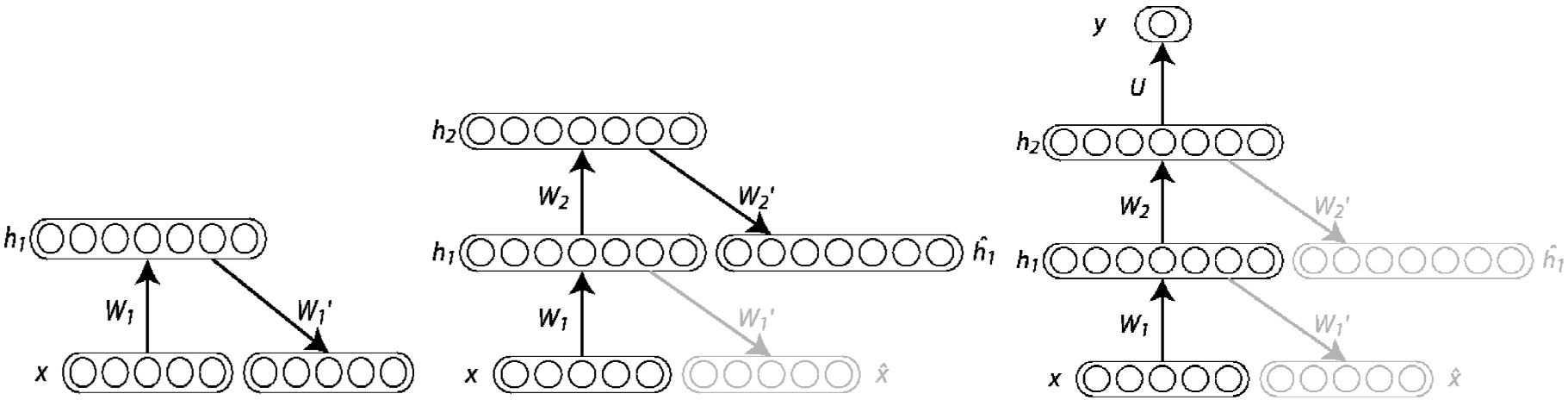


Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)

