Greedy Layer-Wise Training of Deep Networks

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Thanks to: Yann Le Cun, Geoffrey Hinton, Olivier Delalleau, Nicolas Le Roux

Summary

- Motivation: AI $\Rightarrow$ highly-varying functions
  $\Rightarrow$ non-local + **deep architecture**
- Principle of **greedy layer-wise unsupervised initialization**
- Deep Belief Networks
- Deep Multi-layer Neural Networks
- Experimental study: **why this principle works**
- Extensions of Deep Belief Networks

Grand Goal: AI

- Goal: using ML to reach AI
- *AI tasks*: visual and auditory perception, language understanding, intelligent control, long-term prediction, understanding of high-level abstractions...
- Remains elusive! (and mostly forgotten?)
- 3 considerations:
  - computational efficiency
  - statistical efficiency
  - human-labor efficiency
- Here: focus on algorithms associated with broad priors (i.e., non-parametric) with the hope of discovering principles applicable to vast array of tasks within AI, with no need of hand-crafted solutions for each particular task.

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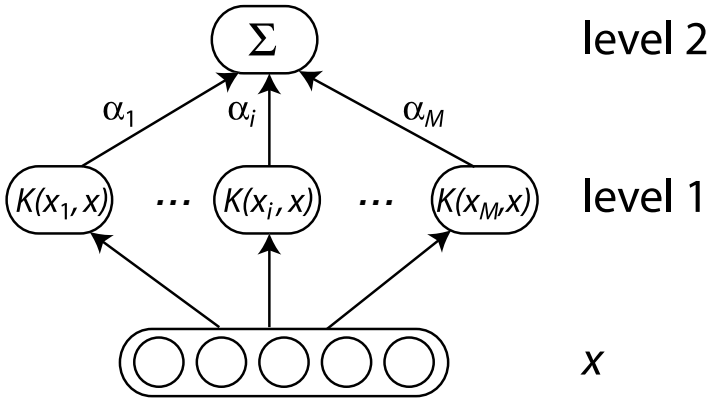
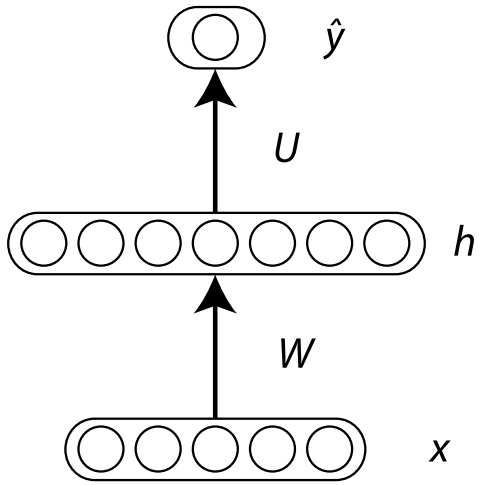
Depth of Architectures

Depth = number of **levels** of composition of adaptable elements:

- kernel machines: shallow
- boosting: generally shallow
- multi-layer neural networks: usually shallow, can be deep?
- decision trees: deep but local estimators (curse of dim.)
- parametric graphical models: human-labor intensive



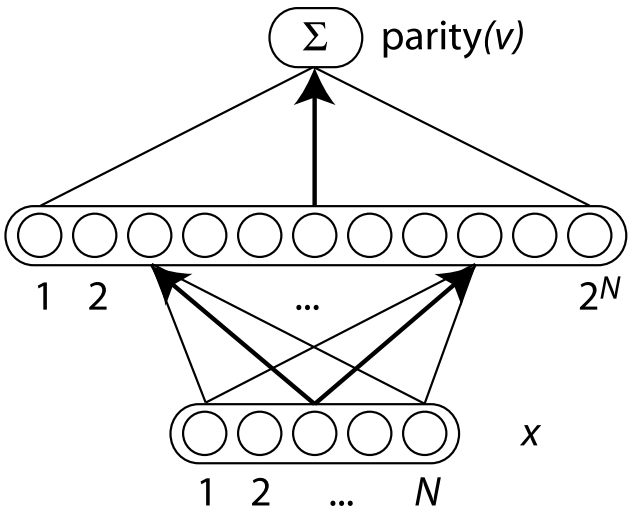


Non-parametric ones can theoretically approximate any continuous function.
But **how efficiently?**
(computational, statistical)

Inefficiency of Shallow Architectures

Shallow architectures may need huge number of elements.

