School of Computer Science
Carnegie Mellon

10-701 Introduction to Machine Learning

Deep Learning

Matt Gormley
Lecture 13
October 19, 2016

Readings:
Bishop Ch. 4.1.7, Ch. 5
Murphy Ch. 16.5, Ch. 28
Mitchell Ch. 4

Reminders

- Homework 3:
  - due 10/24/16

Outline

- **Deep Neural Networks (DNNs)**
  – Three ideas for training a DNN
  – Experiments: MNIST digit classification
  – Autoencoders
  – Pretraining
- **Recurrent Neural Networks (RNNs)**
  – Bidirectional RNNs
  – Deep Bidirectional RNNs
  – Deep Bidirectional LSTMs
  – Connection to forward-backward algorithm
- **Convolutional Neural Networks (CNNs)**
  – Convolutional layers
  – Pooling layers
  – Image recognition

PRE-TRAINING FOR DEEP NETS

Goals for Today's Lecture

1. Explore a **new class of decision functions** (Deep Neural Networks)
2. Consider **variants of this recipe** for training

2. Choose each of these:
   - Decision function

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

   - Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

4. Train with SGD: (take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

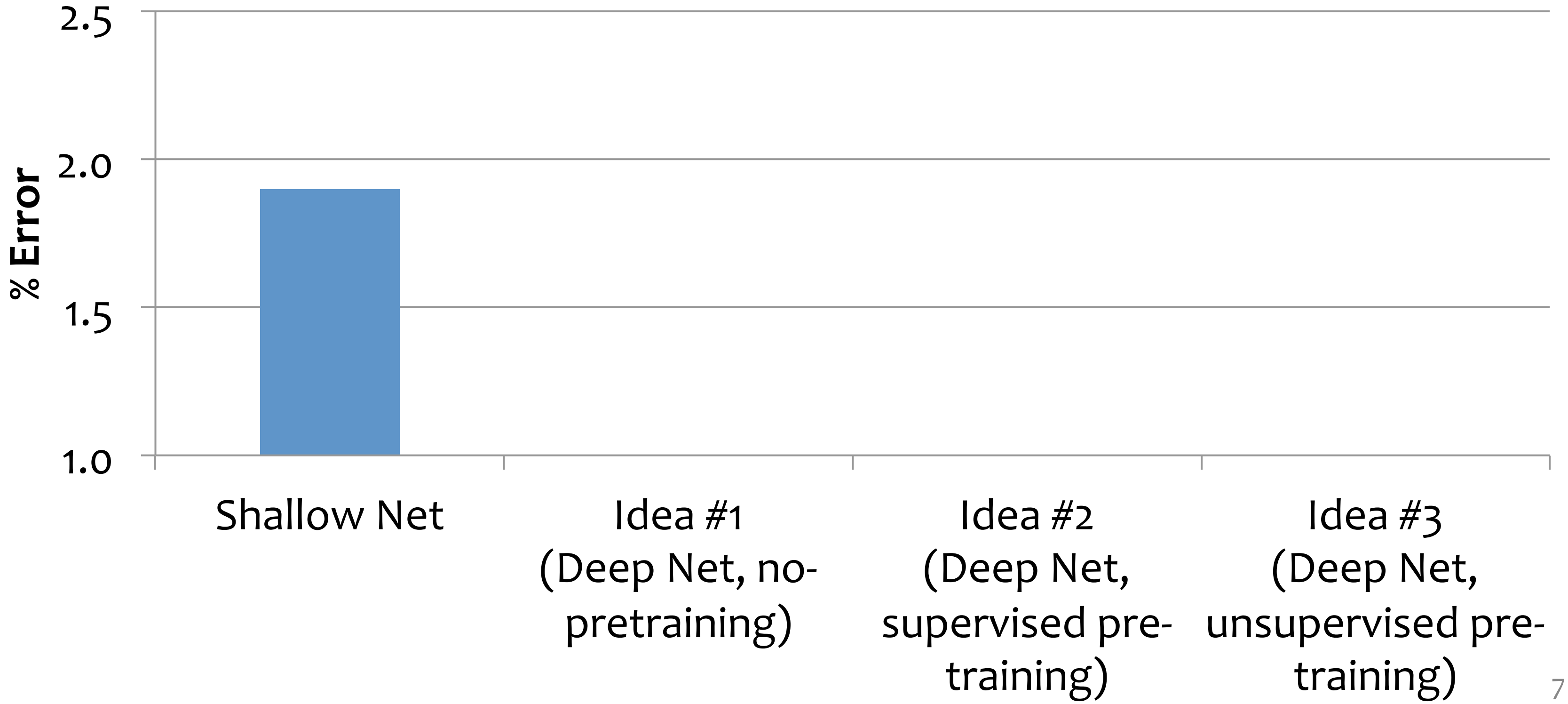
Training

Idea #1: No pre-training

- **Idea #1: (Just like a shallow network)**
  - Compute the supervised gradient by backpropagation.
  - Take small steps in the direction of the gradient (SGD)

Comparison on MNIST

- Results from Bengio et al. (2006) on MNIST digit classification task
- Percent error (lower is better)



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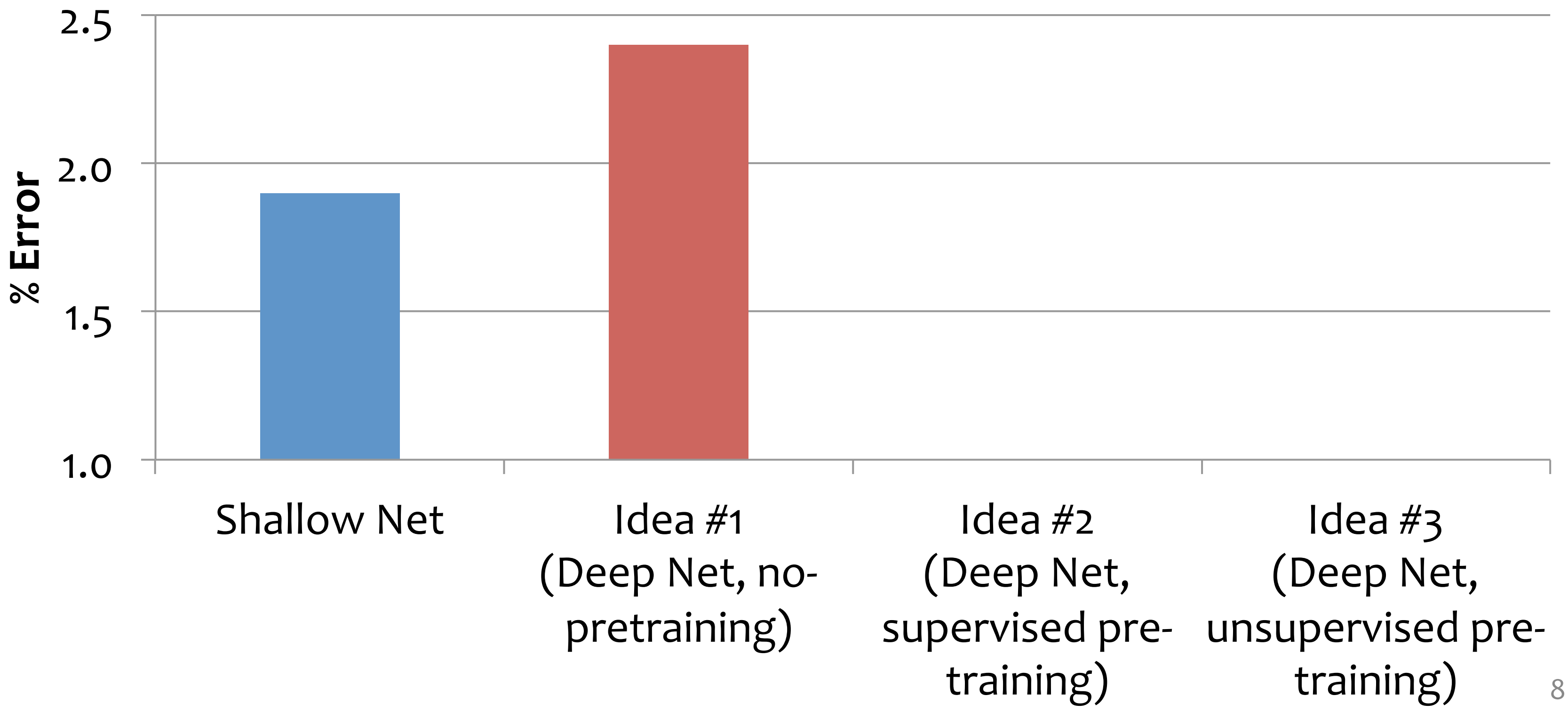

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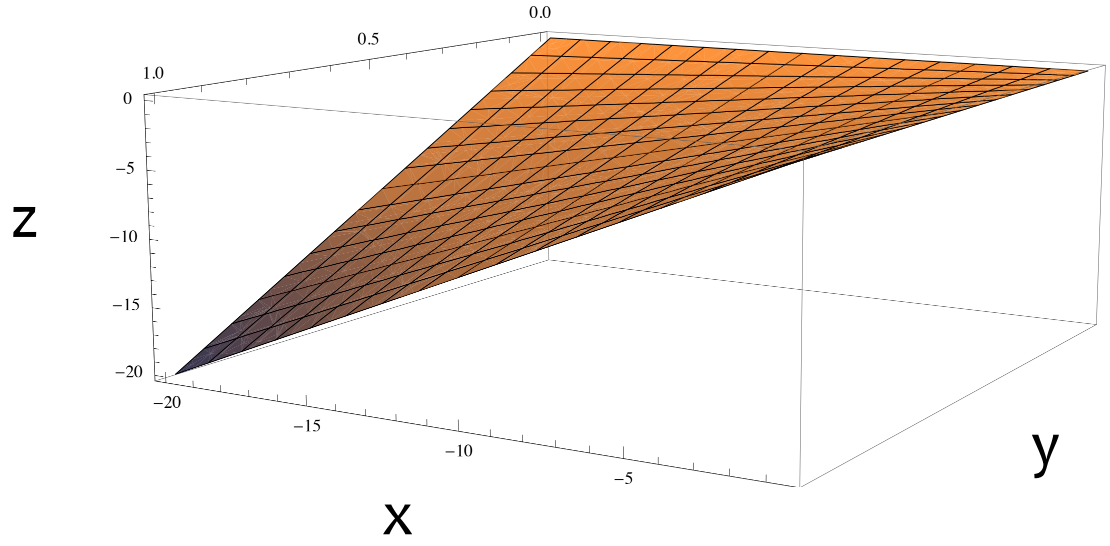
- What goes wrong?
  A. Gets stuck in local optima
     - Nonconvex objective
     - Usually start at a random (bad) point in parameter space
  B. Gradient is progressively getting more dilute
     - "Vanishing gradients"

Training

Problem A: *Nonconvexity*

- Where does the nonconvexity come from?
- Even a simple quadratic z = xy objective is nonconvex:



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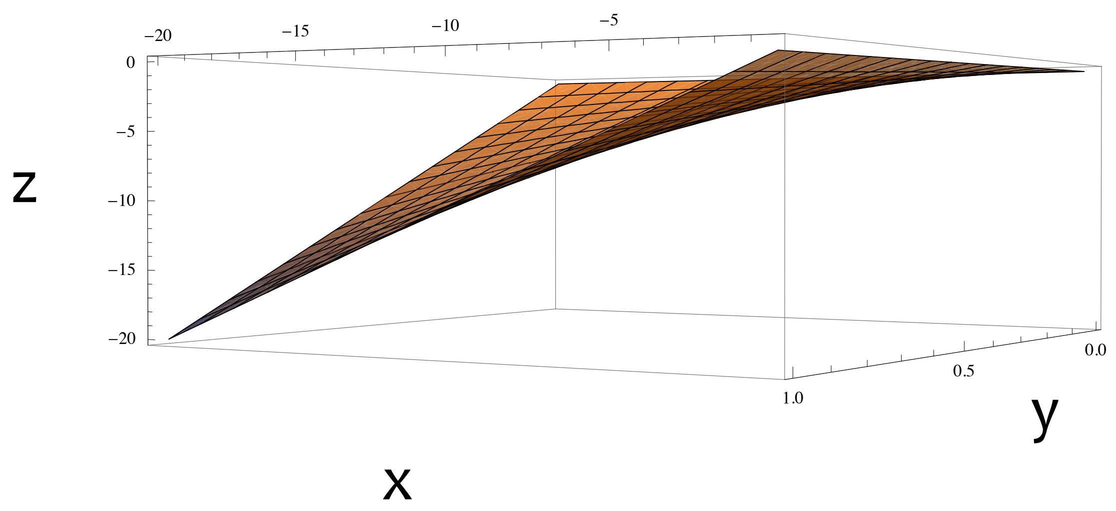
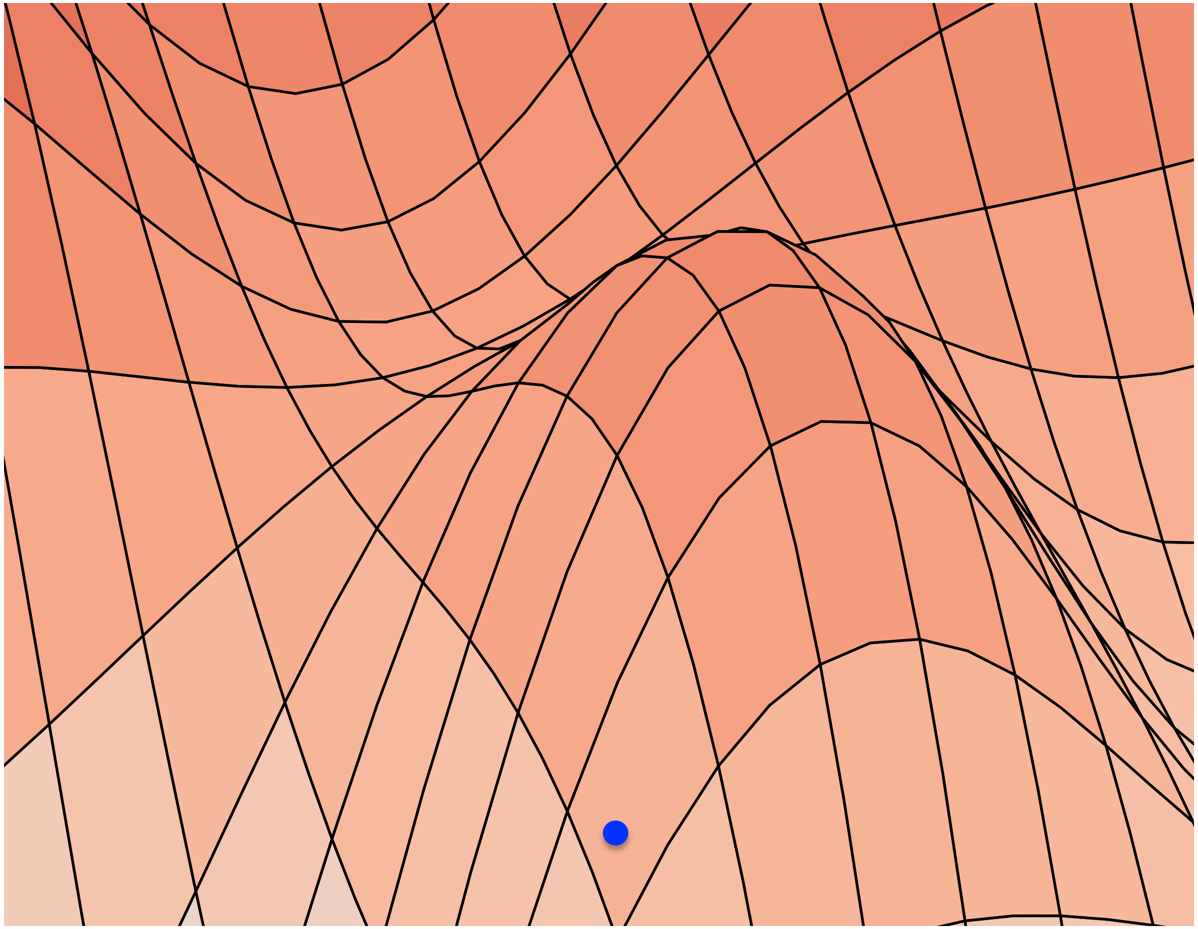