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



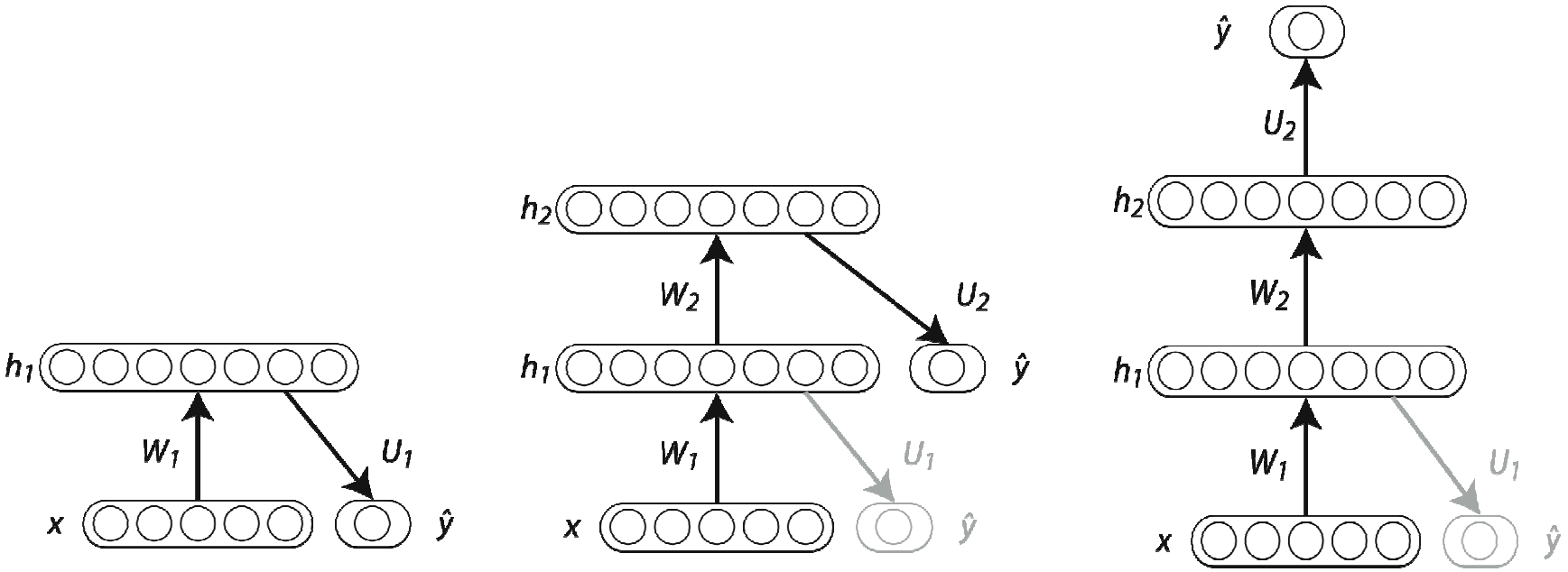
Auto-encoders and CD

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

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

(Bengio & Delalleau 2009)