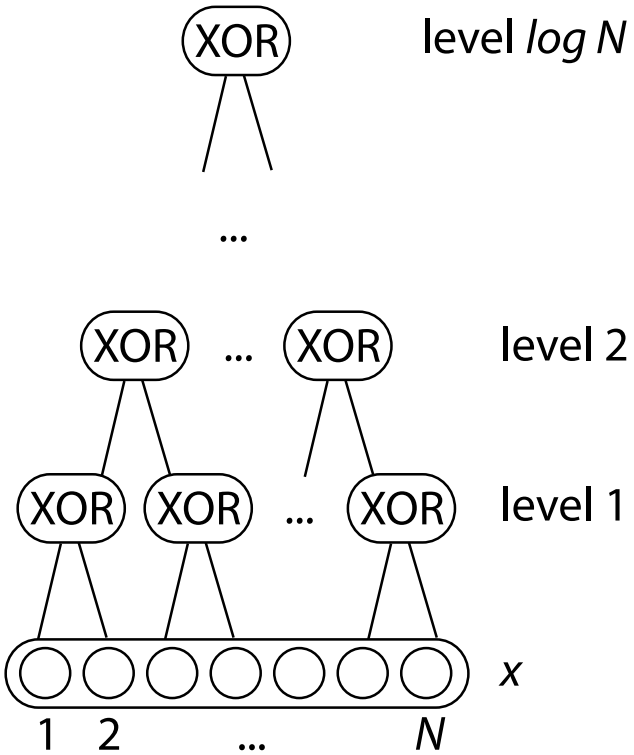
Worst-case can be **exponentially bad**. Many theorems and examples from boolean circuits theory (Hastad 1987): multiplier circuits, parity, etc..



Very fat shallow circuit

$\Rightarrow$ many adjustable elements

$\Rightarrow$ many examples needed



Number of levels should increase with complexity, nb inputs, maybe logarithmic.

Curse of Dimensionality

(Bengio et al 2006):

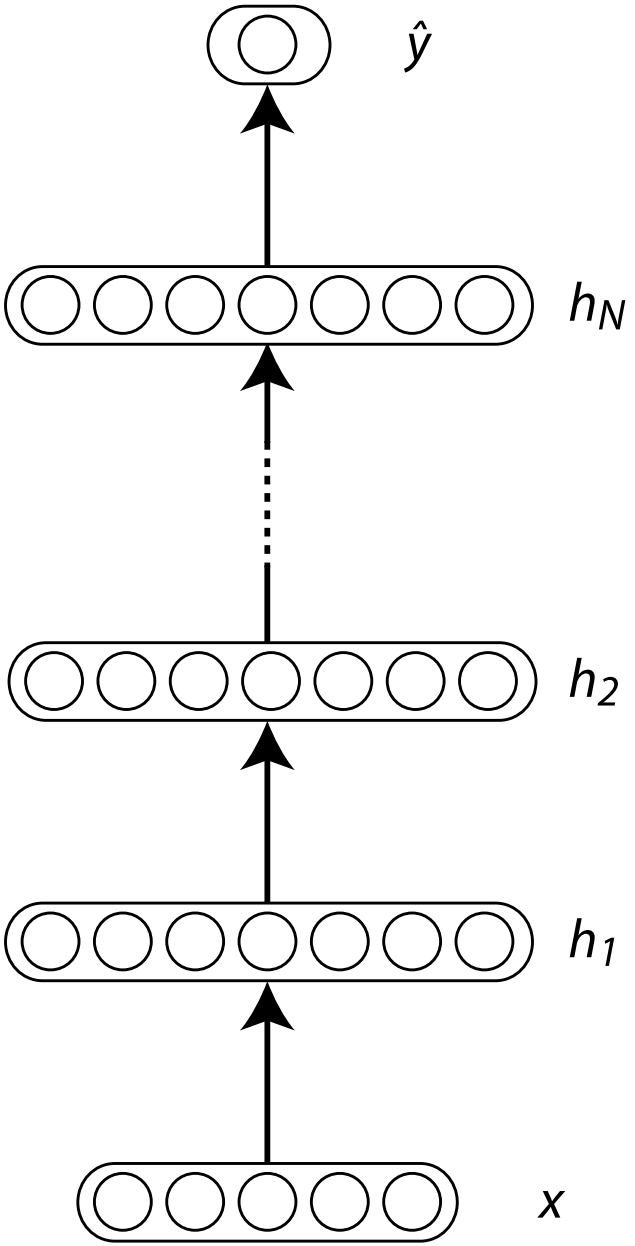
Local kernel machines (= **pattern matchers**) and decision trees **partition the space** and may need

exponential nb of units, i.e. of examples

inefficient at representing **highly-varying functions**, which may otherwise have a compact representation.