Training

Problem A: *Nonconvexity*

Stochastic Gradient Descent…

…climbs to the top of the nearest hill…



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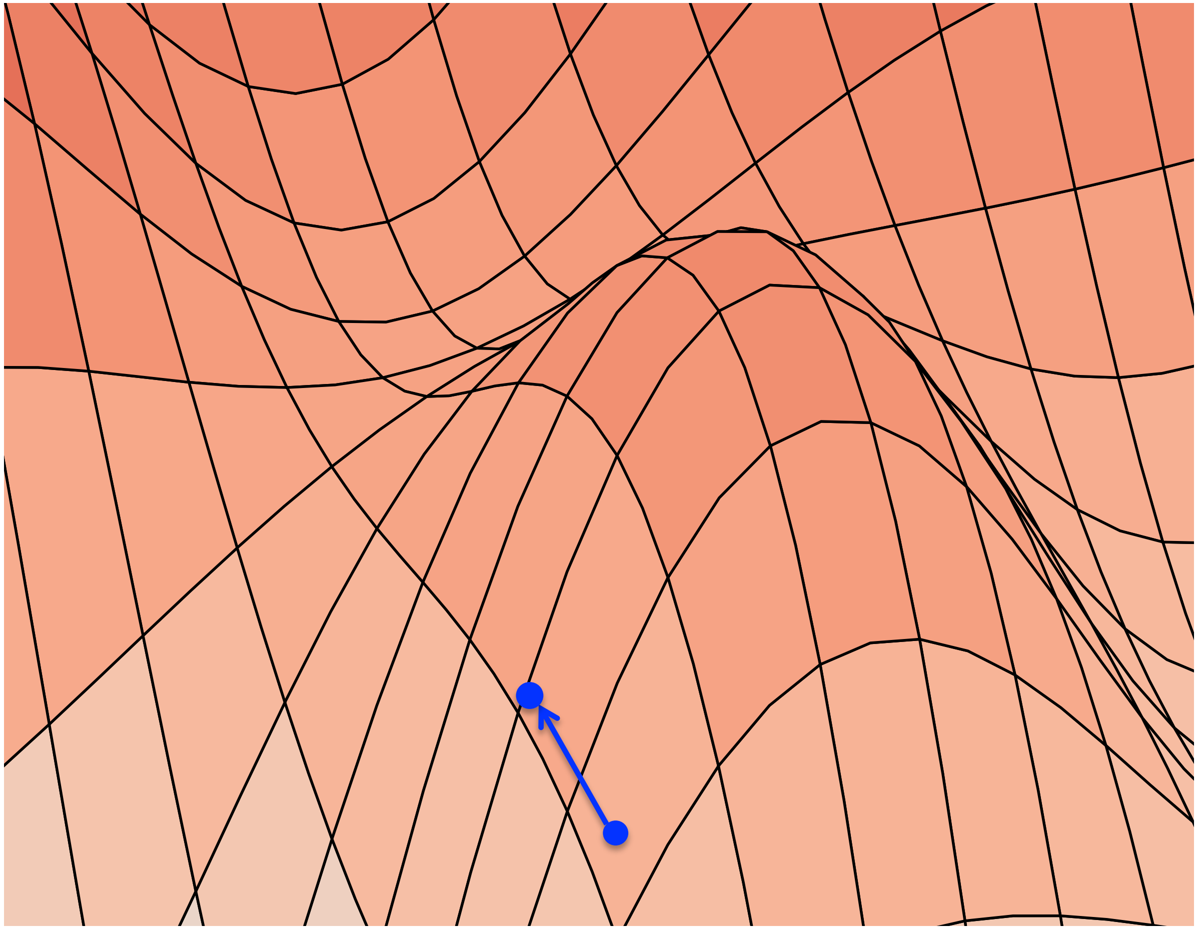

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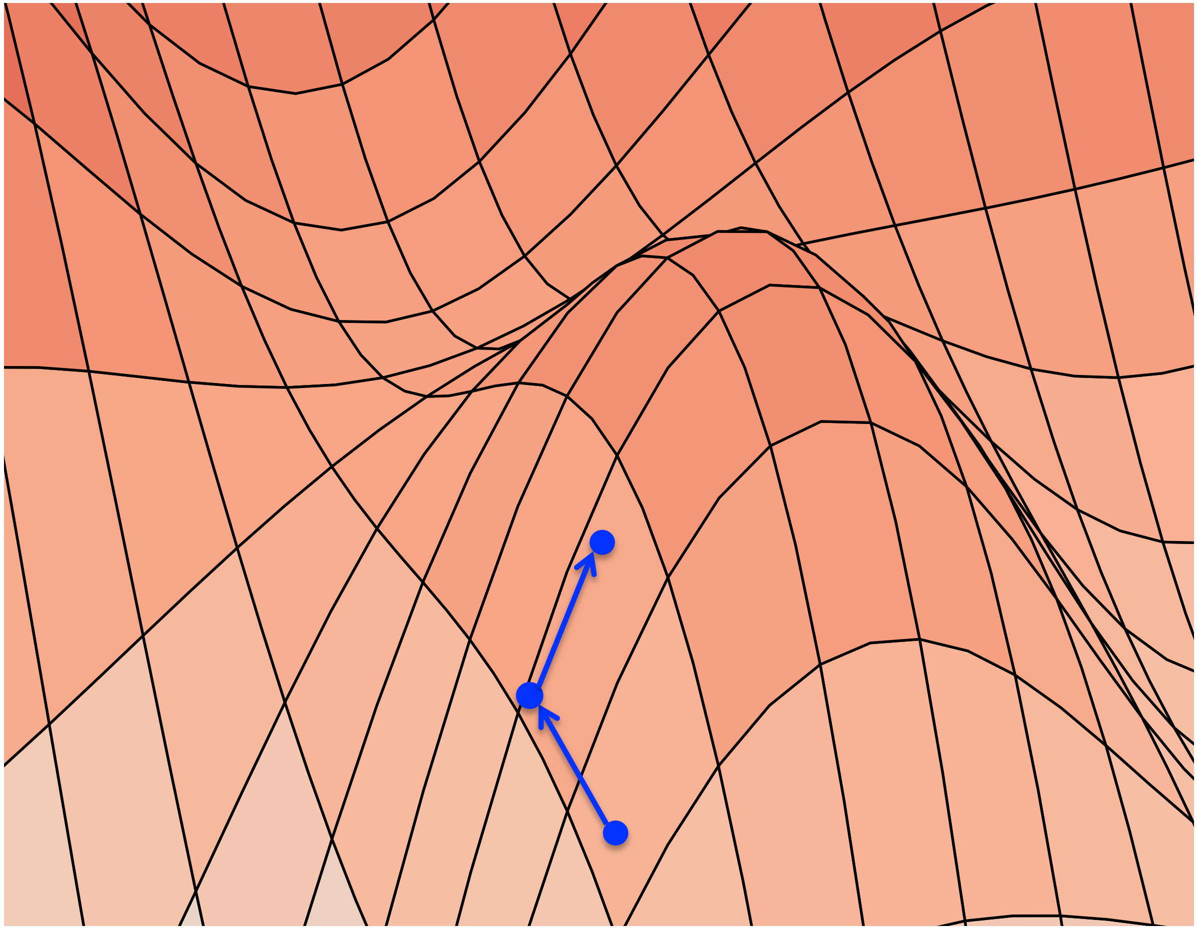

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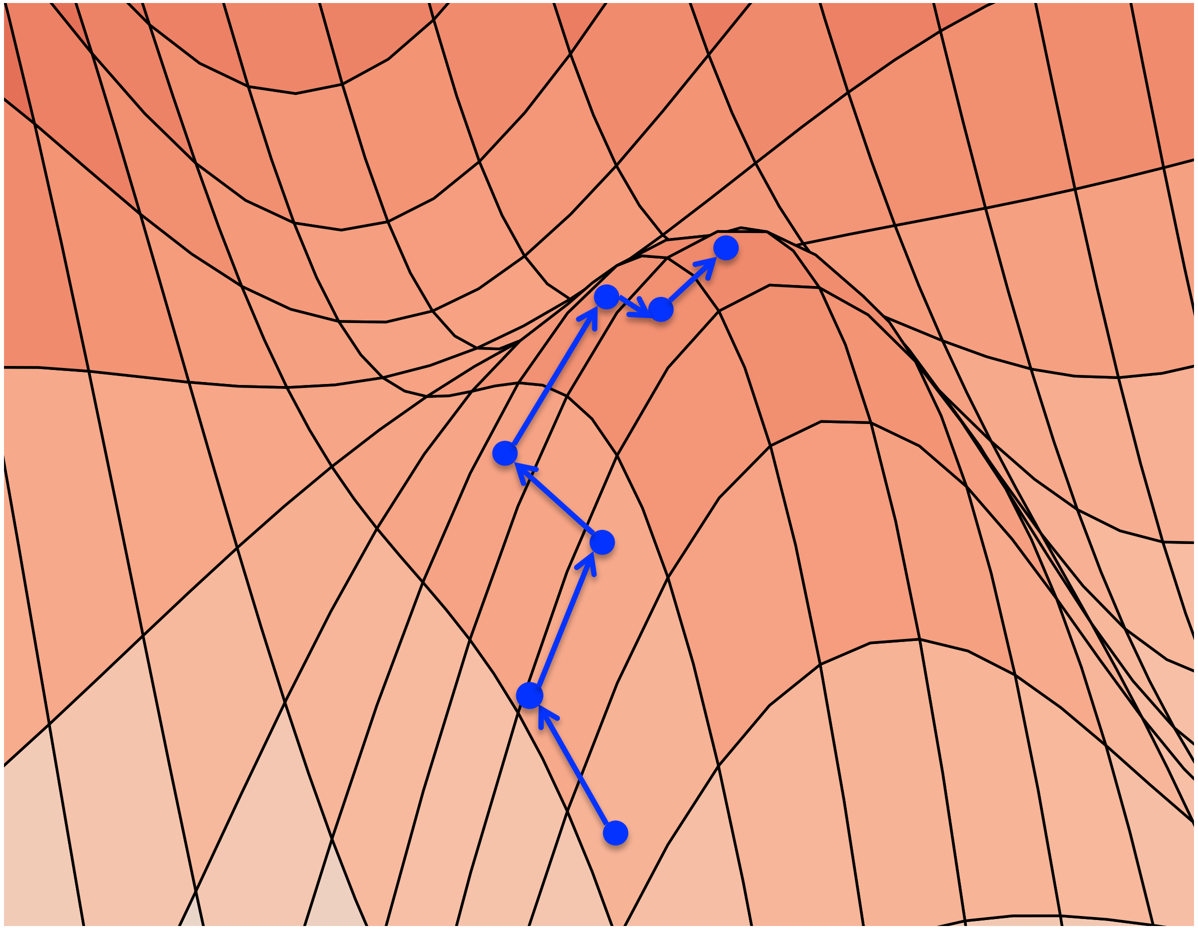


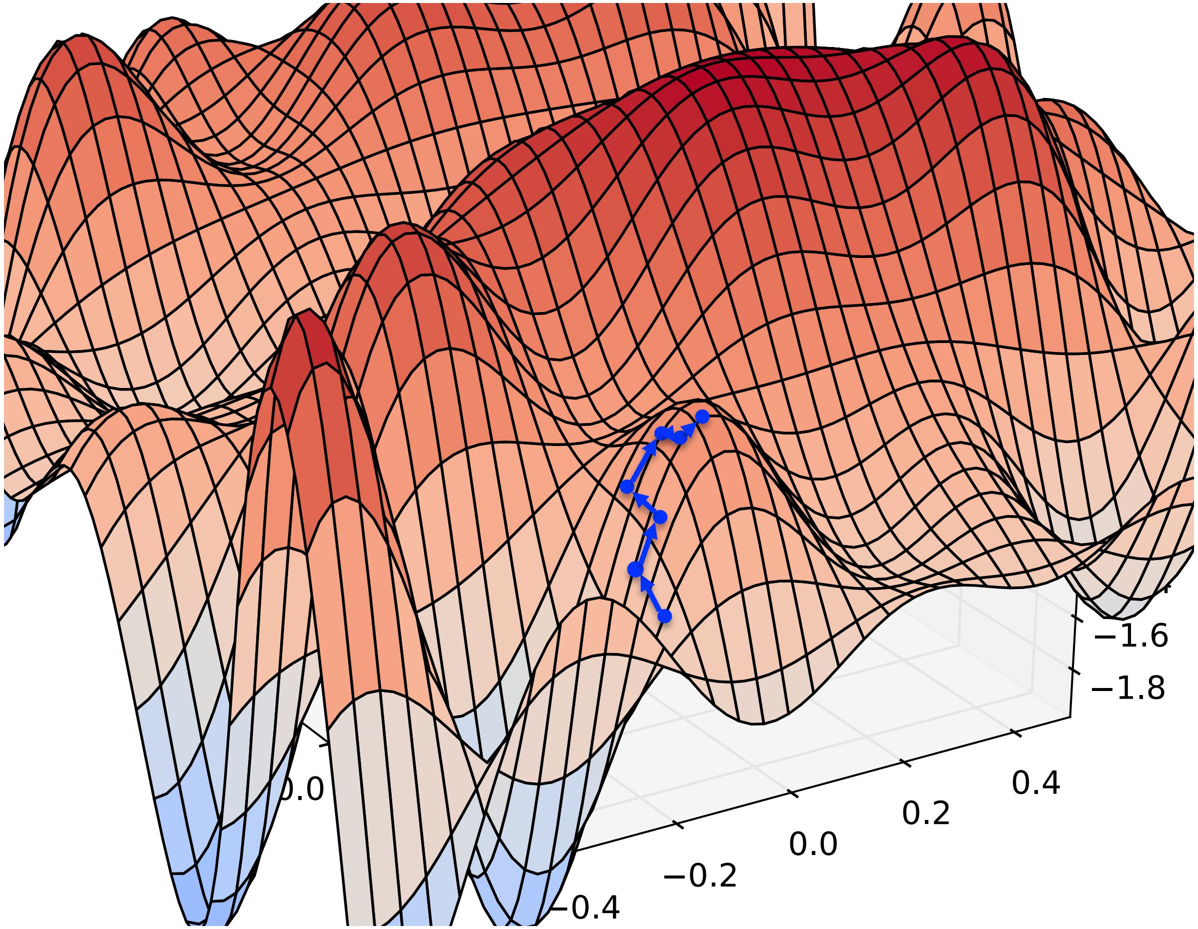
Training

Problem A: *Nonconvexity*

Stochastic Gradient Descent…

… climbs to the top of the nearest hill…

… which might not lead to the top of the mountain

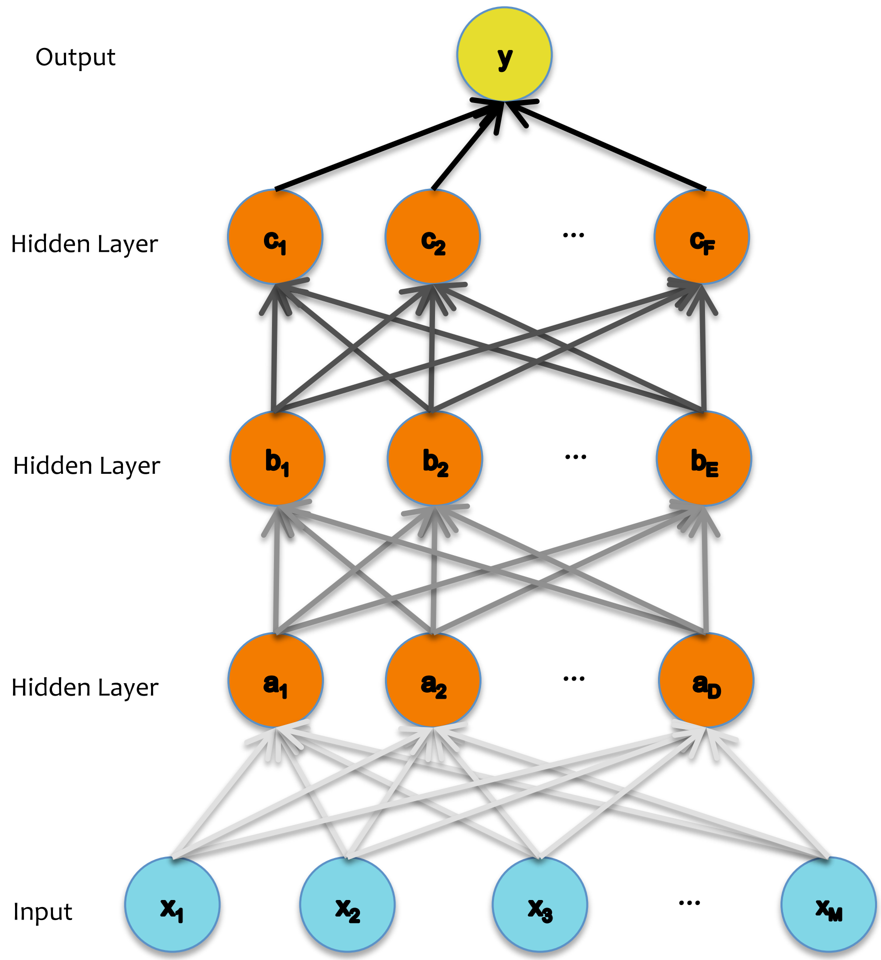


Training

Problem B: *Vanishing Gradients*

The gradient for an edge at the base of the network depends on the gradients of many edges above it

The chain rule multiplies many of these partial derivatives together



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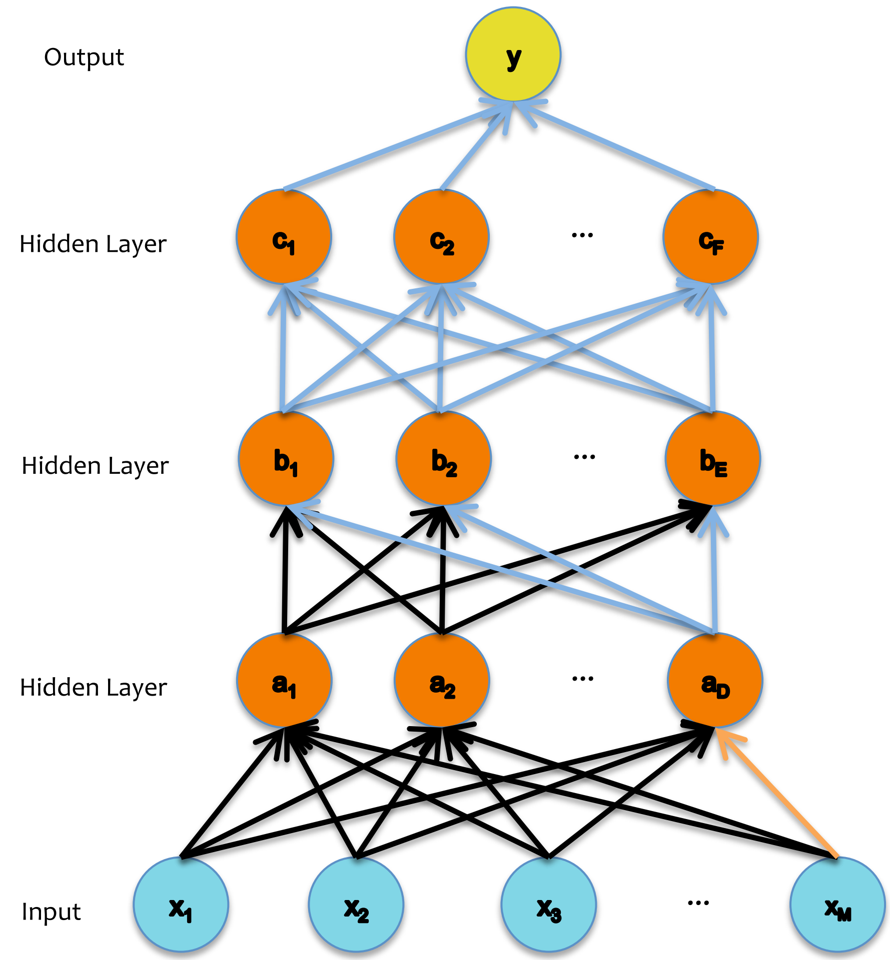