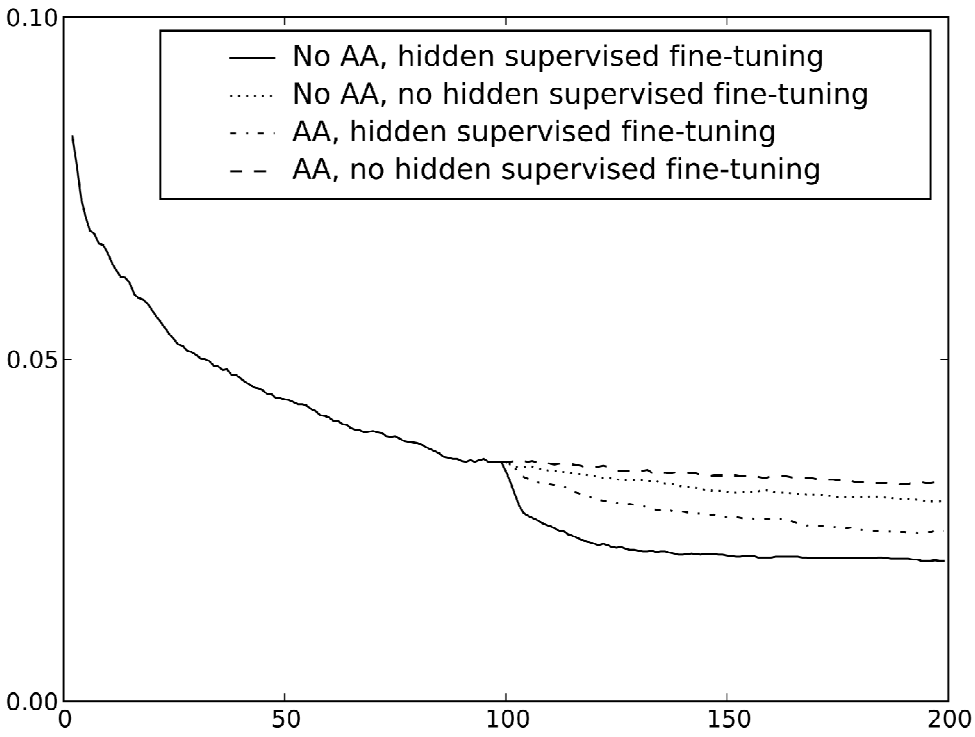
Greedy Layerwise Supervised Training



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



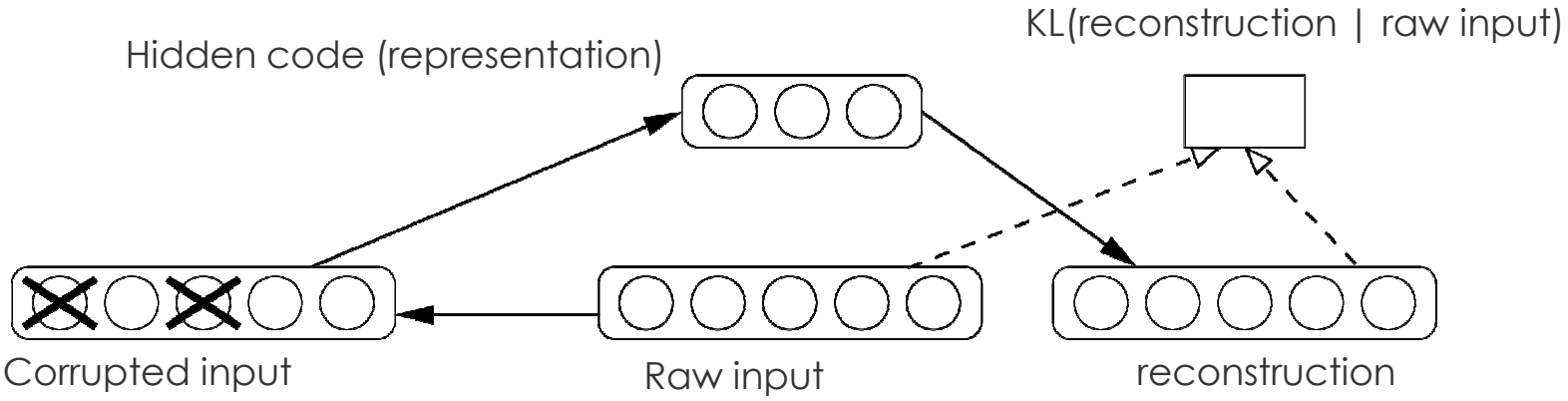
Sparse Auto-Encoders

- (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)