Optimization of Deep Architectures

- What **deep** architectures are known? various kinds of multi-layer neural networks with many layers.
- Except for a very special kind of architectures for machine vision (convolutional networks), deep architectures have been neglected in machine learning.
- Why? **Training gets stuck in mediocre solutions** (Tesauro 92).
- Credit assignment problem?
- No hope?



Greedy Learning of Multiple Levels of Abstractions

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  2. the simpler ones can be learned first (i.e., are also good models of the data).
- Coherent with psychological literature (Piaget 1952).
  We learn baby math before arithmetic before algebra before differential equations . . .
- Also some evidence from neurobiology: (Guillery 2005) *"Is postnatal neocortical maturation hierarchical?"*.

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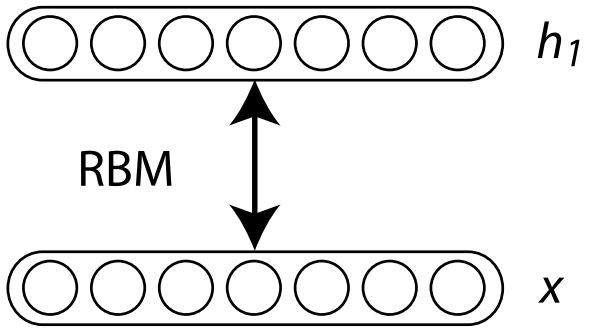

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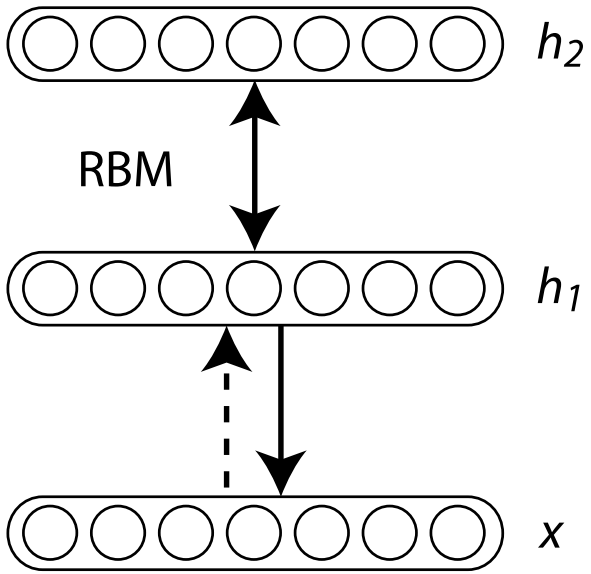

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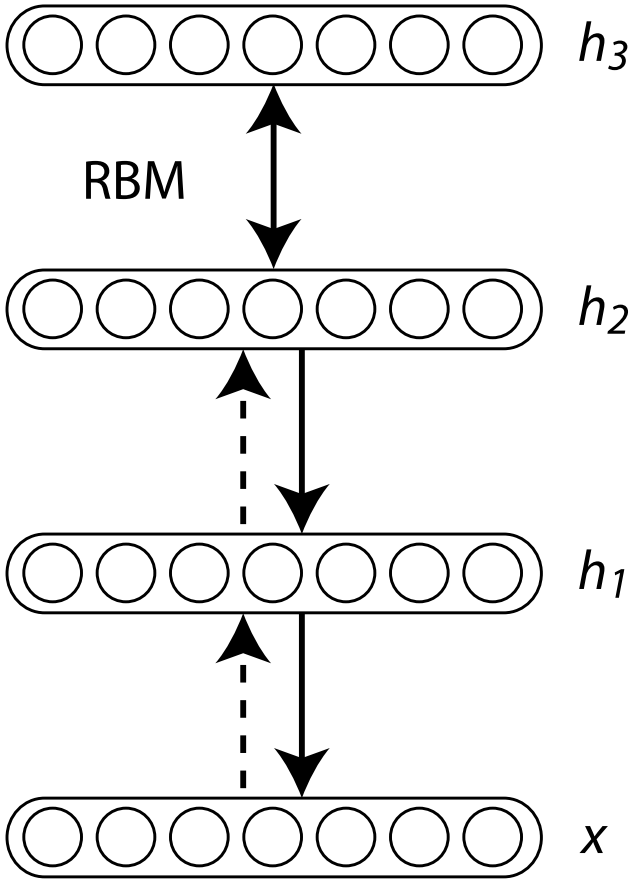

Greedy Layer-Wise Initialization

- The principle of greedy layer-wise initialization proposed by Hinton can be generalized to other algorithms.

- Initialize each layer of a deep multi-layer feedforward neural net as an autoassociator for the output of previous layer.
- Find W which minimizes cross-entropy loss in predicting x from $\hat{x} = \mathrm{sigm}(W' \mathrm{sigm}(Wx))$.