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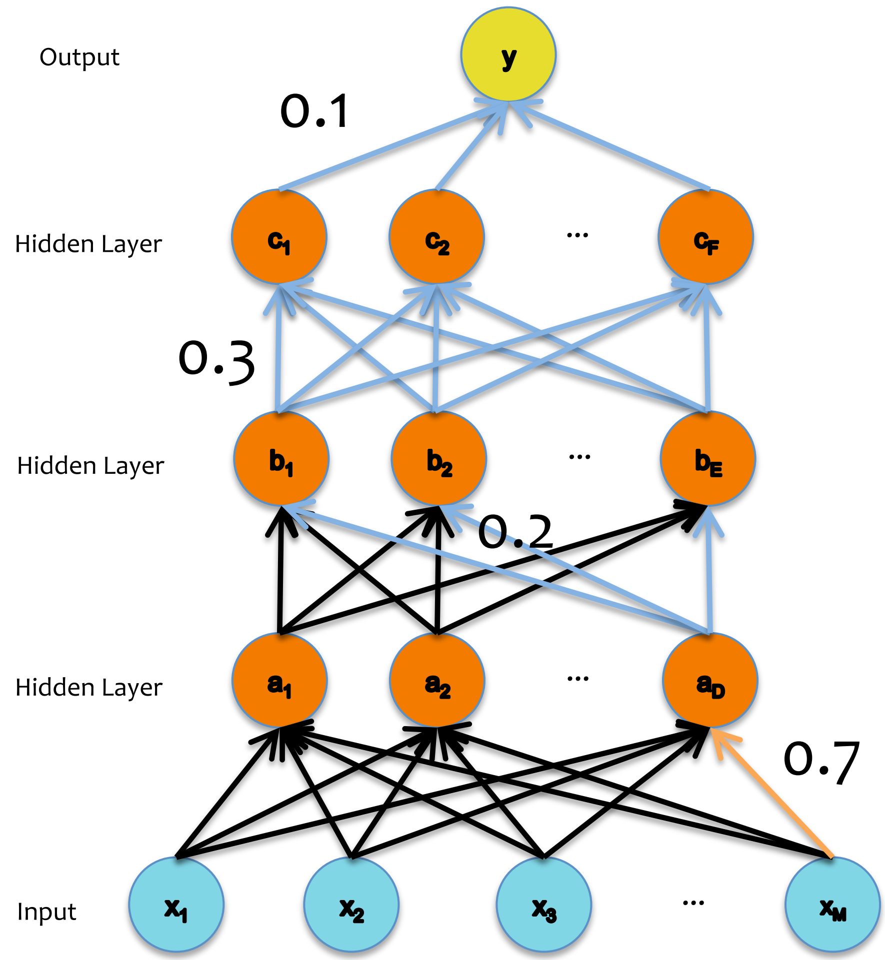

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Idea #2: Supervised Pre-training

- **Idea #2: (Two Steps)**
  - **Train each level** of the model in a **greedy** way
  - Then use our **original idea**

1. Supervised Pre-training
   - Use **labeled** data
   - Work bottom-up
     - Train hidden layer 1. Then fix its parameters.
     - Train hidden layer 2. Then fix its parameters.
     - …
     - Train hidden layer n. Then fix its parameters.
2. Supervised Fine-tuning
   - Use **labeled** data to train following "Idea #1"
   - Refine the features by backpropagation so that they become tuned to the end-task

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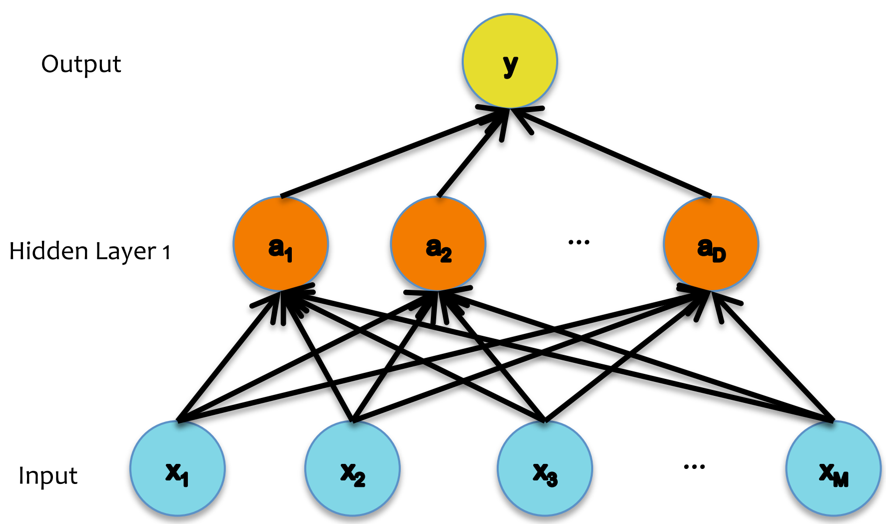

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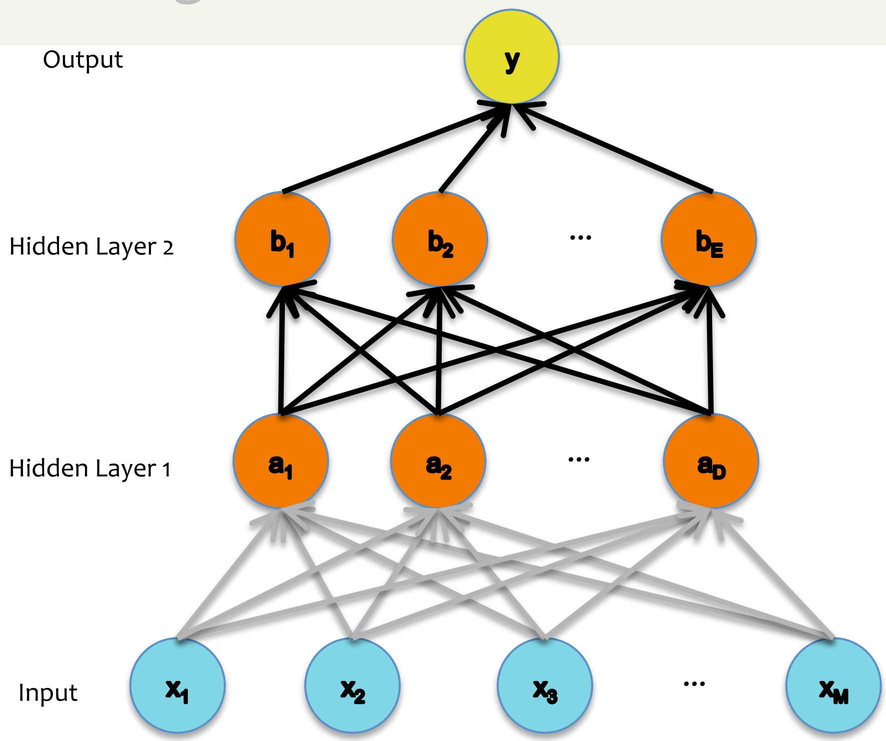

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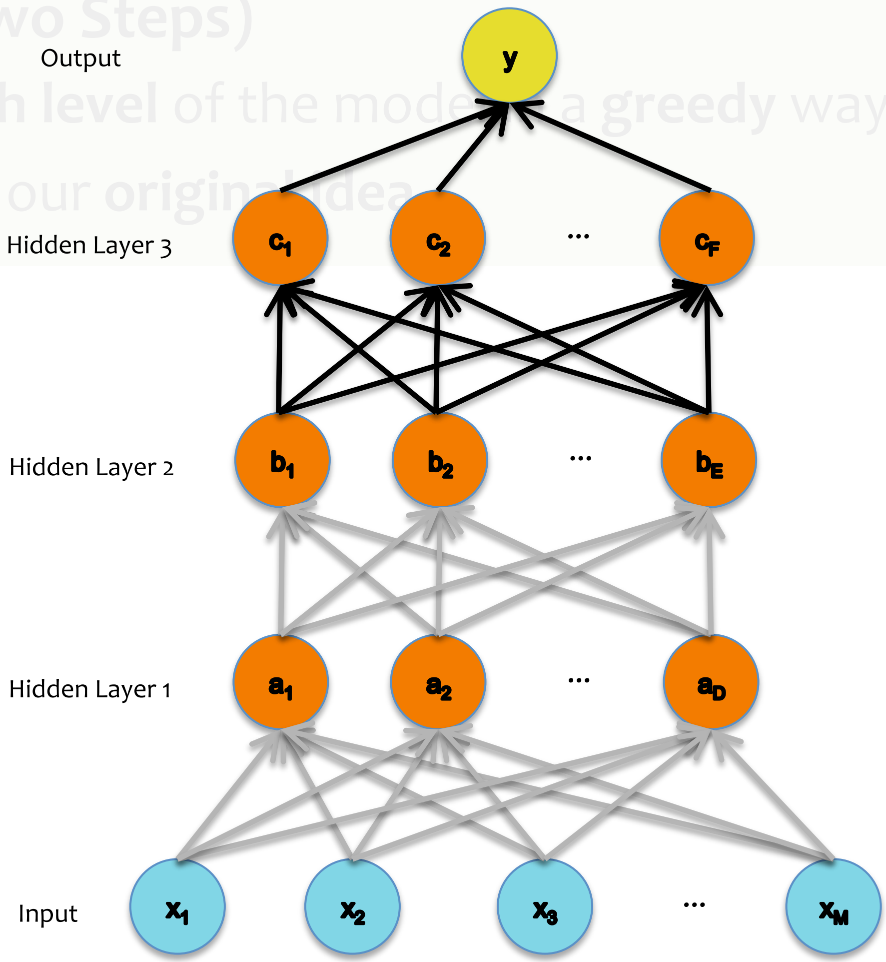

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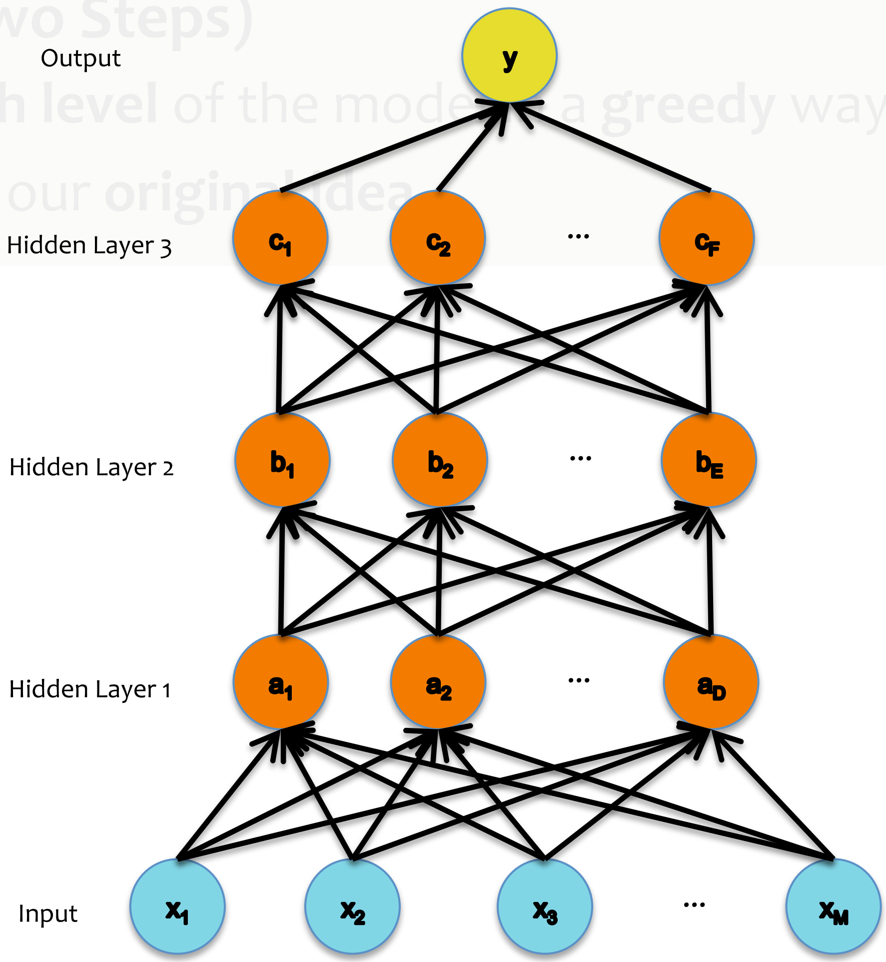

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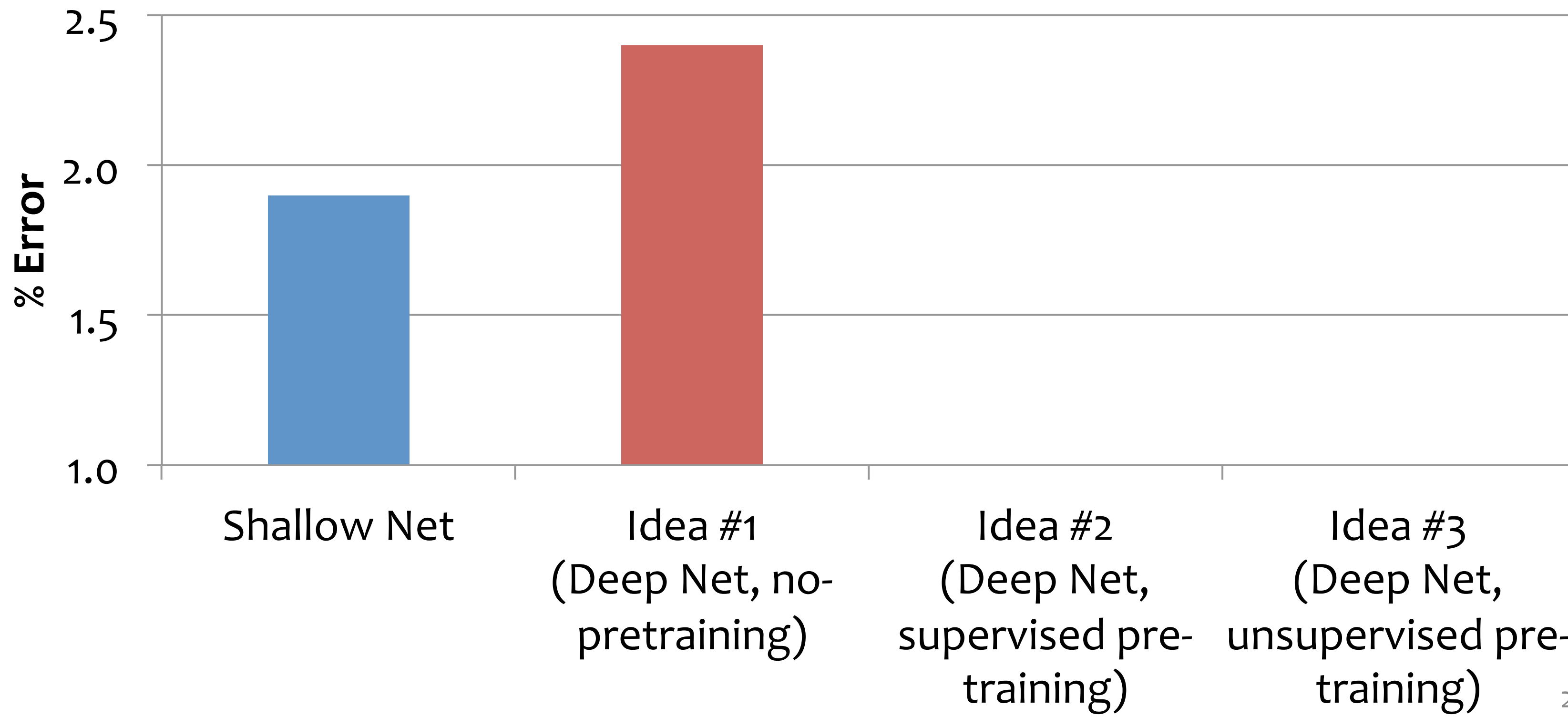