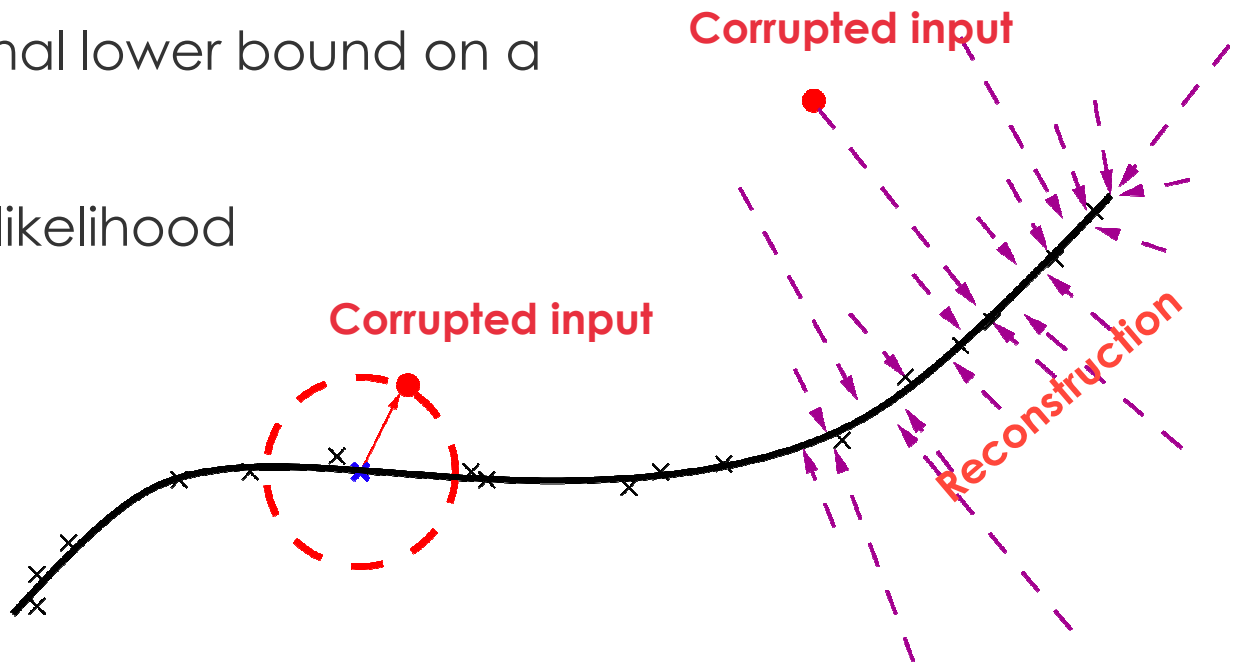
Denoising Auto-Encoder

- (Vincent et al, 2008)
- Corrupt the input
- Reconstruct the uncorrupted input



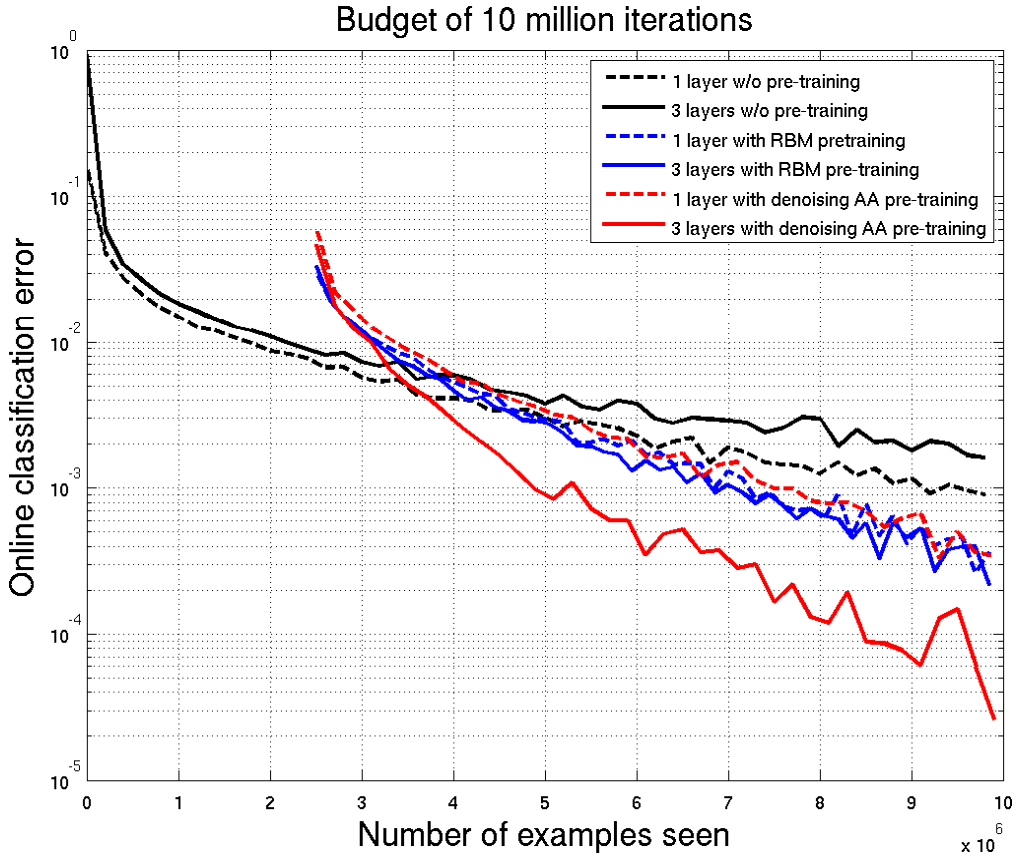