- Feed its hidden activations as input to next layer.
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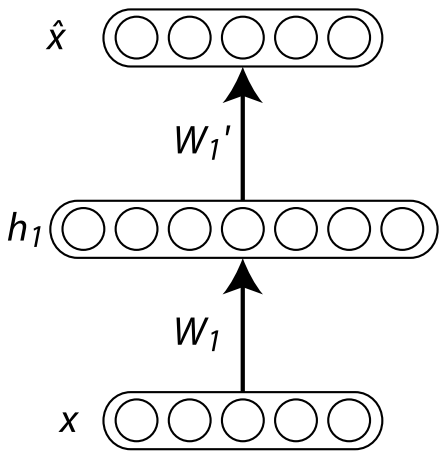

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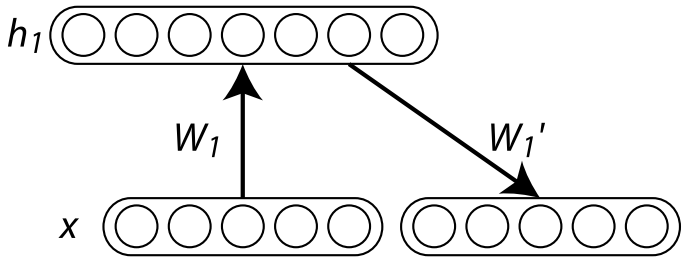

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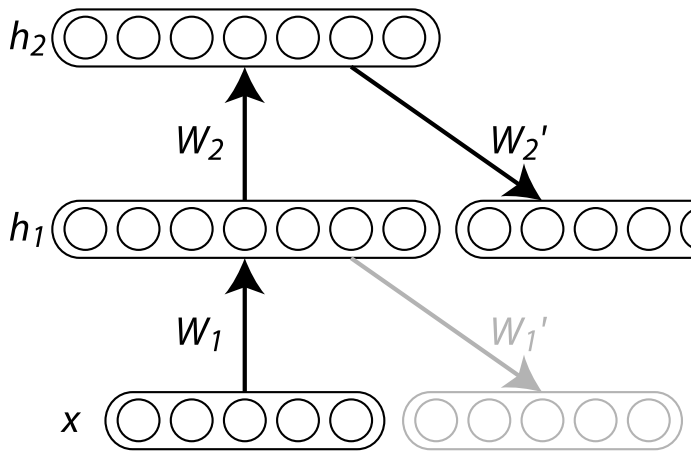

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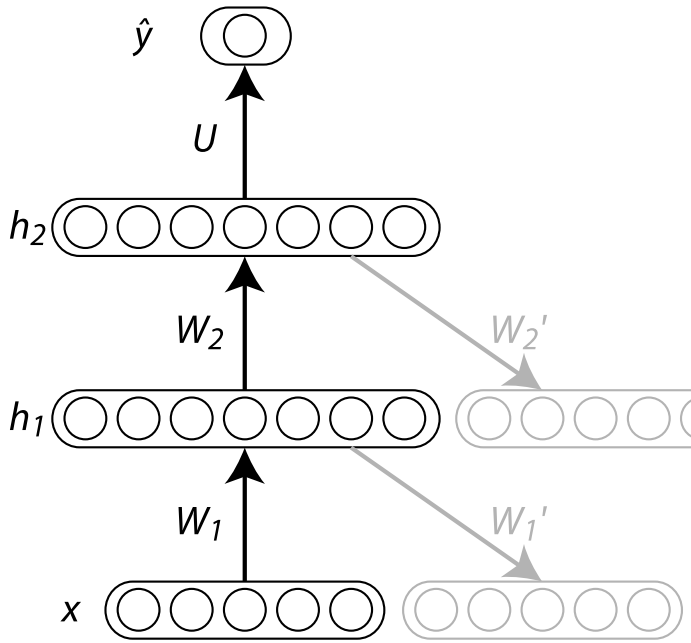

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Greedy Supervised Layer-Wise Initialization

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- Each layer is trained as the hidden layer of a supervised 2-layer neural net.
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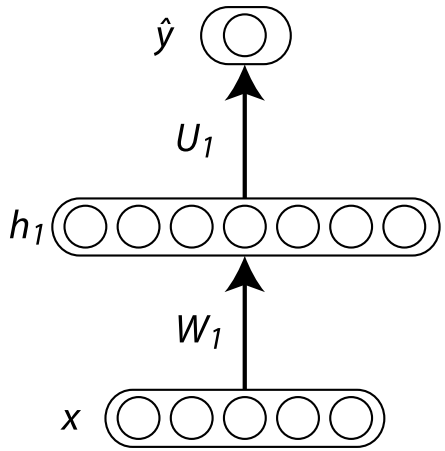
- Propagate data through new hidden layer, train another layer, etc.