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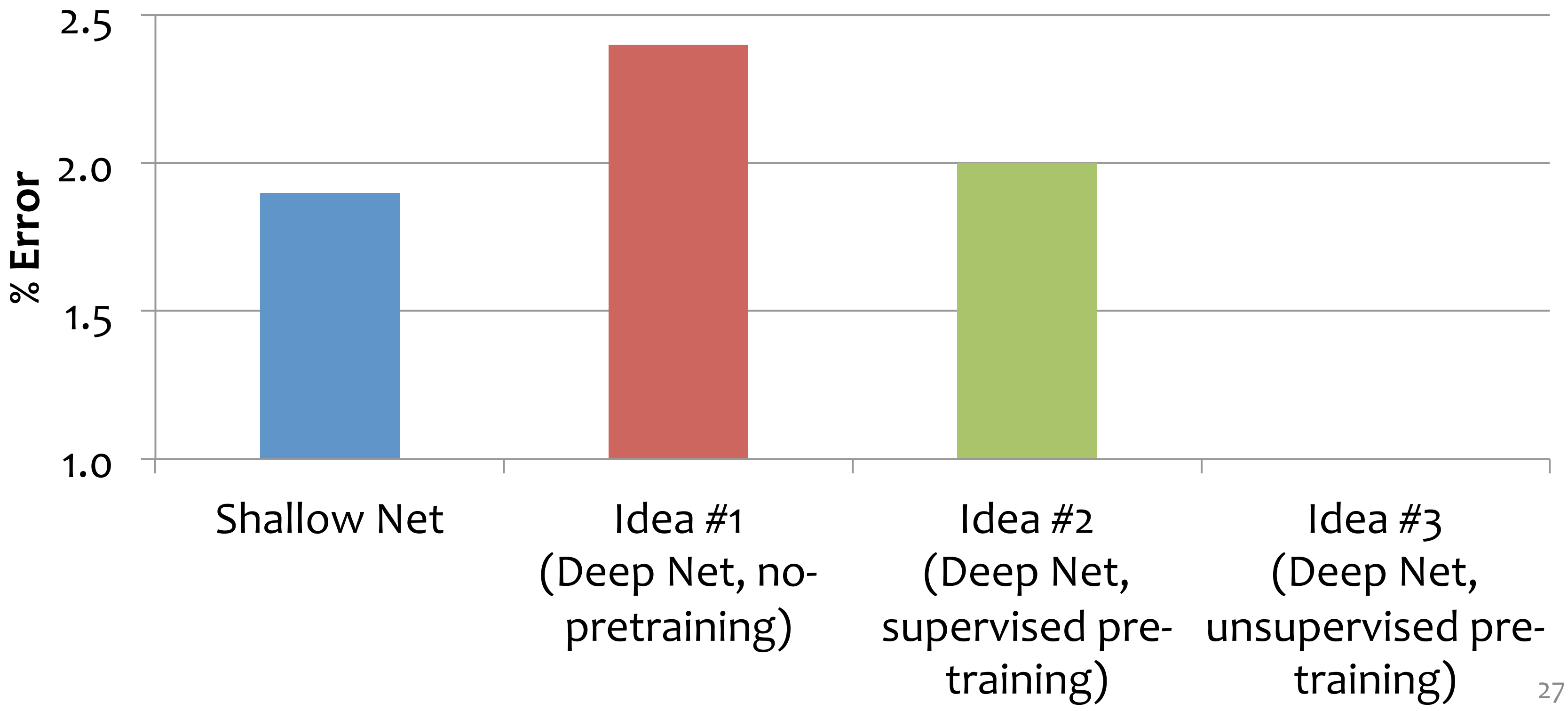

Idea #3: Unsupervised Pre-training

- **Idea #3: (Two Steps)**
  - Use our original idea, but **pick a better starting point**
  - **Train each level** of the model in a **greedy** way

1. Unsupervised Pre-training
   - Use **unlabeled** data
   - Work bottom-up
     - Train hidden layer 1. Then fix its parameters.
     - Train hidden layer 2. Then fix its parameters.
     - …
     - Train hidden layer n. Then fix its parameters.
2. Supervised Fine-tuning
   - Use **labeled** data to train following "Idea #1"
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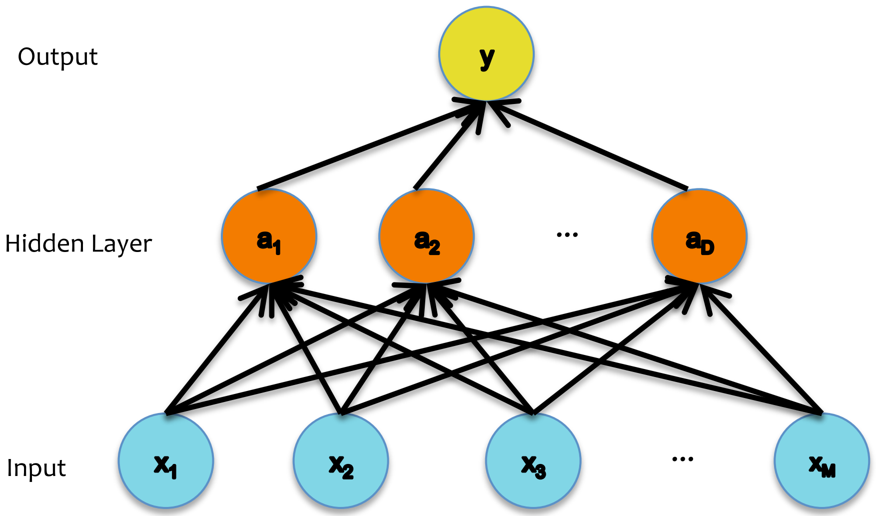
The solution: *Unsupervised pre-training*

Unsupervised pre-training of the first layer:

- What should it predict?
- What else do we observe?
- **The input!**



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Unsupervised pre-training of the first layer:

- What should it predict?
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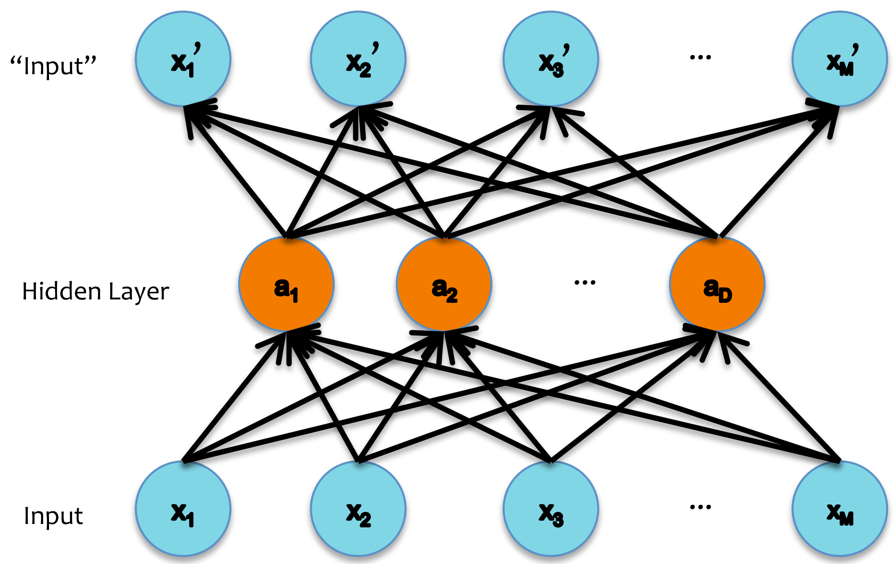
This topology defines an Auto-encoder.



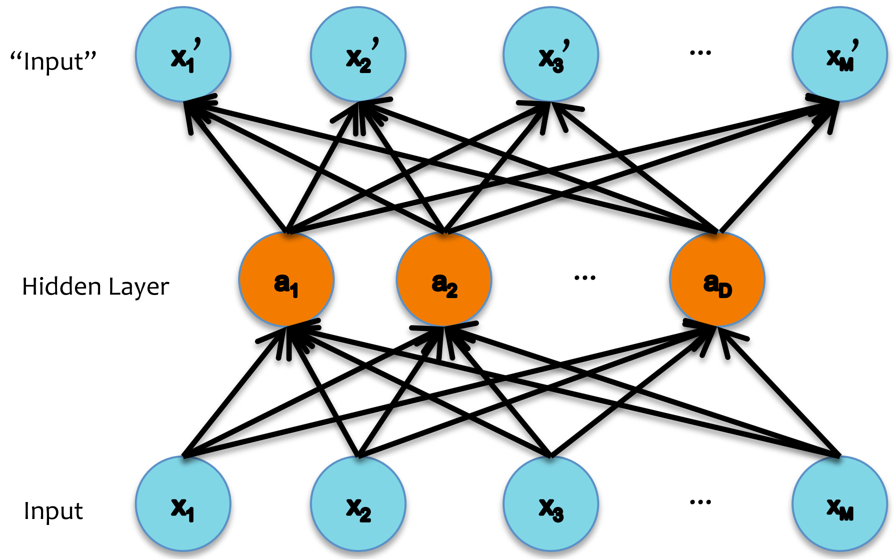
Auto-Encoders

Key idea: Encourage z to give small reconstruction error:

- x' is the *reconstruction* of x
- Loss = || x – DECODER(ENCODER(x)) ||^2
- Train with the same backpropagation algorithm for 2-layer Neural Networks with x_m as both input and output.

DECODER: x' = h(W'z)

ENCODER: z = h(Wx)



Slide adapted from Raman Arora

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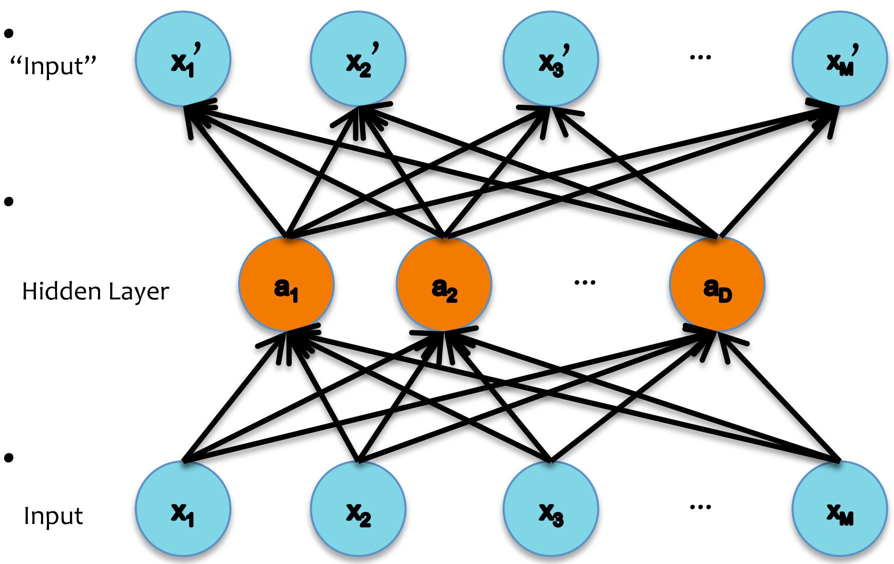

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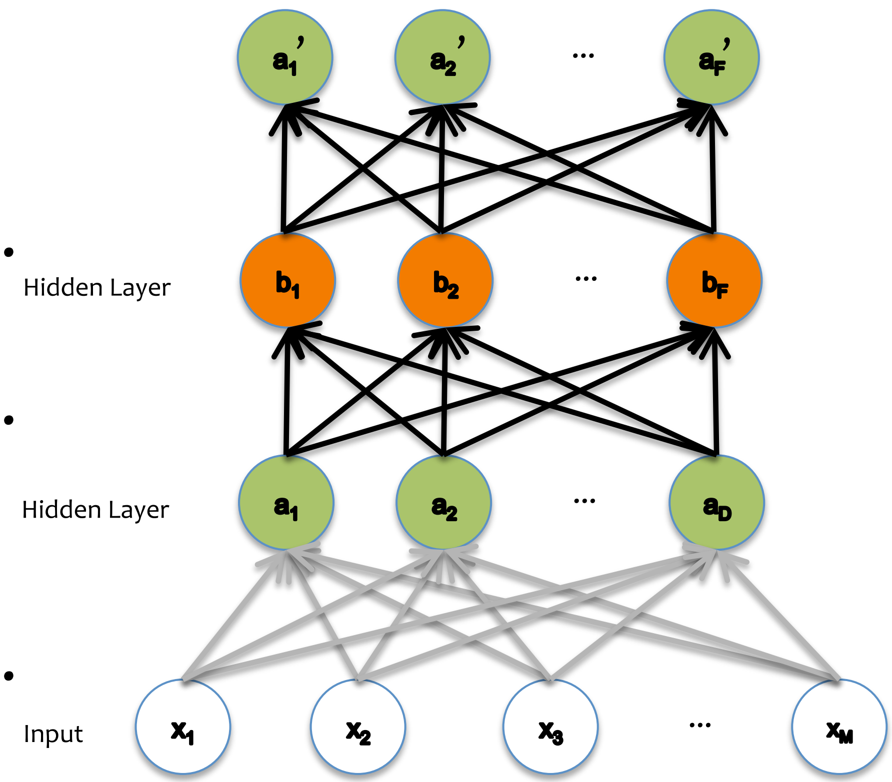

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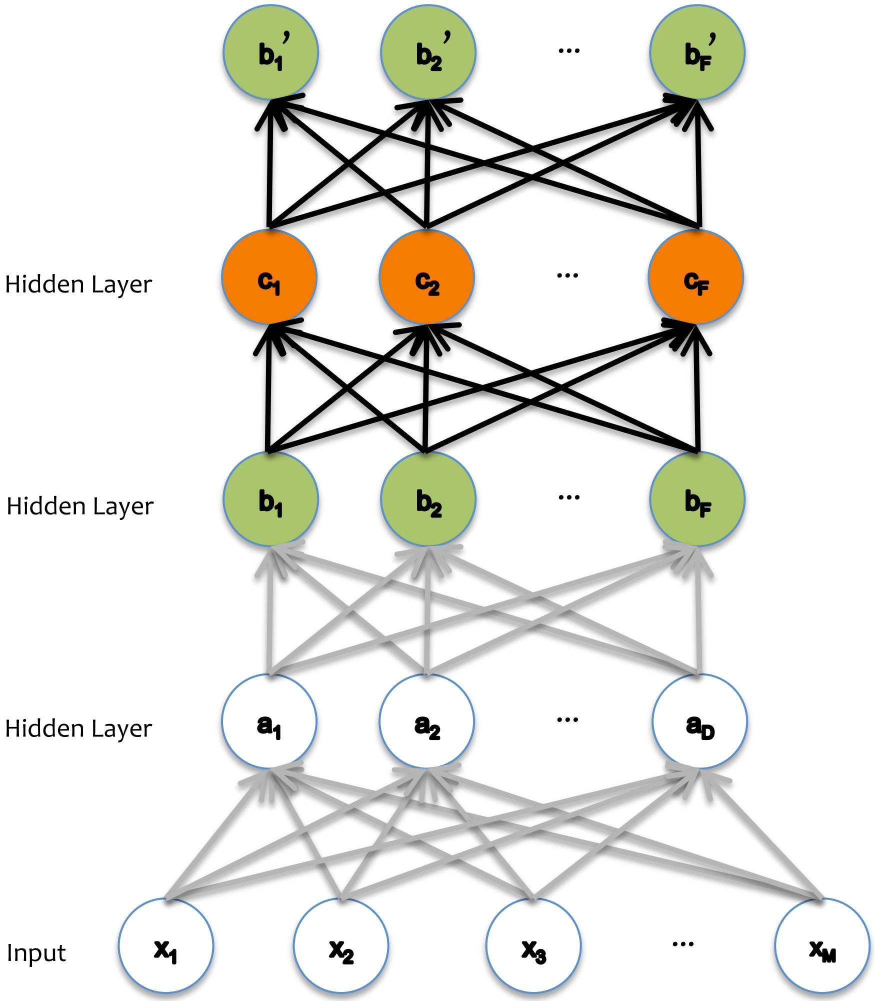

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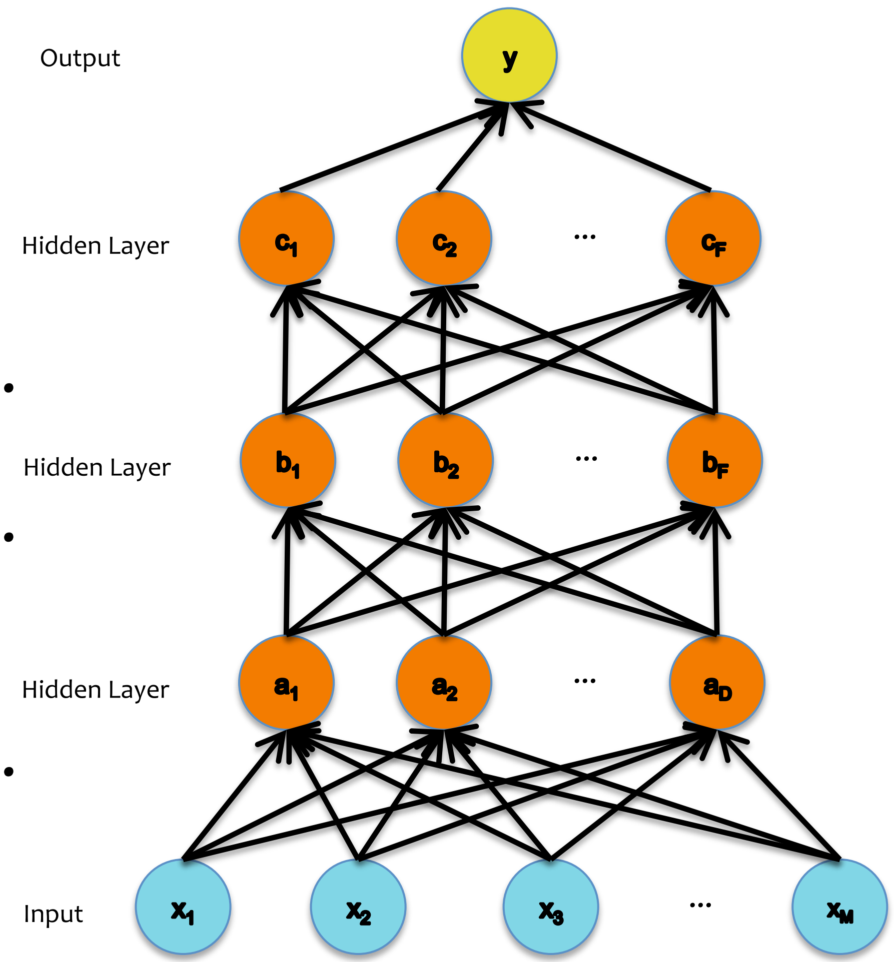
Supervised fine-tuning

Backprop and update all parameters



Deep Network Training

- **Idea #1:**
  1. Supervised fine-tuning only

- **Idea #2:**
  1. Supervised layer-wise pre-training
  2. Supervised fine-tuning

- **Idea #3:**
  1. Unsupervised layer-wise pre-training
  2. Supervised fine-tuning