Denoising Auto-Encoder

- 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

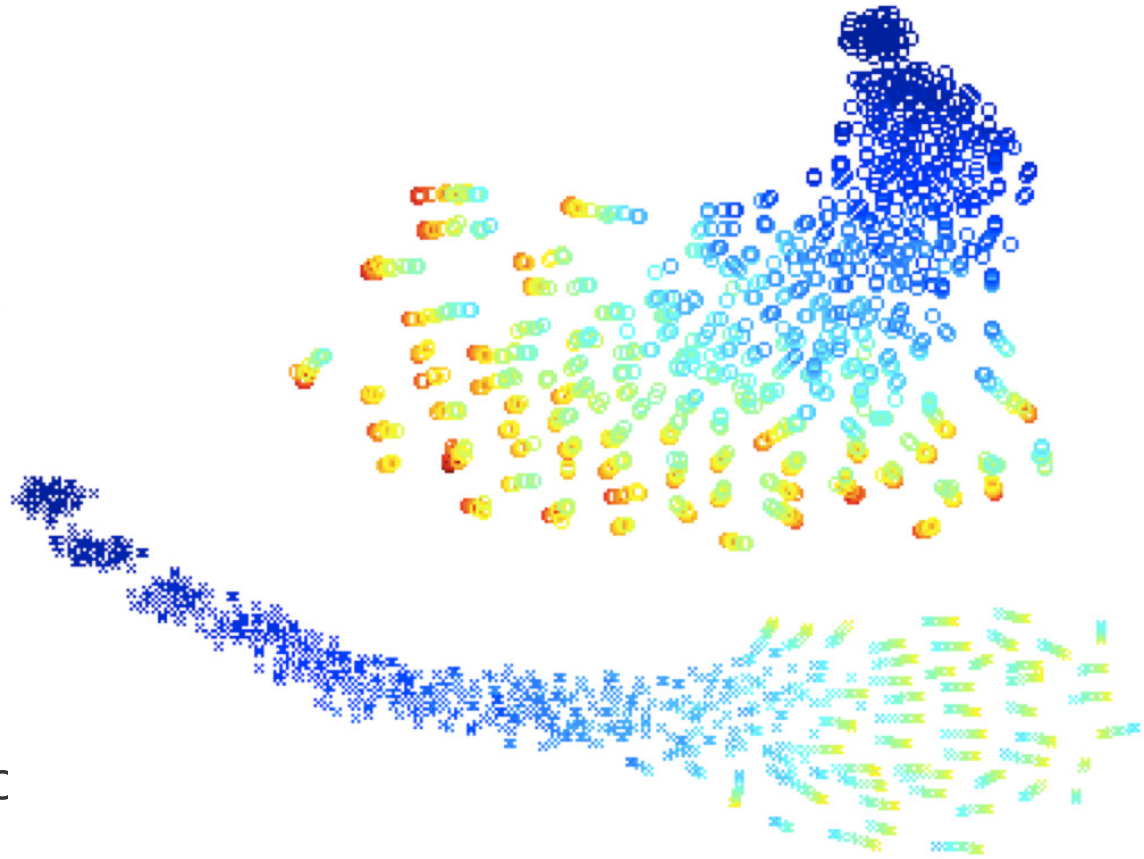
Why is Unsupervised Pre-Training Working So Well?