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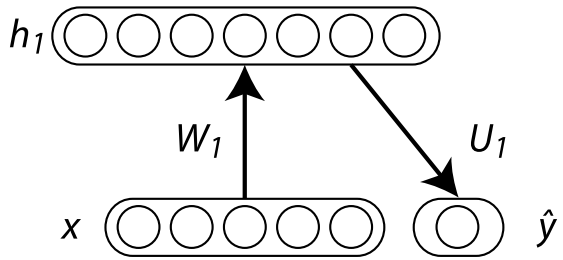

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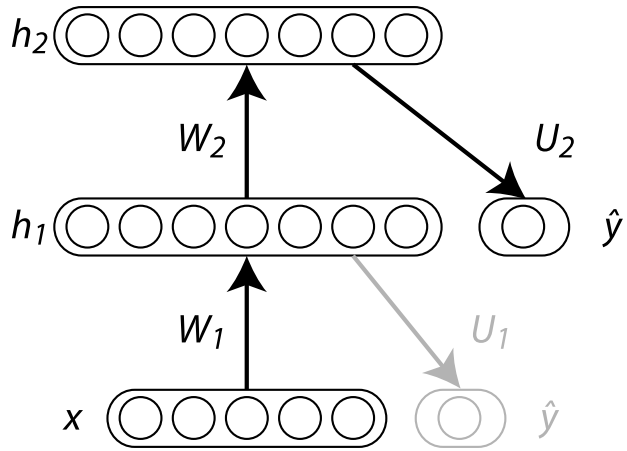

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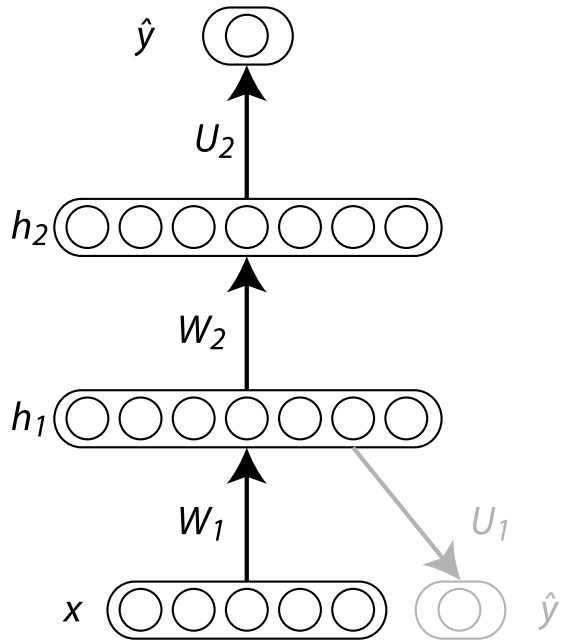

Experiments on Greedy Layer-Wise Initialization

	train.	test.
Deep Belief Net, unsupervised pre-training	0%	1.2%
Deep net, autoassociator pre-training	0%	1.4%
Deep net, supervised pre-training	0%	2.0%
Deep net, no pre-training	.004%	2.4%
Shallow net, no pre-training	.004%	1.9%

Classification error on MNIST digits benchmark training, validation, and test sets, with the best hyper-parameters according to validation error.

Deep nets with 3 to 5 hidden layers.
Selects around 500 hidden units per layer.

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Supervised greedy is **too greedy**.
Greedy unsupervised initialization works great.

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Classification error on MNIST with 20 hidden units on top layer:

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Because

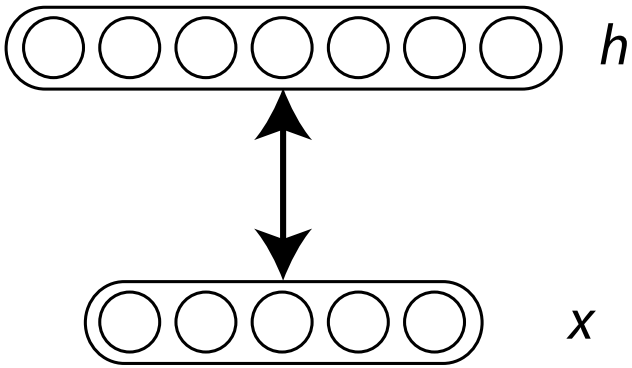
1. last fat hidden layer did all the work
2. using a poor representation (output of all previous layers)