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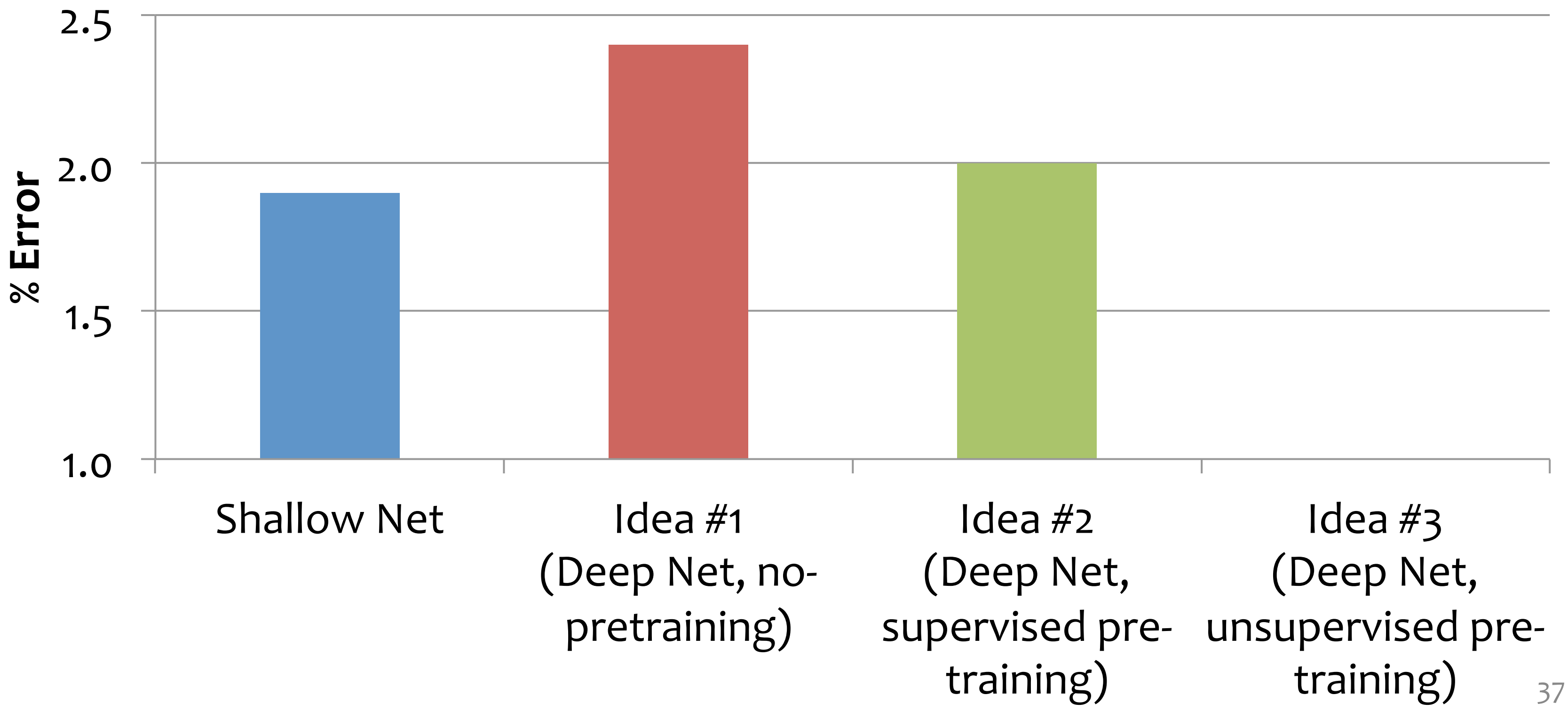

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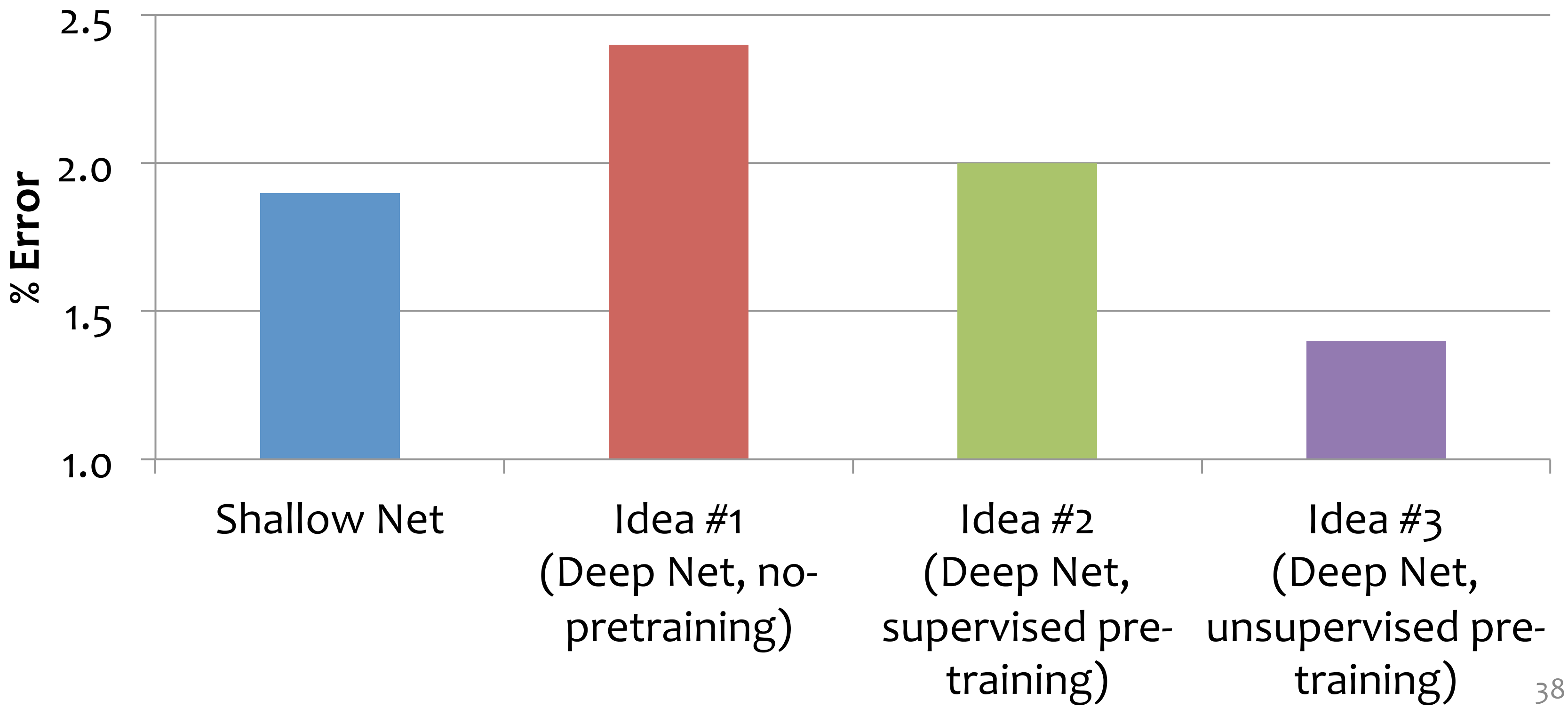


Training

Is layer-wise pre-training always necessary?

In 2010, a record on a hand-writing recognition task was set by standard supervised backpropagation (our Idea #1).

How? A very fast implementation on GPUs.

See Ciresen et al. (2010)

Deep Learning

- Goal: learn features at different levels of abstraction
- Training can be tricky due to…
  - Nonconvexity
  - Vanishing gradients
- Unsupervised layer-wise pre-training can help with both!

RECURRENT NEURAL NETWORKS

Recurrent Neural Networks (RNNs)

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\mathbf{h} = (h_1, h_2, \ldots, h_T), h_i \in \mathcal{R}^J$

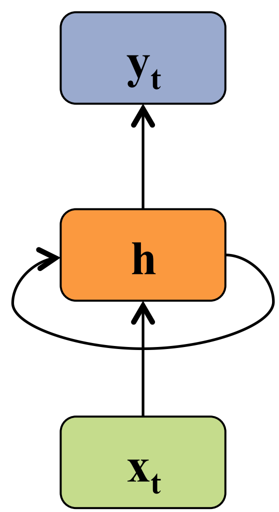
outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

Definition of the RNN:

$$h_t = \mathcal{H}\left(W_{xh}x_t + W_{hh}h_{t-1} + b_h\right)$$

$$y_t = W_{hy}h_t + b_y$$



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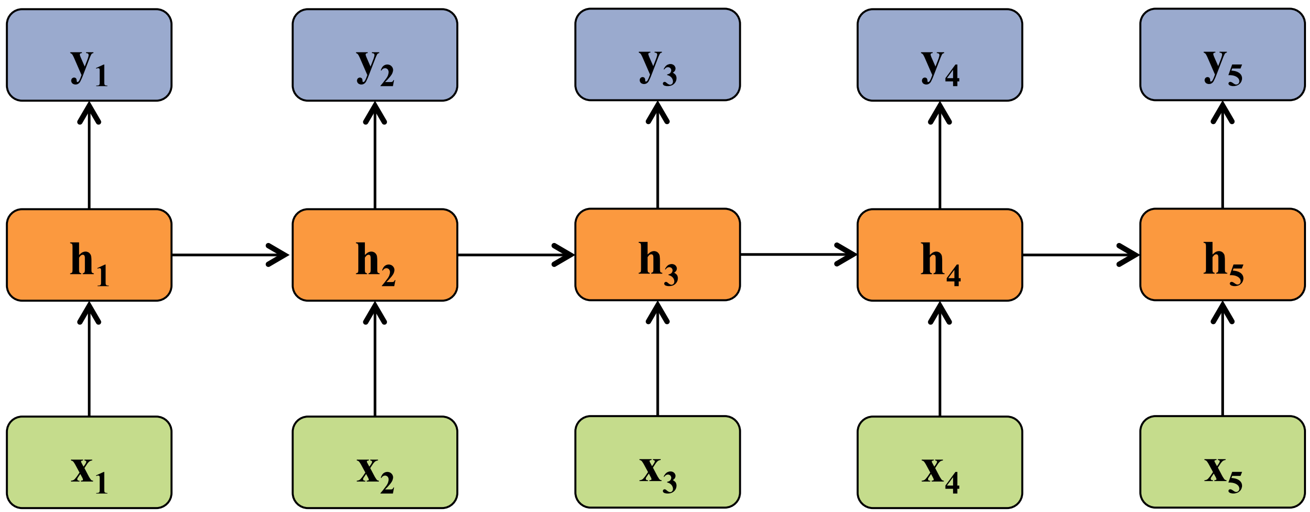

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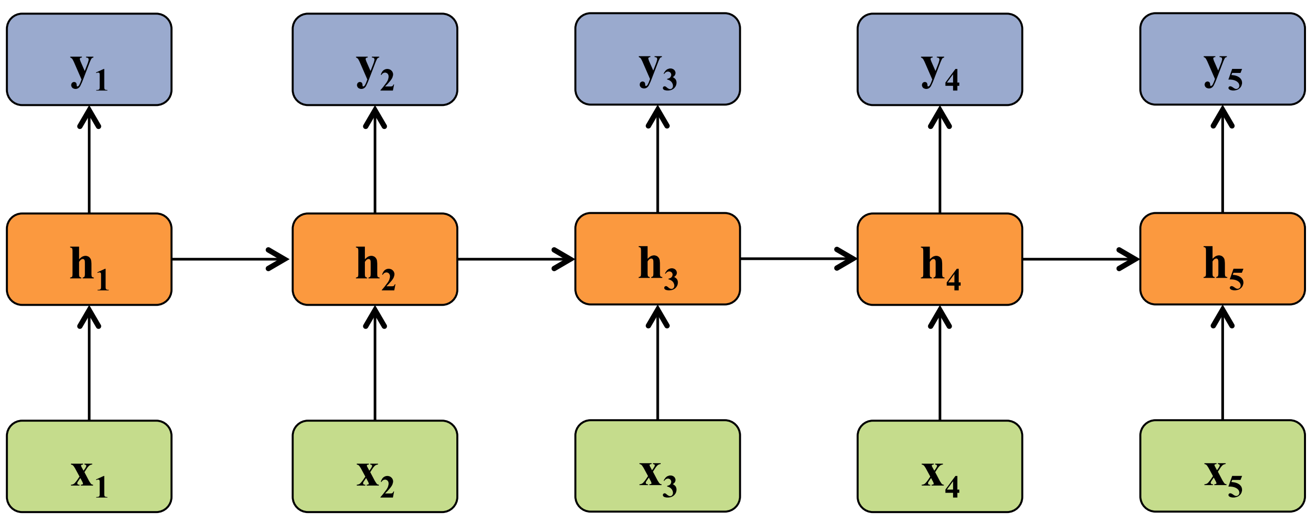

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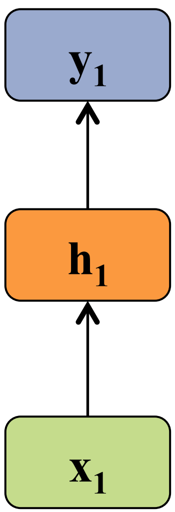

- If $T=1$, then we have a standard feed-forward **neural net with one hidden layer**
- All of the deep nets from last lecture (DNN, DBN, DBM) required **fixed size inputs/outputs**

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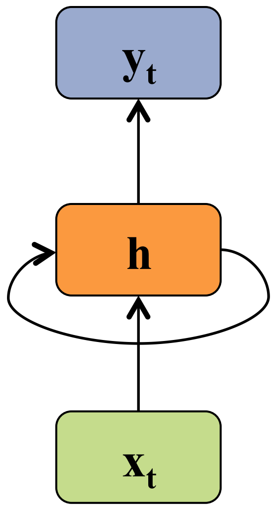
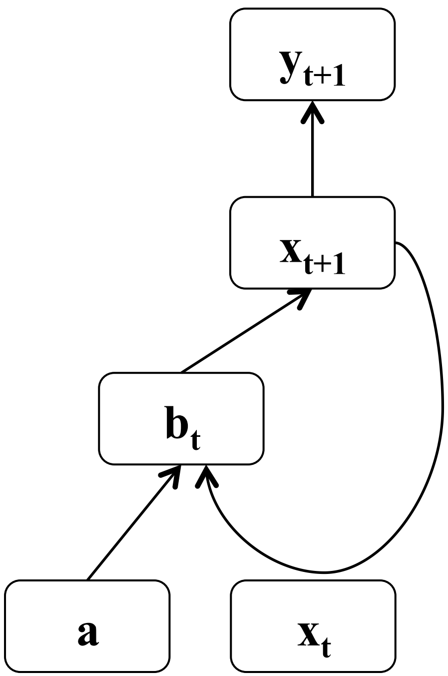
- By unrolling the RNN through time, we can **share parameters** and accommodate **arbitrary length** input/output pairs
- Applications: **time-series data** such as sentences, speech, stock-market, signal data, etc.



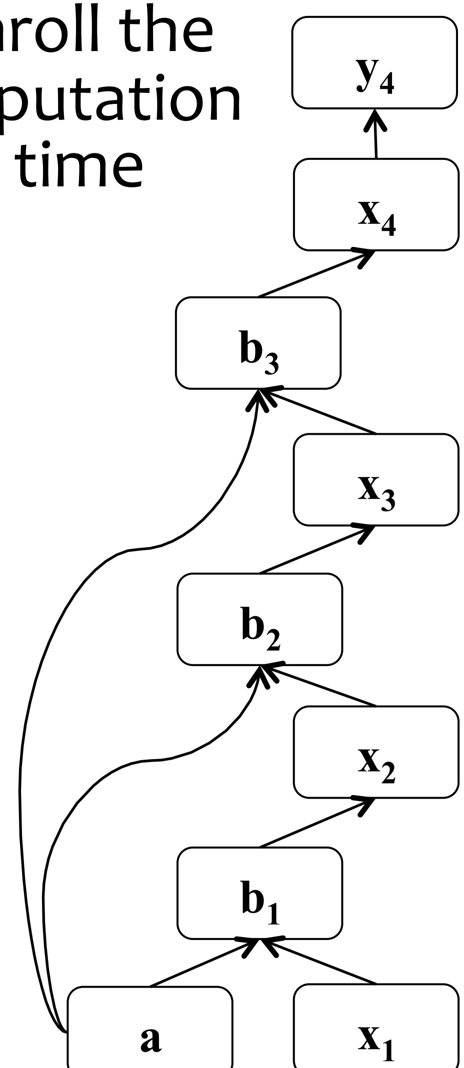
Background: Backprop through time

Recurrent neural network:



BPTT:

1. Unroll the computation over time



2. Run backprop through the resulting feed-forward network

(Robinson & Fallside, 1987)
(Werbos, 1988)
(Mozer, 1995)

Bidirectional RNN

$$\text{inputs: } \mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$$

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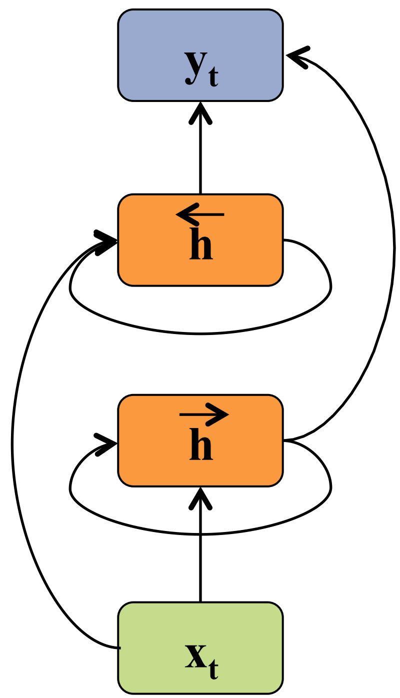
$$y_t = W_{\overrightarrow{h}y} \overrightarrow{h}_t + W_{\overleftarrow{h}y} \overleftarrow{h}_t + b_y$$