- 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

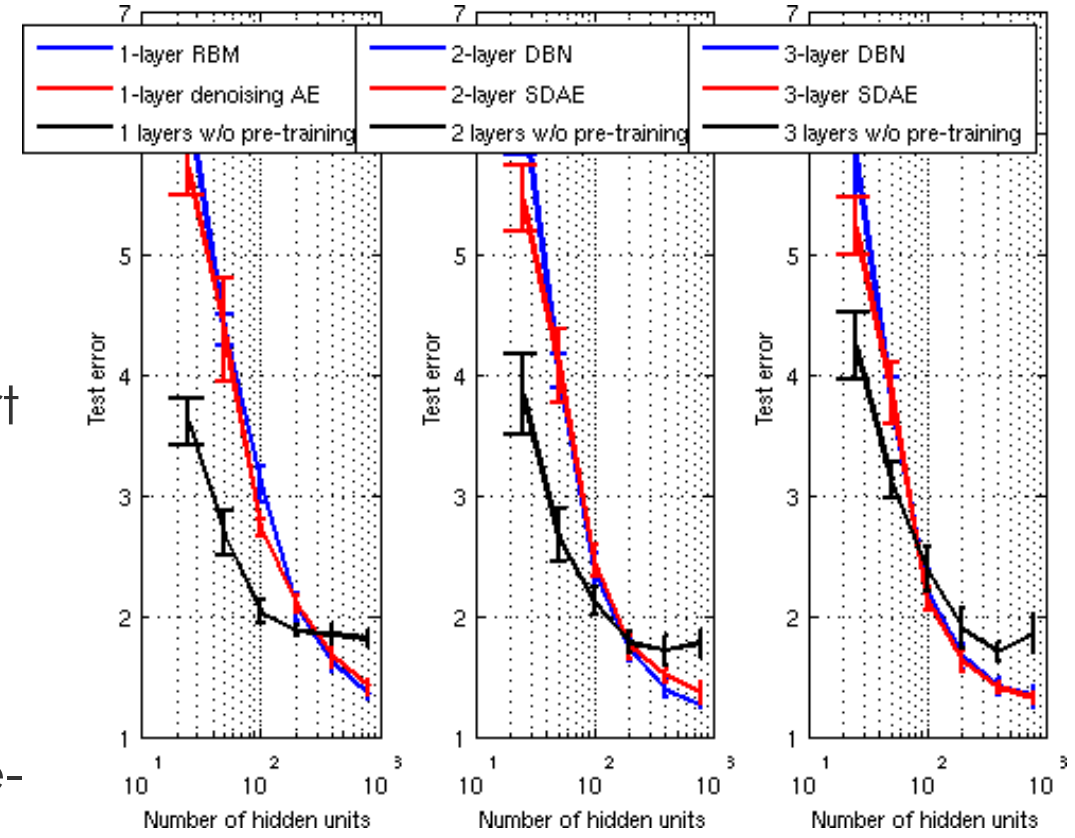
Learning Trajectories in Function Space

- 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



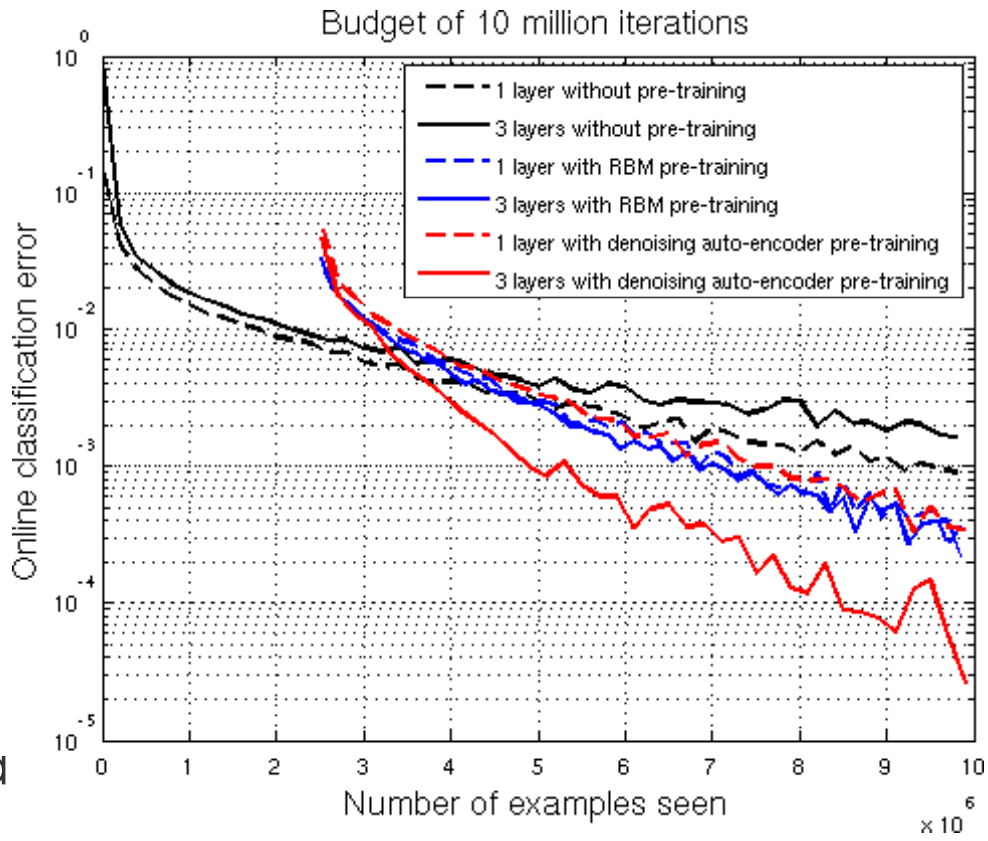
Unsupervised learning as regularizer

- 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

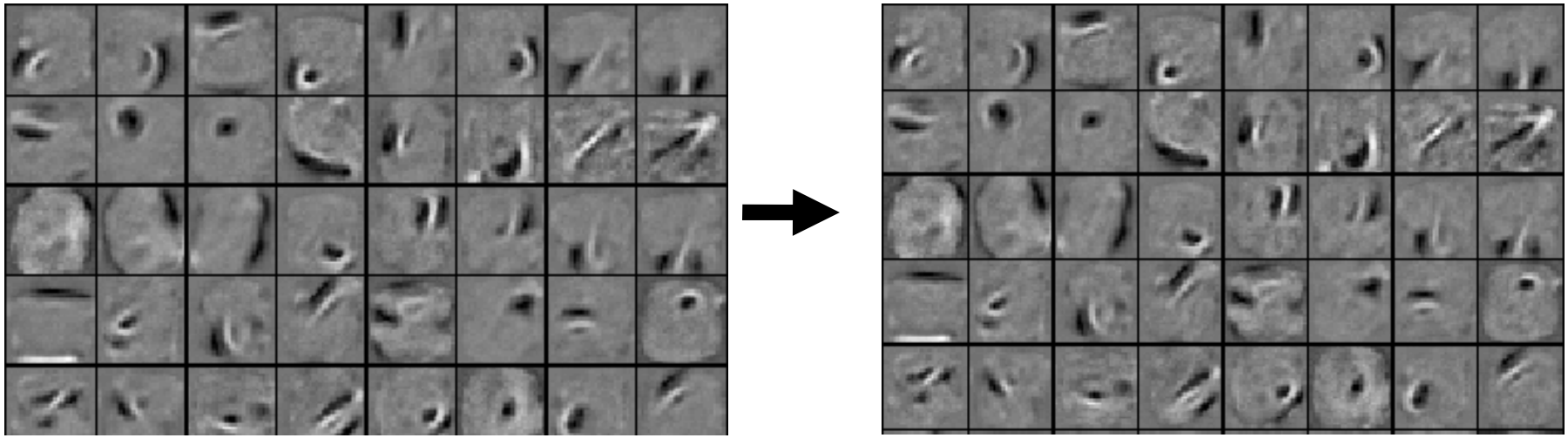


Better optimization of online error

- 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

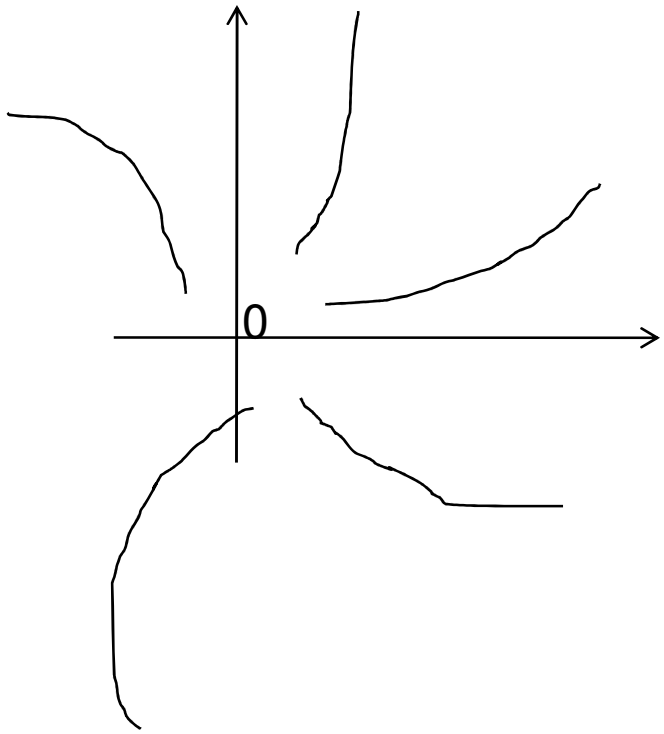


Before fine-tuning

After fine-tuning

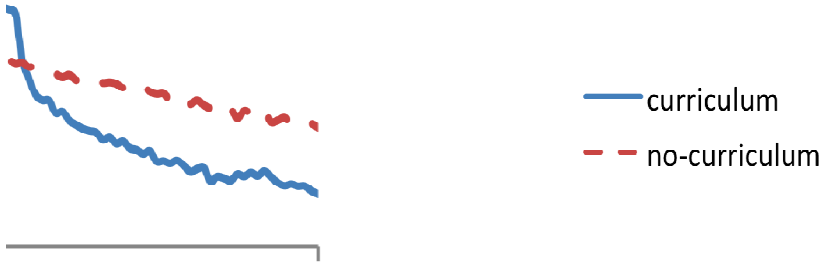
Learning Dynamics of Deep Nets

- 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



The order and selection of examples makes a difference

- 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

- 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 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

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?

THANK YOU FOR YOUR ATTENTION!

- Questions?
- Comments?