Yes it is really an **optimization** problem
and a **representation** problem

Restricted Boltzmann Machines

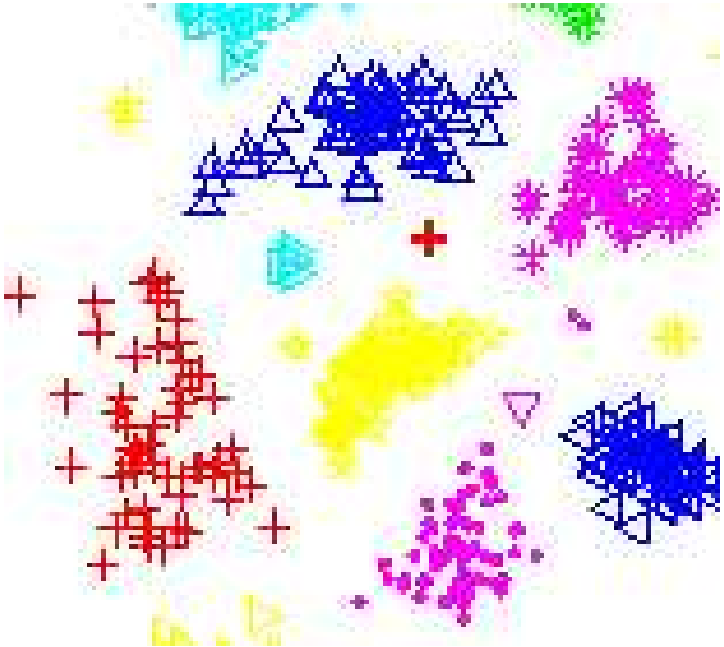
Bi-partite Boltzmann machine:

$$P(V = v, H = h) \propto e^{-\mathcal{E}(v,h)} = e^{v'b + h'c + h'Wv}$$



- Conditionals $P(v|h)$ and $P(h|v)$ easy to derive, and factorize.
- Contrastive divergence provides good estimator of log-likelihood gradient.
- Originally for binary variables; we extend it **easily** to continuous variables by slightly changing energy function and range of values (see poster).

Combining Supervised & Unsupervised



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$\Rightarrow$ **input distribution structure reveals the target class.**

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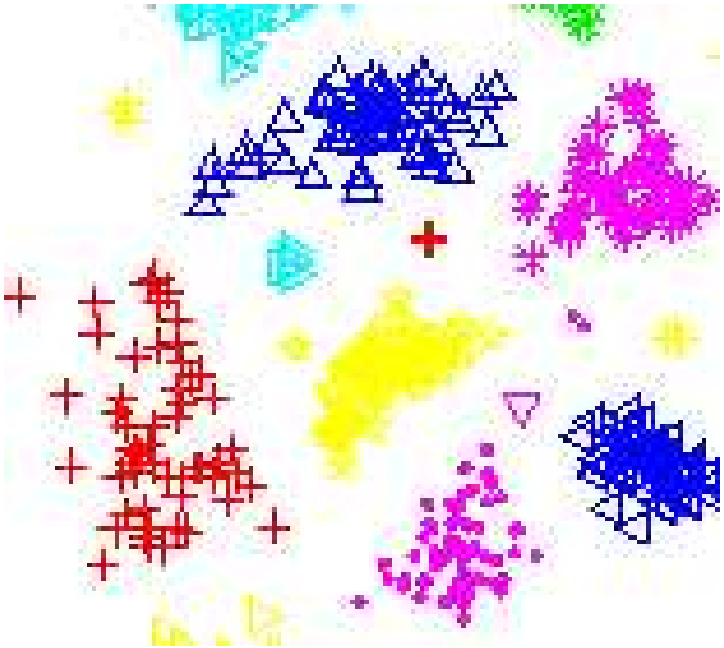