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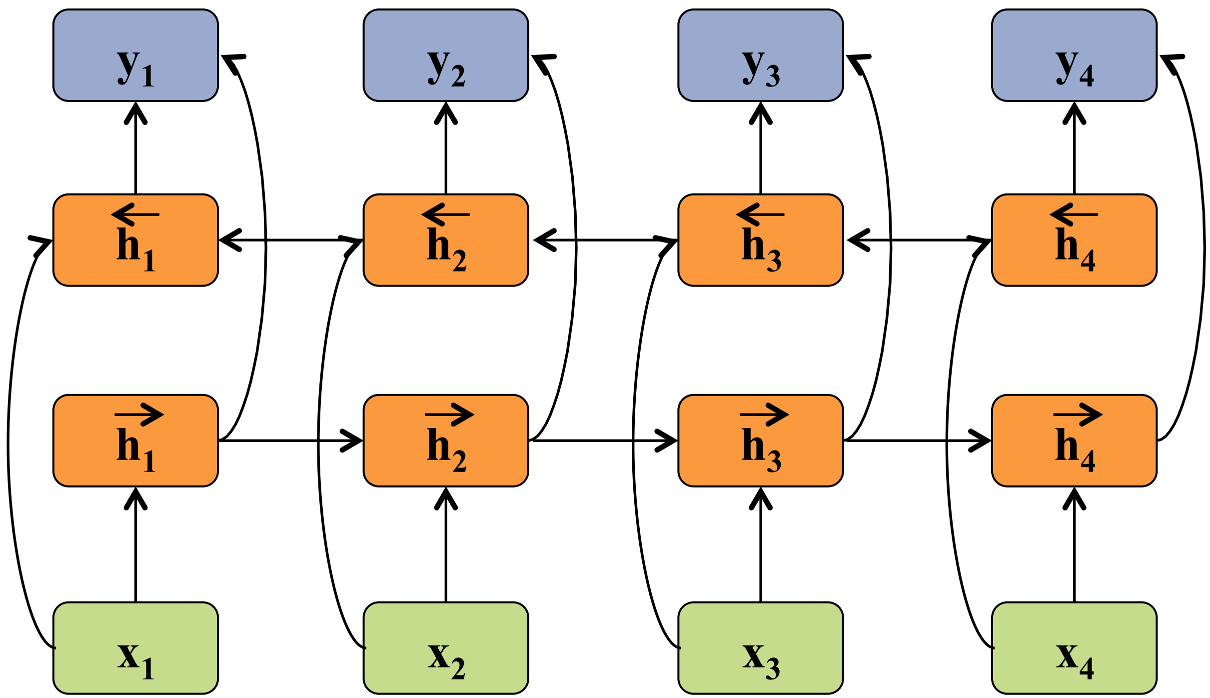
$$\overleftarrow{h}_t = \mathcal{H}\left(W_{x\overleftarrow{h}} x_t + W_{\overleftarrow{h}\overleftarrow{h}} \overleftarrow{h}_{t+1} + b_{\overleftarrow{h}}\right)$$

$$y_t = W_{\overrightarrow{h}y} \overrightarrow{h}_t + W_{\overleftarrow{h}y} \overleftarrow{h}_t + b_y$$



Bidirectional RNN

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\overrightarrow{\mathbf{h}}$ and $\overleftarrow{\mathbf{h}}$

outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

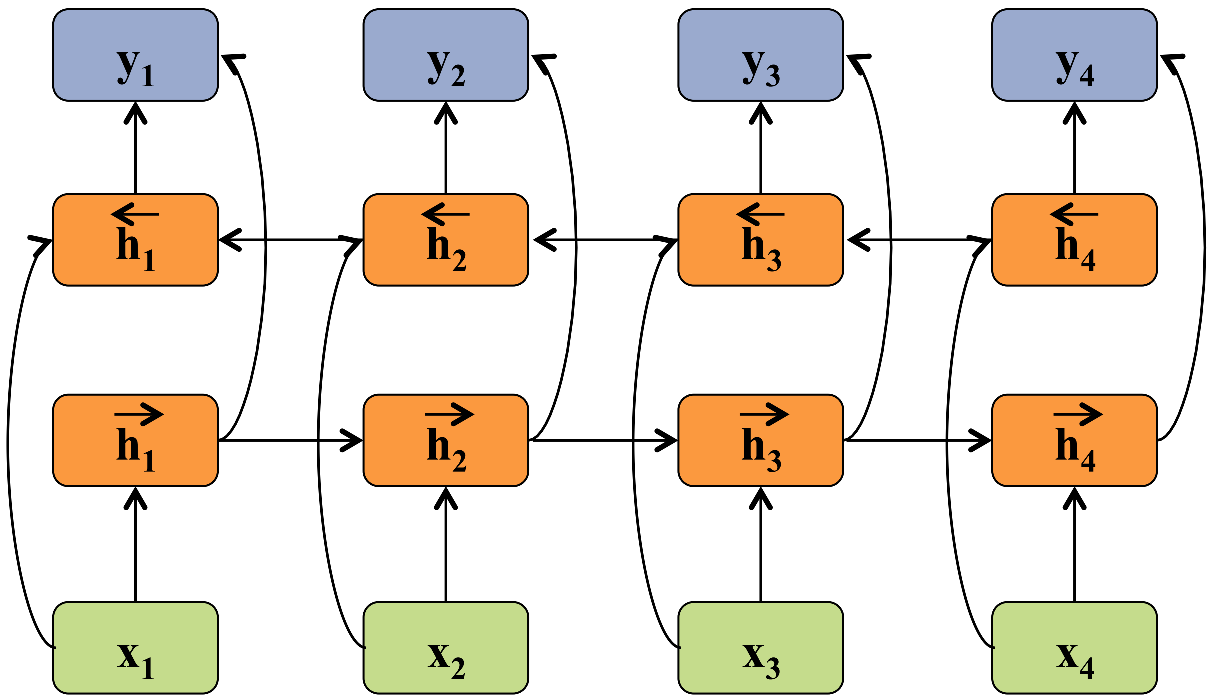
nonlinearity: $\mathcal{H}$

Recursive Definition:

$$\overrightarrow{h}_t = \mathcal{H}\left(W_{x\overrightarrow{h}} x_t + W_{\overrightarrow{h}\overrightarrow{h}} \overrightarrow{h}_{t-1} + b_{\overrightarrow{h}}\right)$$

$$\overleftarrow{h}_t = \mathcal{H}\left(W_{x\overleftarrow{h}} x_t + W_{\overleftarrow{h}\overleftarrow{h}} \overleftarrow{h}_{t+1} + b_{\overleftarrow{h}}\right)$$

$$y_t = W_{\overrightarrow{h}y} \overrightarrow{h}_t + W_{\overleftarrow{h}y} \overleftarrow{h}_t + b_y$$



Bidirectional RNN

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

hidden units: $\overrightarrow{\mathbf{h}}$ and $\overleftarrow{\mathbf{h}}$

outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

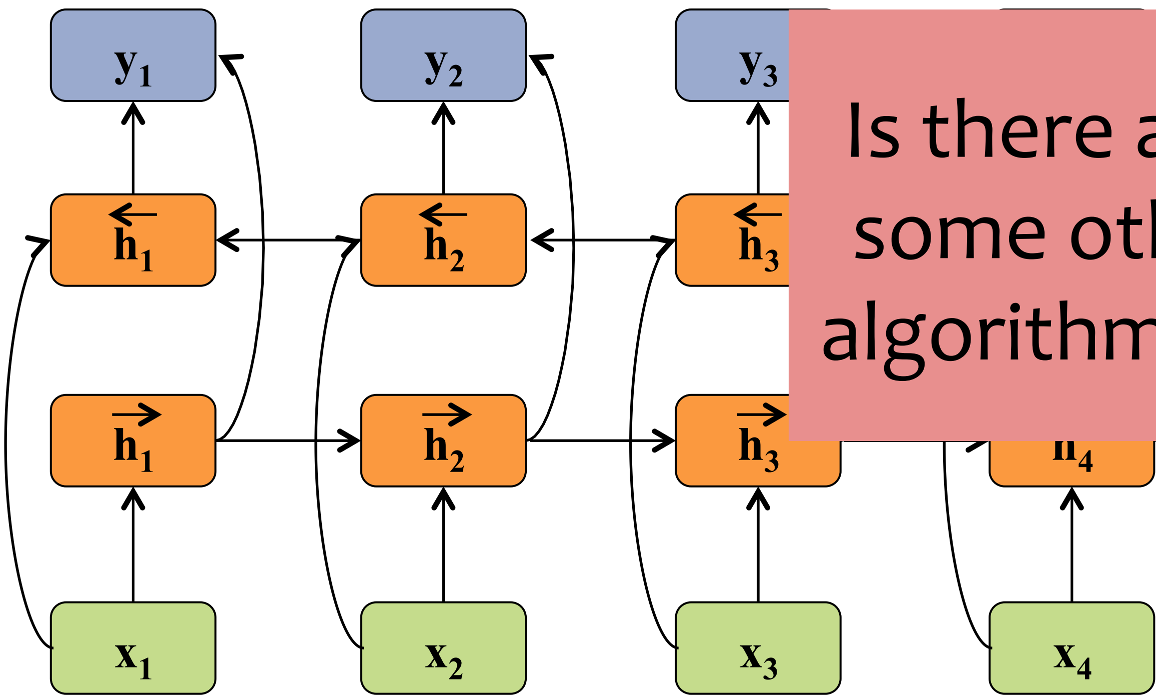
nonlinearity: $\mathcal{H}$

Recursive Definition:

$$\overrightarrow{h}_t = \mathcal{H}\left(W_{x\overrightarrow{h}} x_t + W_{\overrightarrow{h}\overrightarrow{h}} \overrightarrow{h}_{t-1} + b_{\overrightarrow{h}}\right)$$

$$\overleftarrow{h}_t = \mathcal{H}\left(W_{x\overleftarrow{h}} x_t + W_{\overleftarrow{h}\overleftarrow{h}} \overleftarrow{h}_{t+1} + b_{\overleftarrow{h}}\right)$$

$$y_t = W_{\overrightarrow{h}y} \overrightarrow{h}_t + W_{\overleftarrow{h}y} \overleftarrow{h}_t + b_y$$



Is there an analogy to some other recursive algorithm(s) we know?

Deep RNNs

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

Recursive Definition:

$$h_t^n = \mathcal{H}\left(W_{h^{n-1}h^n} h_t^{n-1} + W_{h^n h^n} h_{t-1}^n + b_h^n\right)$$

$$y_t = W_{h^N y} h_t^N + b_y$$

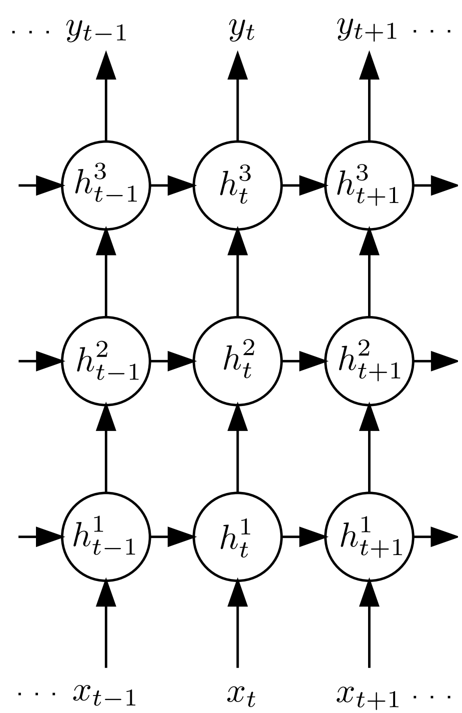


Figure from (Graves et al., 2013)

Deep Bidirectional RNNs

inputs: $\mathbf{x} = (x_1, x_2, \ldots, x_T), x_i \in \mathcal{R}^I$

outputs: $\mathbf{y} = (y_1, y_2, \ldots, y_T), y_i \in \mathcal{R}^K$

nonlinearity: $\mathcal{H}$

- Notice that the upper level hidden units have input from **two previous layers** (i.e. wider input)
- Likewise for the output layer
- What analogy can we draw to DNNs, DBNs, DBMs?

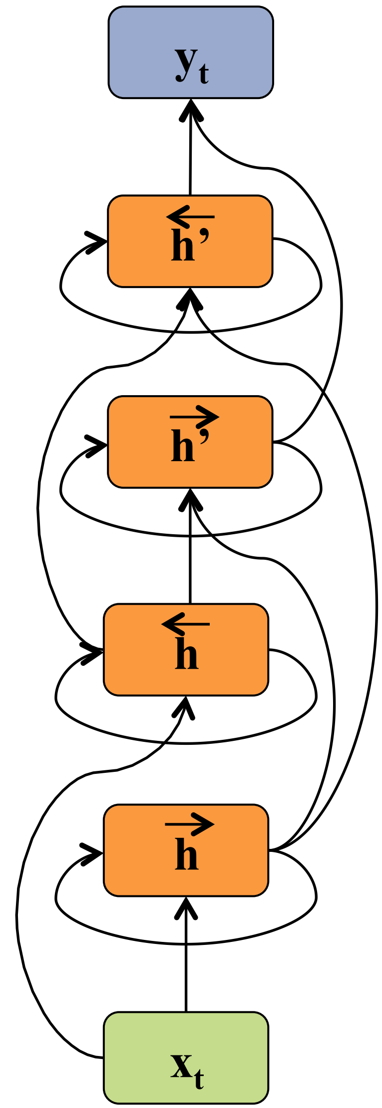
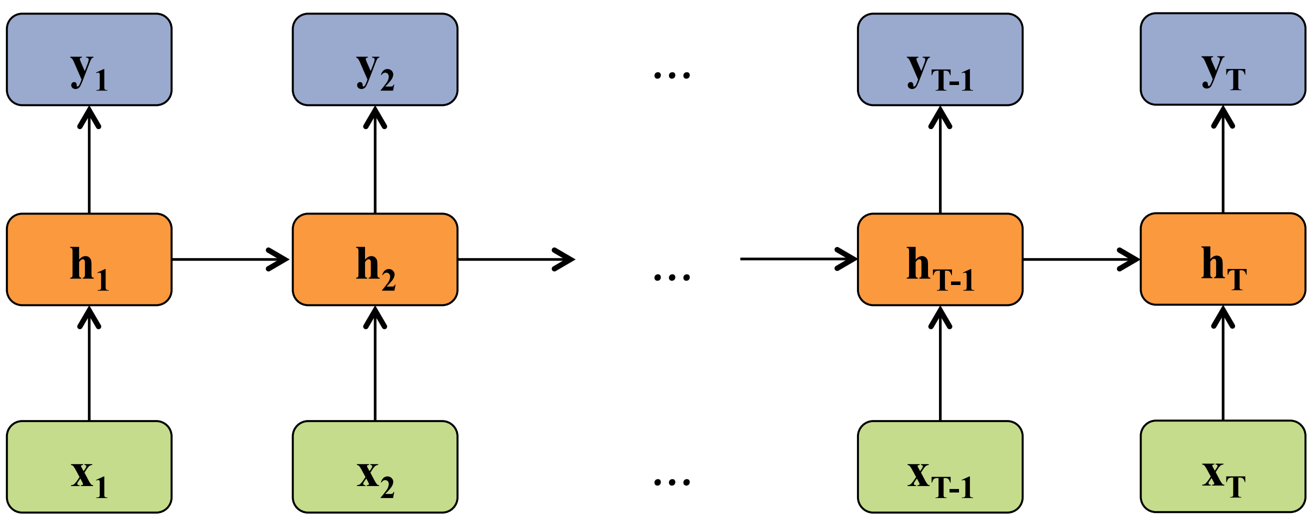


Figure from (Graves et al., 2013)

Long Short-Term Memory (LSTM)

Motivation:

- Standard RNNs have trouble learning long distance dependencies
- LSTMs combat this issue



Long Short-Term Memory (LSTM)

Motivation:

- Vanishing gradient problem for Standard RNNs
- Figure shows sensitivity (darker = more sensitive) to the input at time t=1

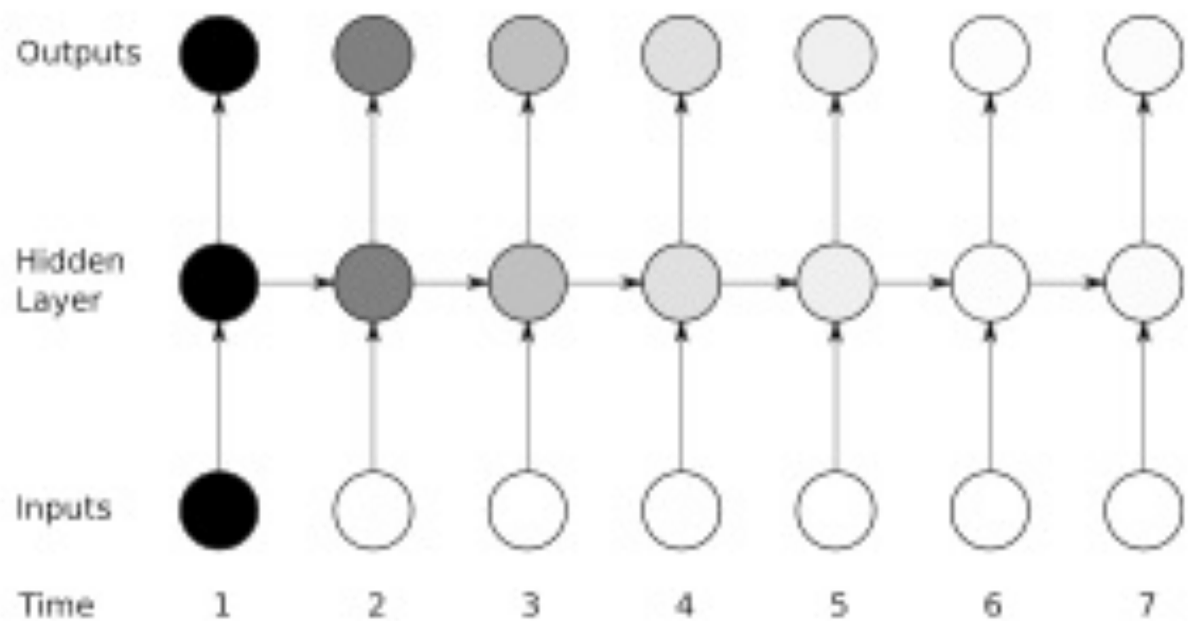


Figure from (Graves, 2012)

