Greedy Layer-Wise Training of Deep Networks

Yoshua Bengio, Pascal Lamblin, Dan Popovici, Hugo Larochelle

U. Montreal

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

Summary

- Motivation: AI $\Rightarrow$ learning high-level abstractions
  $\Rightarrow$ 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

- Ambitious 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! (did we turn our back on it?)
- 3 considerations:
  - computational efficiency
  - statistical efficiency
  - human-labor efficiency 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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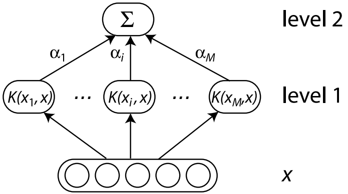
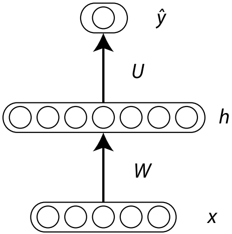
Depth of Architectures

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



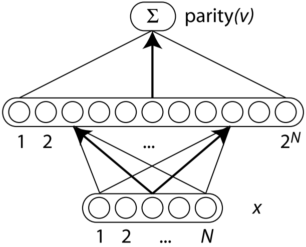
Non-parametric ones can theoretically approximate any continuous function. But **how efficiently?** (computational, statistical)



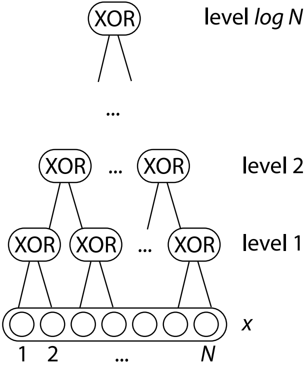
Inefficiency of Shallow Architectures

Mathematical results from complexity theory of boolean circuits:

Functions representable compactly by a deep circuit often need circuits of exponential size to be represented by a shallow circuit (Hastad 1987)



Very fat shallow circuit
⇒ many adjustable elements
⇒ many examples needed



Brain has a deep architecture

Number of levels should not be fixed but data-dependent.

Curse of Dimensionality

(Bengio et al 2006):

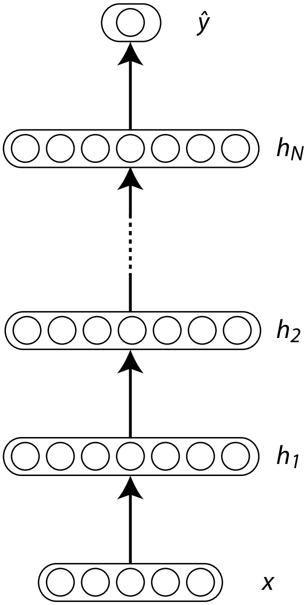
Local kernel machines (= **pattern matchers**) and decision trees **partition the space** and may need

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

- Learning AI $\Rightarrow$ **learning abstractions**
- General principle: **Greedily learning simple things first, higher-level abstractions on top of lower-level ones.**
- **Implicit prior**: restrict to functions that
  1. can be represented as a composition of simpler ones such that
  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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Deep Belief Networks

Hinton et al (2006) recently introduced a deep graphical model that provides more evidence that this principle works:

- beats state-of-the-art statistical learning in experiments on a large machine learning benchmark task (knowledge-free MNIST)
  See also Ranzato et al spotlight/poster tomorrow
- Each layer tries to model distribution of its input (unsupervised training as Restricted Boltzmann Machine)
- H = hidden causes,
  $P(h|x)$ = representation of x.
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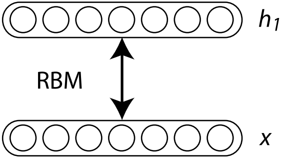

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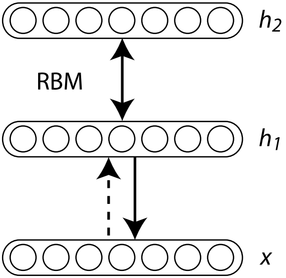

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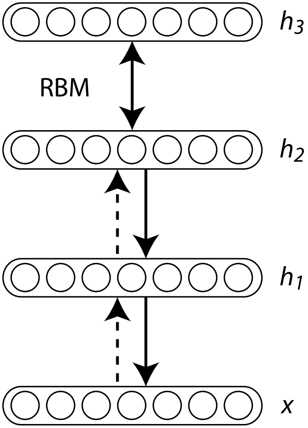

Greedy Layer-Wise Initialization

- 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.
- Sigmoid and small weights (weight decay or stochastic gradient) prevent autoassociator from learning the identity.

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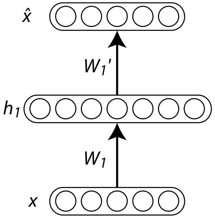

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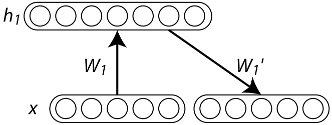

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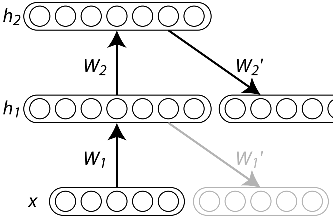

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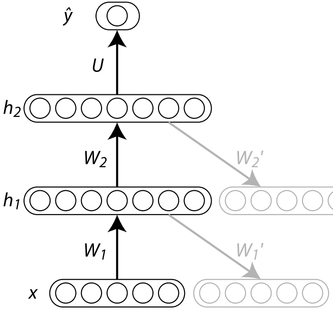

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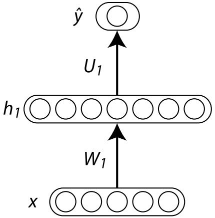
Greedy Supervised Layer-Wise Initialization

Why not use supervised learning at each stage?