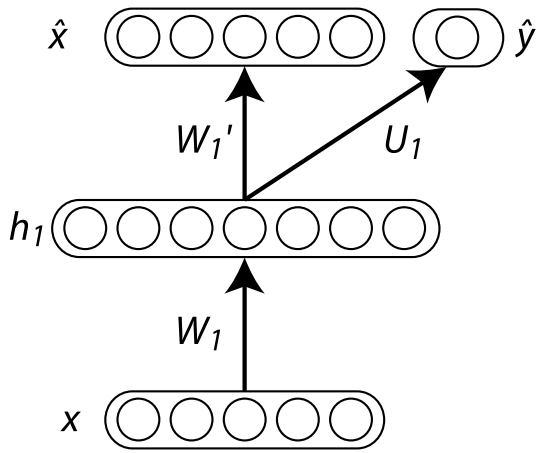

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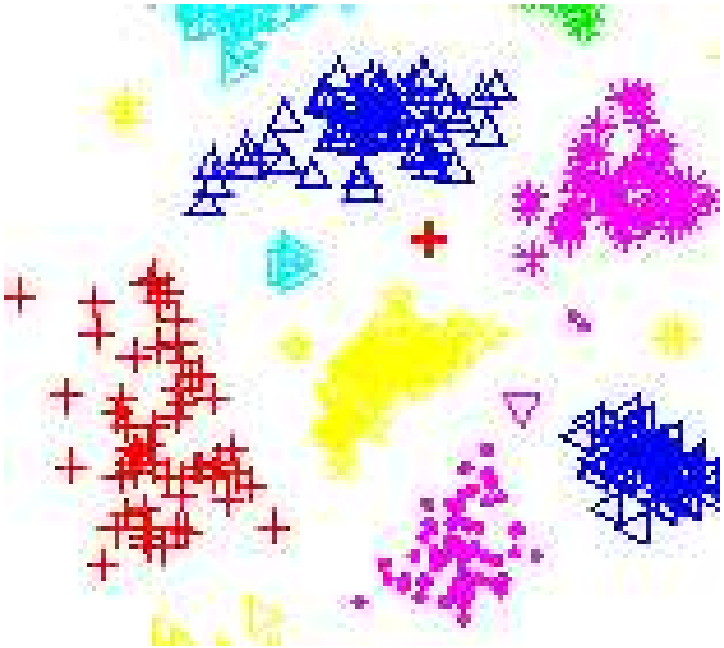

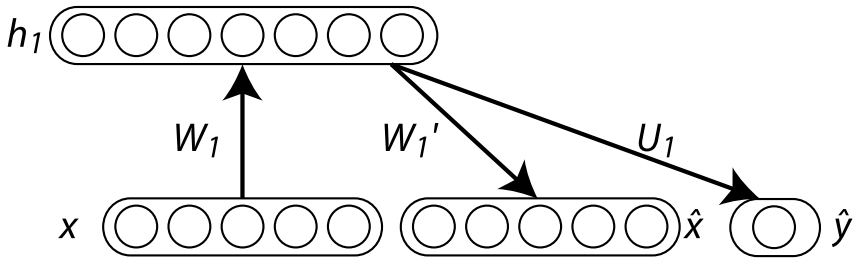

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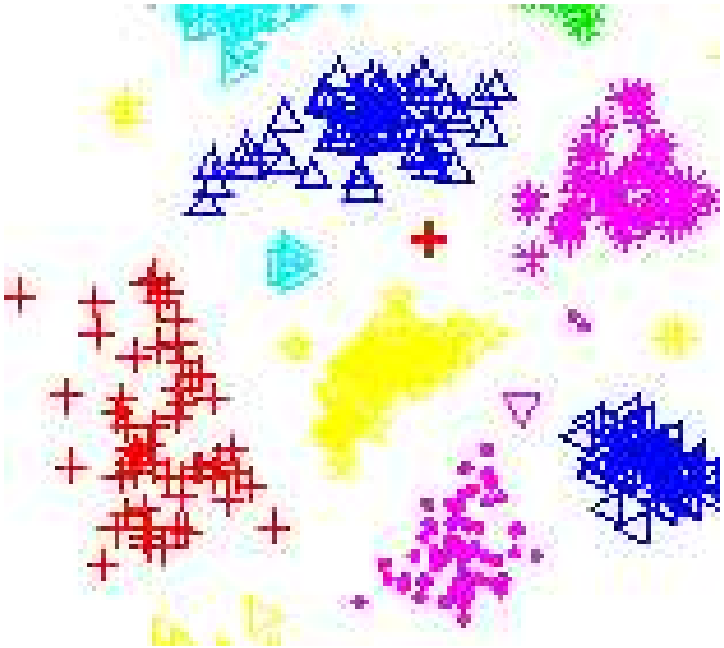