Long Short-Term Memory (LSTM)

Motivation:

- LSTM units have a rich internal structure
- The various "gates" determine the propagation of information and can choose to "remember" or "forget" information

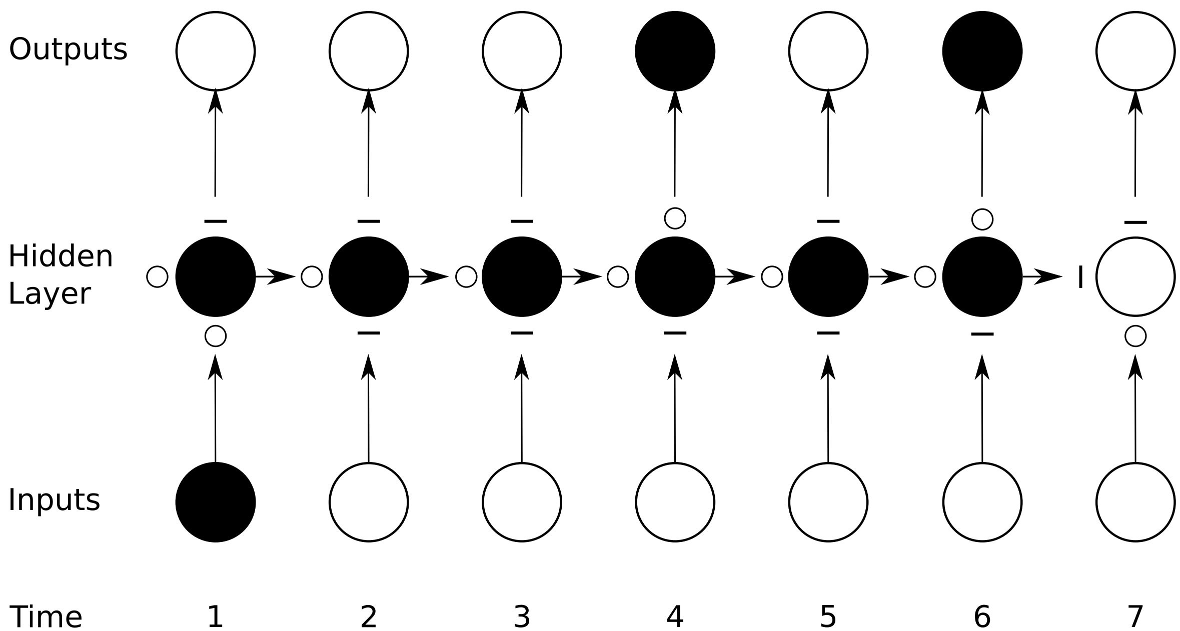
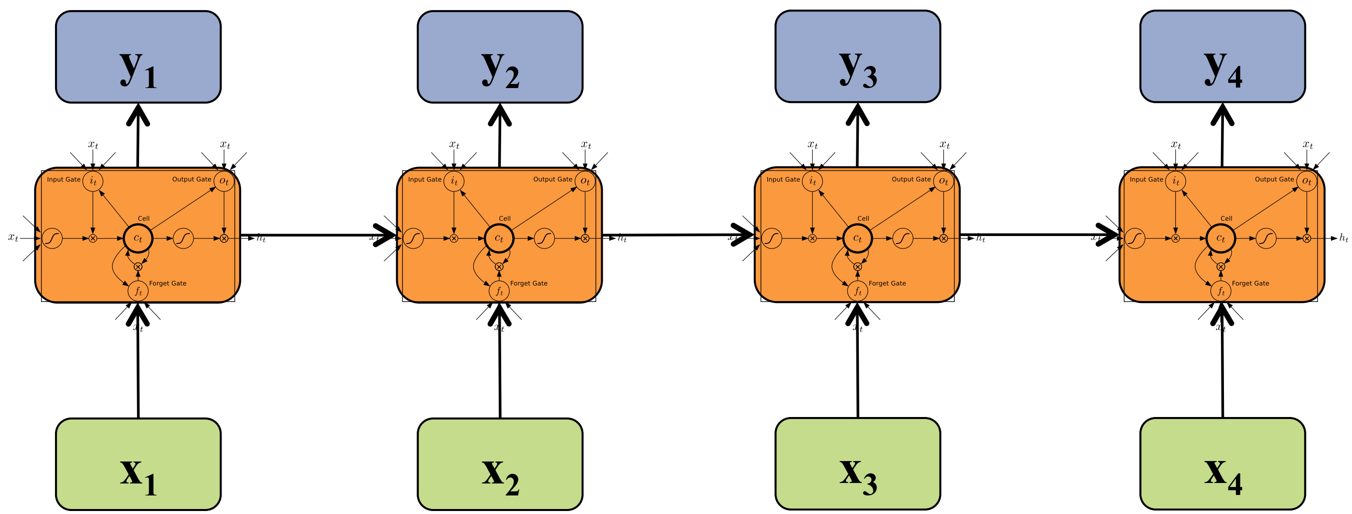


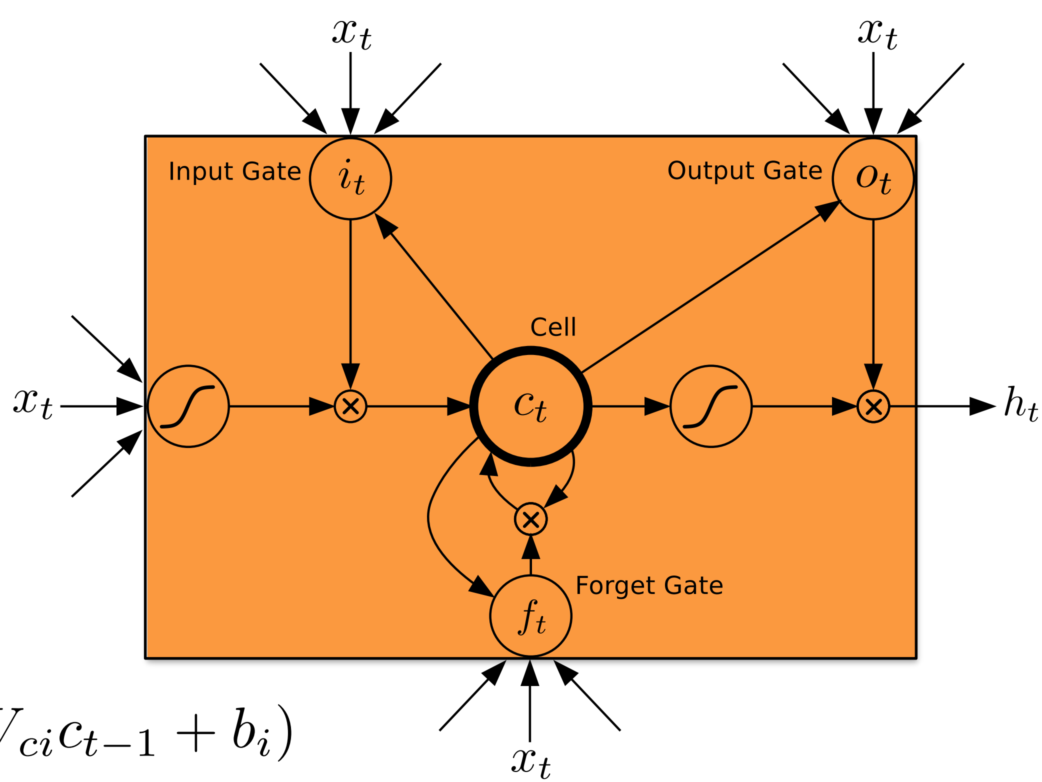
Figure from (Graves, 2012)

Long Short-Term Memory (LSTM)



Long Short-Term Memory (LSTM)

- **Input gate:** masks out the standard RNN inputs
- **Forget gate:** masks out the previous cell
- **Cell:** stores the input/forget mixture
- **Output gate:** masks out the values of the next hidden



$$i_t = \sigma\left(W_{xi}x_t + W_{hi}h_{t-1} + W_{ci}c_{t-1} + b_i\right)$$

$$f_t = \sigma\left(W_{xf}x_t + W_{hf}h_{t-1} + W_{cf}c_{t-1} + b_f\right)$$

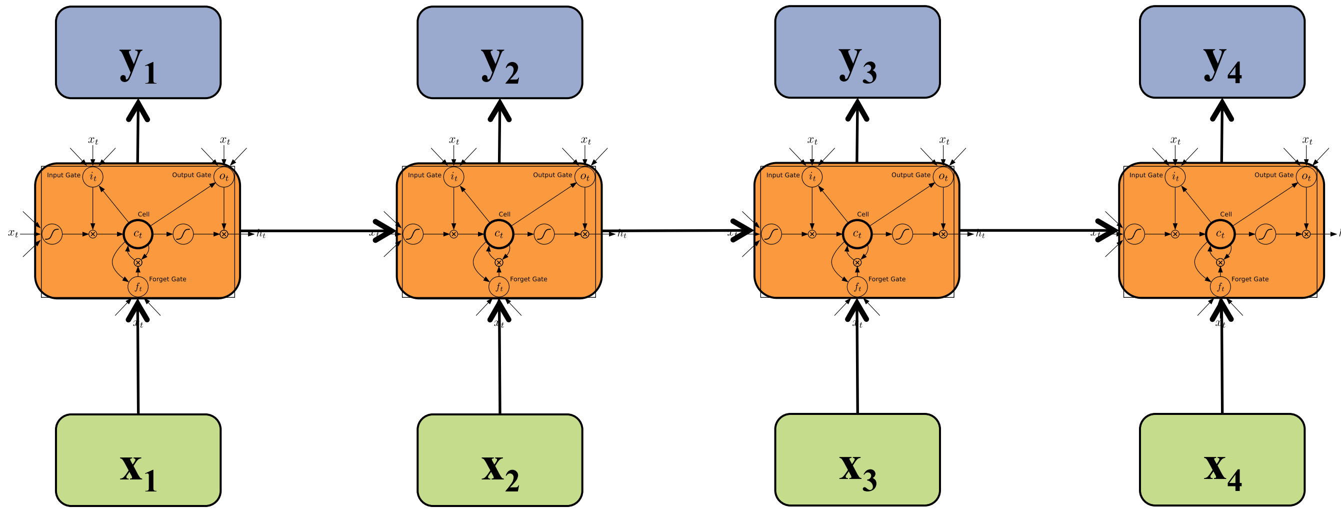
$$c_t = f_t c_{t-1} + i_t \tanh\left(W_{xc}x_t + W_{hc}h_{t-1} + b_c\right)$$

$$o_t = \sigma\left(W_{xo}x_t + W_{ho}h_{t-1} + W_{co}c_t + b_o\right)$$

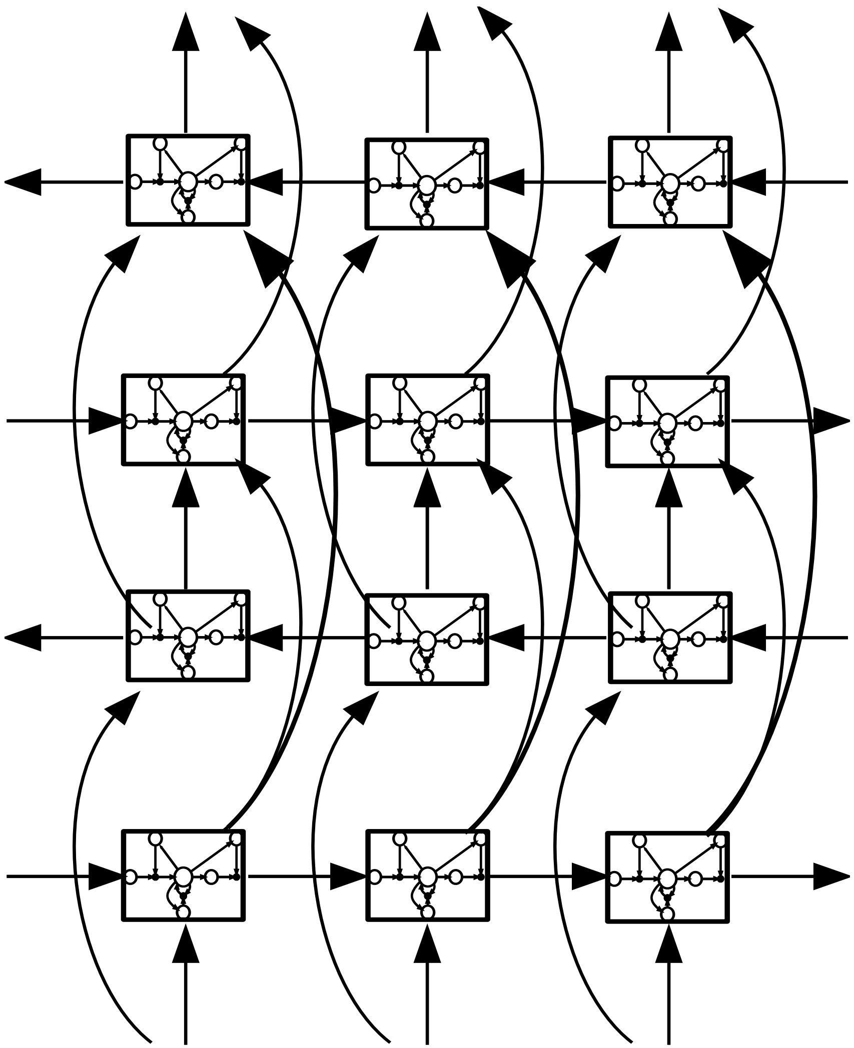
$$h_t = o_t \tanh(c_t)$$

Figure from (Graves et al., 2013)

Long Short-Term Memory (LSTM)



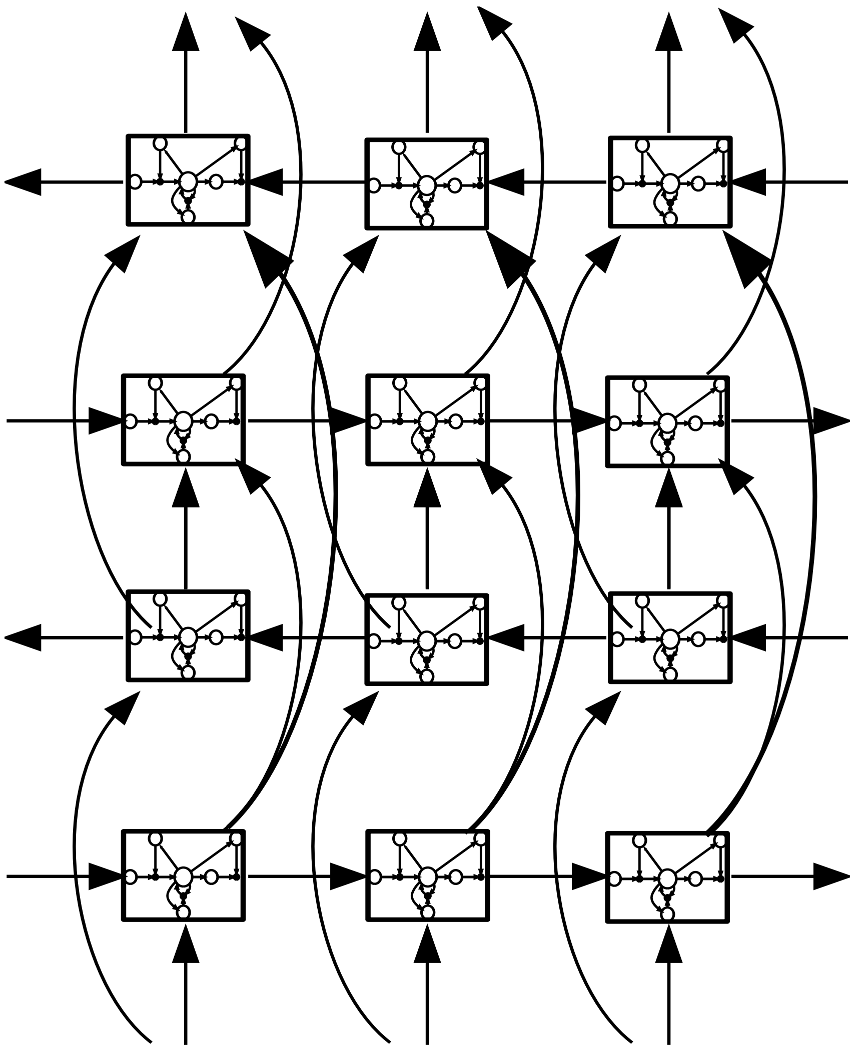
Deep Bidirectional LSTM (DBLSTM)



- Figure: input/output layers not shown
- **Same general topology** as a Deep Bidirectional RNN, but with **LSTM units** in the hidden layers
- No additional **representational power** over DBRNN, but **easier to learn** in practice

Figure from (Graves et al., 2013)

Deep Bidirectional LSTM (DBLSTM)



How important is this particular architecture?

Jozefowicz et al. (2015) **evaluated 10,000 different LSTM-like architectures** and found several variants that worked just as well on several tasks.