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



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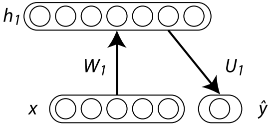

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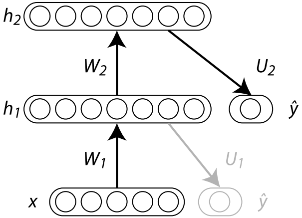

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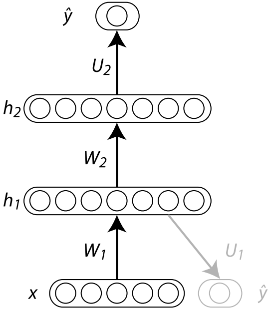

Experiments on Greedy Layer-Wise Initialization

	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.

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

Why 0 train error even with deep net / no-pretraining?

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Is it Really an Optimization Problem?

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

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Deep net, autoassociator pre-training	0%	**1.6%**
Deep net, supervised pre-training	0%	1.9%
Deep net, no pre-training	.59%	2.2%
Shallow net, no pre-training	3.6%	5.0%

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

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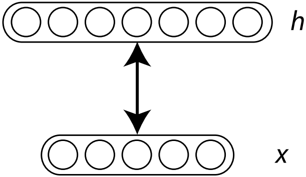
Restricted Boltzmann Machines

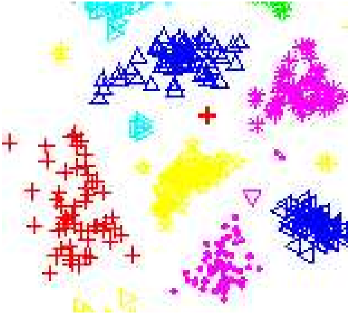
Bi-partite Boltzmann machine:

$$P(X = x, H = h) \propto e^{-\mathcal{E}(x,h)} = e^{x'b + h'c + h'Wx}$$



- Conditionals $P(x|h)$ and $P(h|x)$ 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



MNIST: nice clusters in the distribution
⇒ **input distribution structure reveals the target class.**
$f_1(x) = P(Y|x)$ related to $f_2(x) = P(x)$

Otherwise? Simple solution:
combine supervised & unsupervised layer-wise greedy initialization.

Just add the two stochastic gradient updates.

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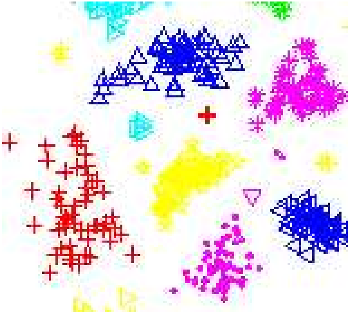

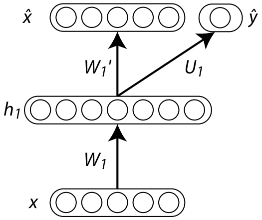

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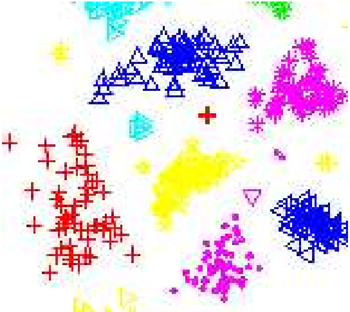

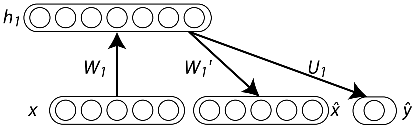

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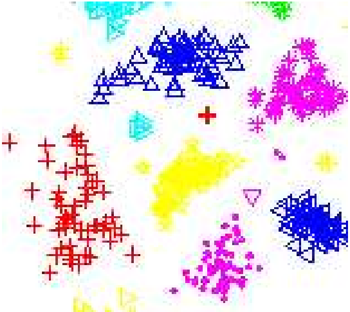

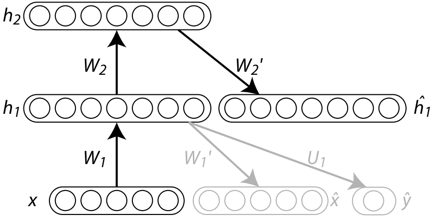

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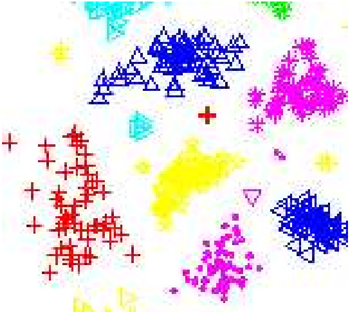

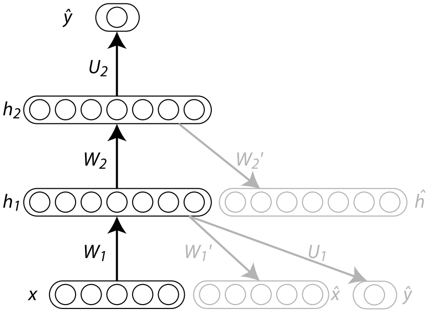

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More experimental results

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

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

Conclusions

- For AI $\Rightarrow$ must learn **high level abstractions** efficiently
  $\Rightarrow$ deep architectures (statistical efficiency)
- Deep architectures not trainable? computational efficiency? new methods appear to **break through the obstacle**
- Basic principle: greedy layer-wise unsupervised (or adding unsupervised and supervised criteria)
- **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
- Come see the poster!

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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
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Conclusions

- For AI $\Rightarrow$ must learn **high level abstractions** efficiently
  $\Rightarrow$ deep architectures (statistical efficiency)
- Deep architectures not trainable? computational efficiency? new methods appear to **break through the obstacle**
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