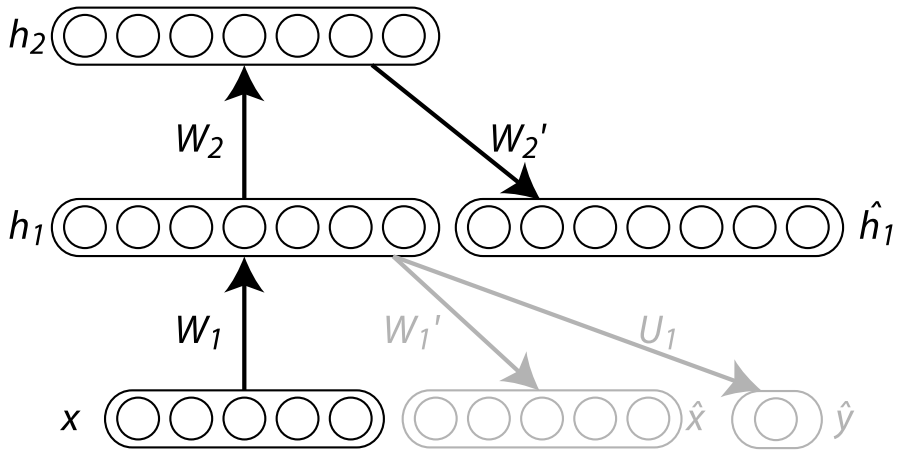

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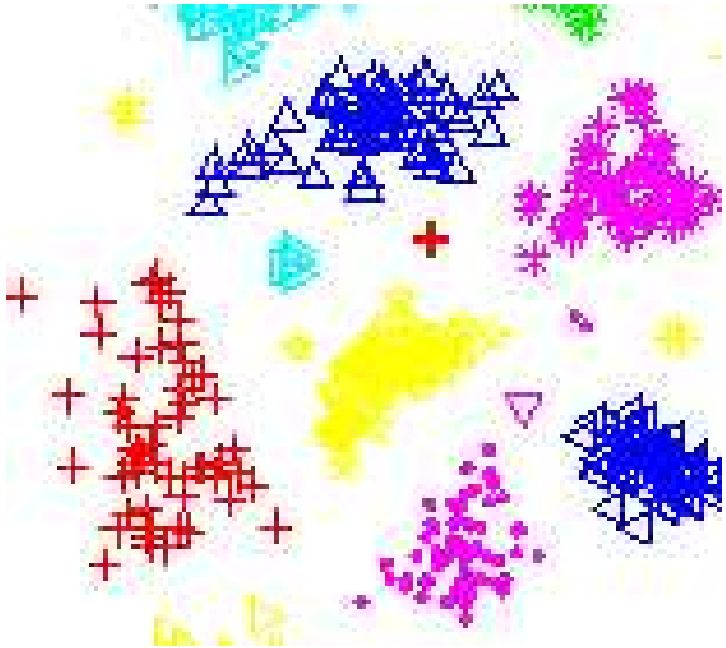

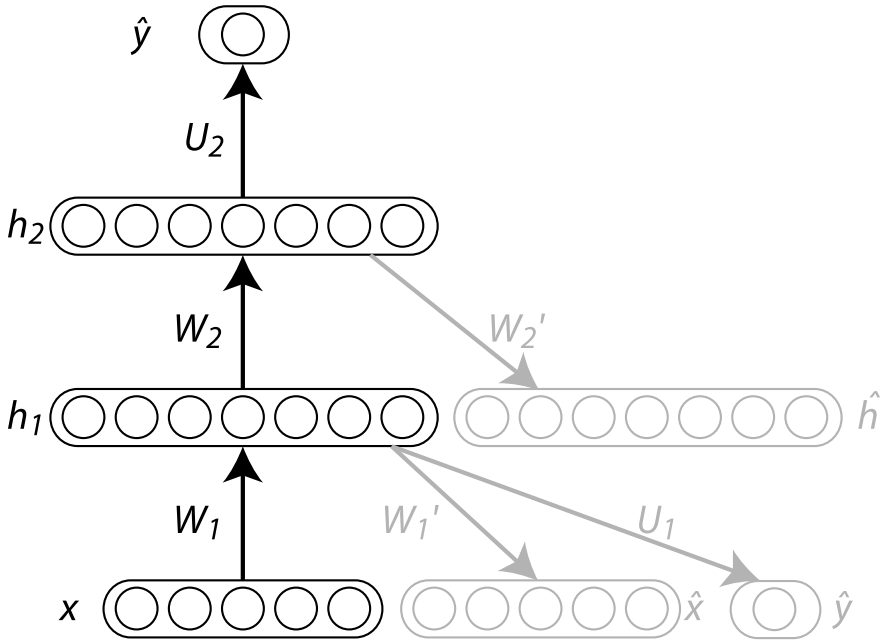

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More experimental results

	Abalone MSE	**Cotton** class. error
1. Deep Network, no pre-training	4.2	43.0%
2. Logistic regression	·	45.0%
3. DBN, Bin inputs, unsup	4.47	45.0%
4. DBN, Bin inputs, partially sup	4.28	43.7%
5. DBN, Gauss inputs, unsup	4.19	35.8%
6. DBN, Gauss inputs, partially sup	4.18	31.4%

MSE on Abalone task and classification error on Cotton task, showing improvement with Gaussian vs binomial units and partial supervision

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- **Principle works about as well with symmetric autoassociators** in feedforward neural net
- The unsupervised part is important: regularizes and makes sure to propagate most information about input, **purely supervised is too greedy**.
- Easy extensions of Deep Belief Nets: continuous-valued units / partially supervised initialization when input density is not revealing of target