Figure from (Graves et al., 2013)

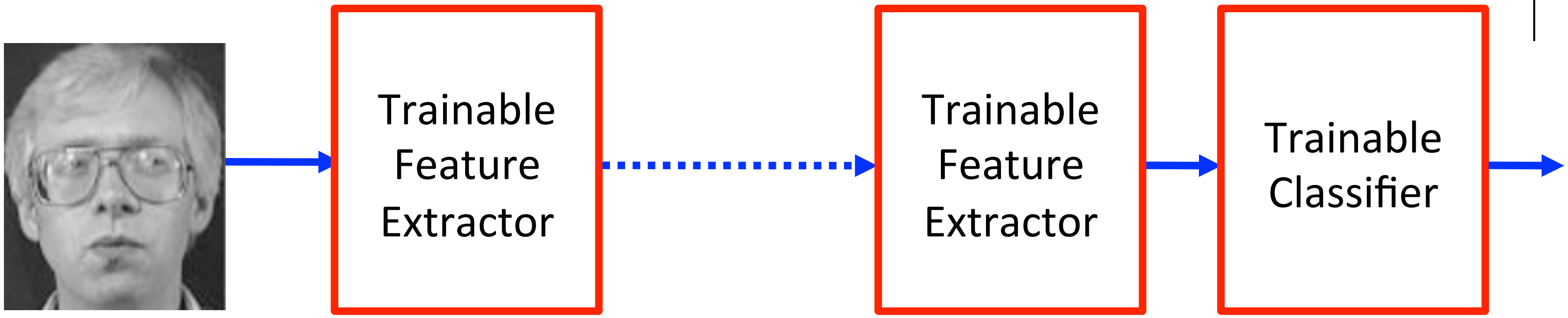
CONVOLUTIONAL NEURAL NETS

Expressive Capabilities of ANNs

- Boolean functions:
  - Every Boolean function can be represented by network with single hidden layer
  - But might require exponential (in number of inputs) hidden units

- Continuous functions:
  - Every bounded continuous function can be approximated with arbitrary small error, by network with one hidden layer [Cybenko 1989; Hornik et al 1989]
  - Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988].

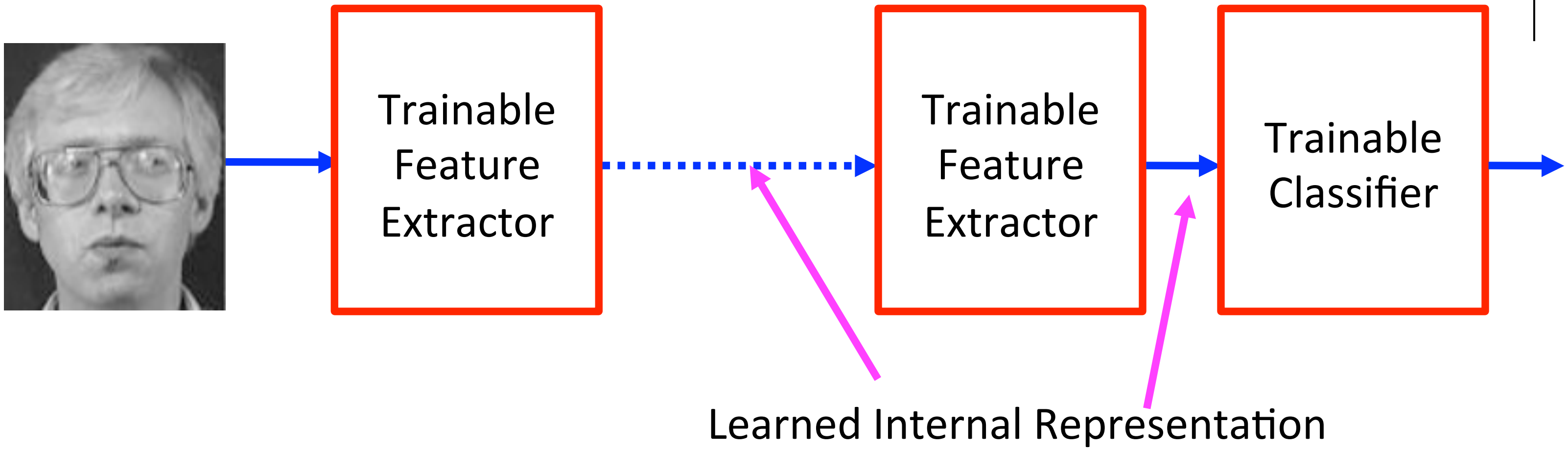
Using ANN to hierarchical representation



Good Representations are hierarchical

- In Language: hierarchy in syntax and semantics
  - Words->Parts of Speech->Sentences->Text
  - Objects,Actions,Attributes...-> Phrases -> Statements -> Stories
- In Vision: part-whole hierarchy
  - Pixels->Edges->Textons->Parts->Objects->Scenes

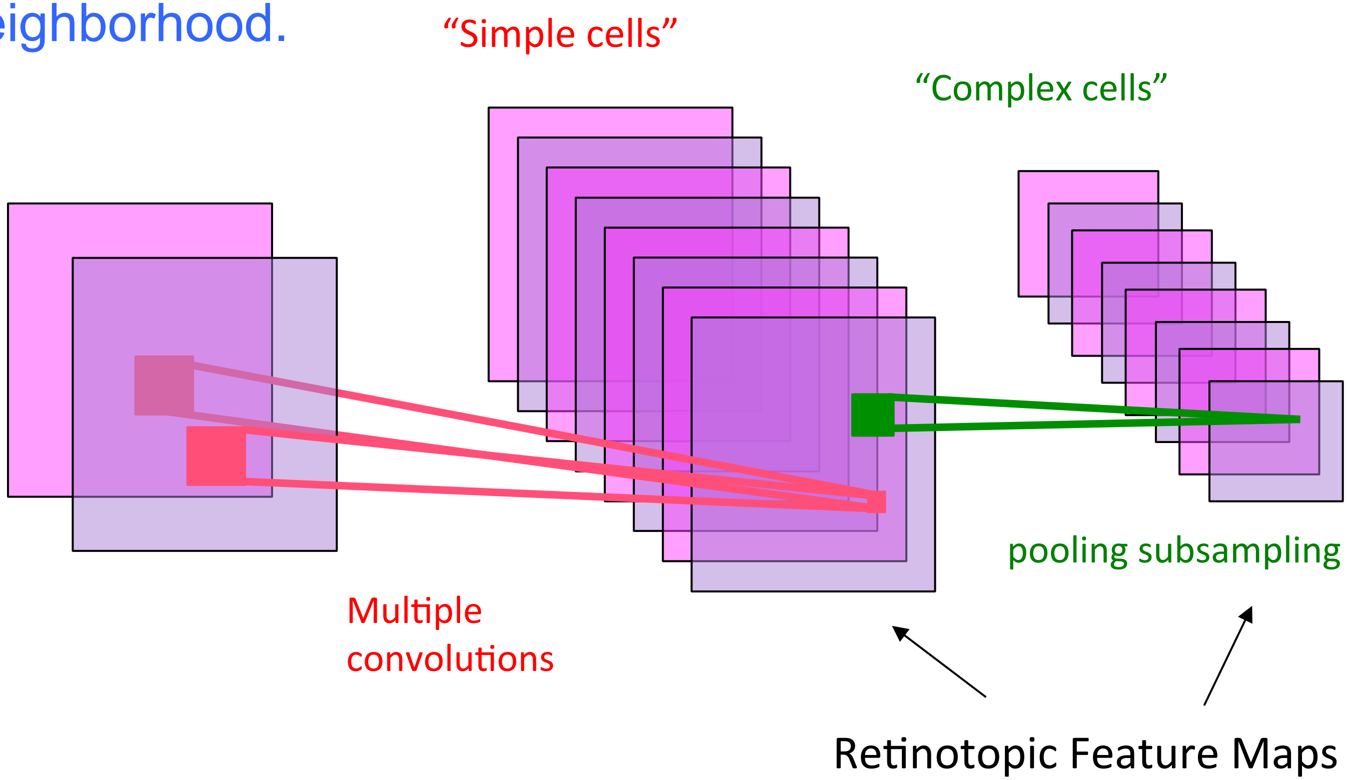
"Deep" learning: learning hierarchical representations



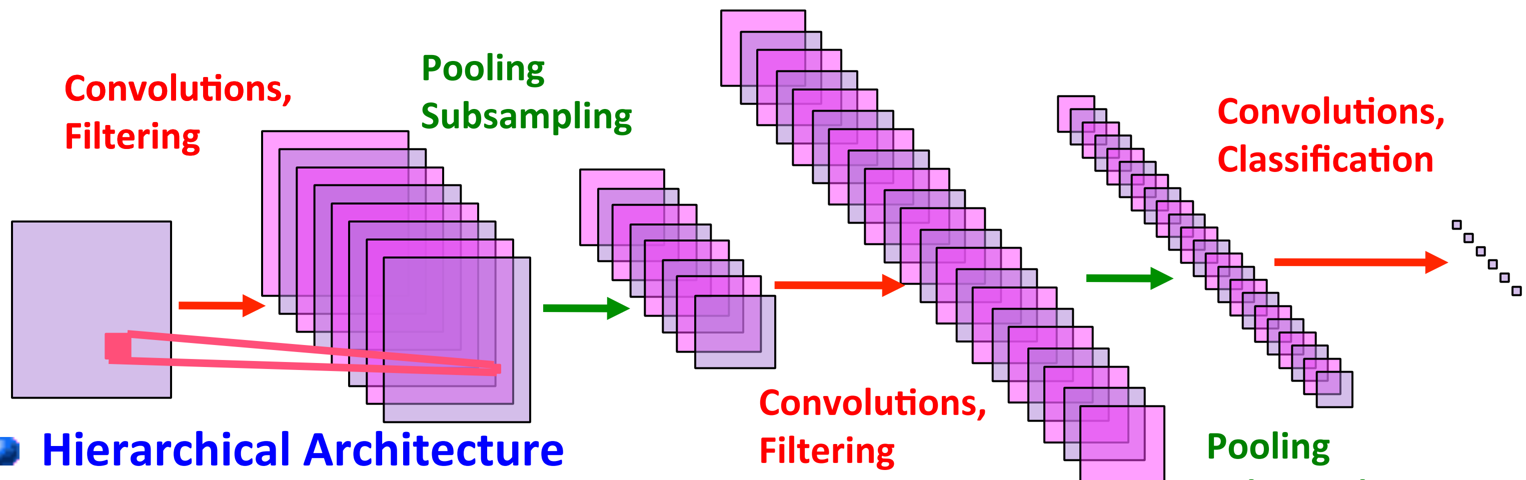
- Deep Learning: learning a hierarchy of internal representations
- From low-level features to mid-level invariant representations, to object identities
- Representations are increasingly invariant as we go up the layers
- using multiple stages gets around the specificity/invariance dilemma

Filtering+NonLinearity+Pooling = 1 stage of a Convolutional Net

- [Hubel & Wiesel 1962]:
  - simple cells detect local features
  - complex cells "pool" the outputs of simple cells within a retinotopic neighborhood.

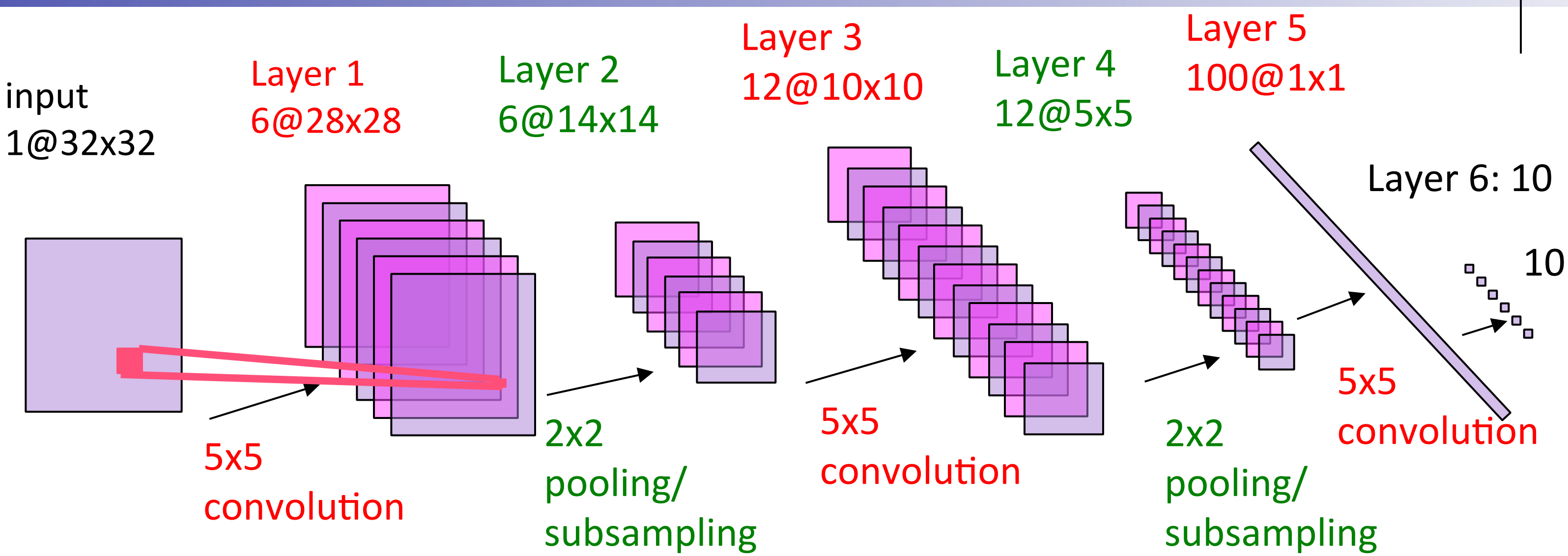


Convolutional Network: Multi-Stage Trainable Architecture



- **Hierarchical Architecture**
  - Representations are more global, more invariant, and more abstract as we go up the layers
- **Alternated Layers of Filtering and Spatial Pooling**
  - Filtering detects conjunctions of features
  - Pooling computes local disjunctions of features
- **Fully Trainable**
  - All the layers are trainable

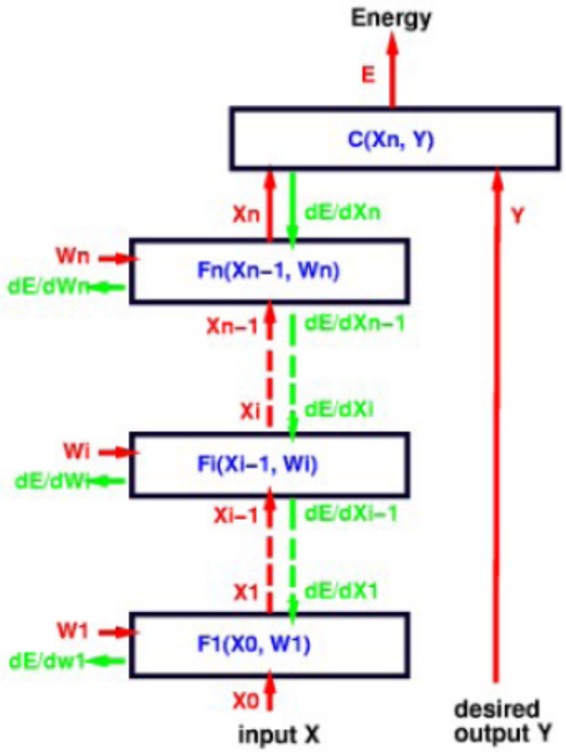
Convolutional Net Architecture for Hand-writing recognition



- Convolutional net for handwriting recognition (400,000 synapses)
  - Convolutional layers (simple cells): all units in a feature plane share the same weights
  - Pooling/subsampling layers (complex cells): for invariance to small distortions.
  - Supervised gradient-descent learning using back-propagation
  - The entire network is trained end-to-end. All the layers are trained simultaneously.
  - [LeCun et al. Proc IEEE, 1998]

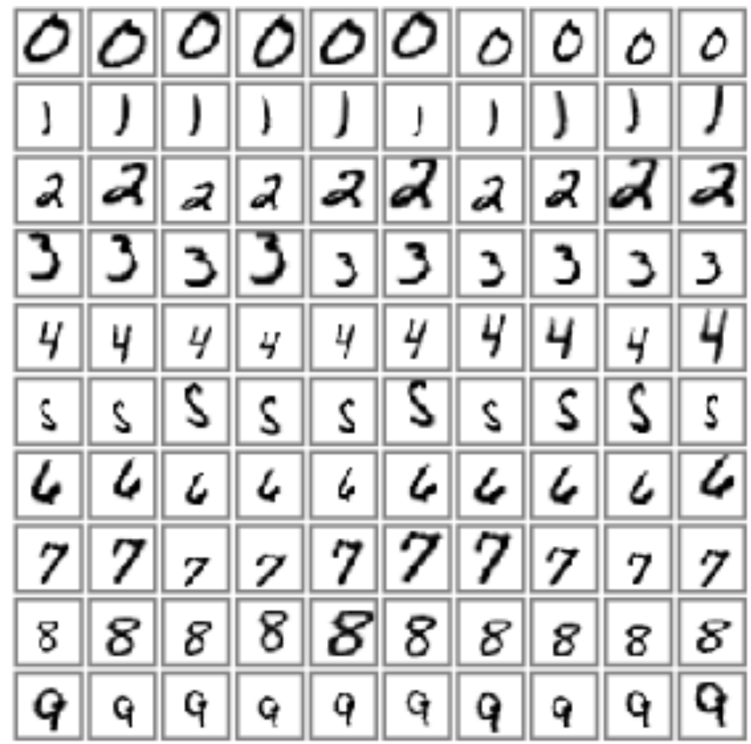
How to train?

To compute all the derivatives, we use a backward sweep called the **back-propagation algorithm** that uses the recurrence equation for $\frac{\partial E}{\partial X_i}$



- $\frac{\partial E}{\partial X_n} = \frac{\partial C(X_n, Y)}{\partial X_n}$
- $\frac{\partial E}{\partial X_{n-1}} = \frac{\partial E}{\partial X_n} \frac{\partial F_n(X_{n-1}, W_n)}{\partial X_{n-1}}$
- $\frac{\partial E}{\partial W_n} = \frac{\partial E}{\partial X_n} \frac{\partial F_n(X_{n-1}, W_n)}{\partial W_n}$
- $\frac{\partial E}{\partial X_{n-2}} = \frac{\partial E}{\partial X_{n-1}} \frac{\partial F_{n-1}(X_{n-2}, W_{n-1})}{\partial X_{n-2}}$
- $\frac{\partial E}{\partial W_{n-1}} = \frac{\partial E}{\partial X_{n-1}} \frac{\partial F_{n-1}(X_{n-2}, W_{n-1})}{\partial W_{n-1}}$
- ....etc, until we reach the first module.
- we now have all the $\frac{\partial E}{\partial W_i}$ for $i \in [1, n]$.

Application: MNIST Handwritten Digit Dataset



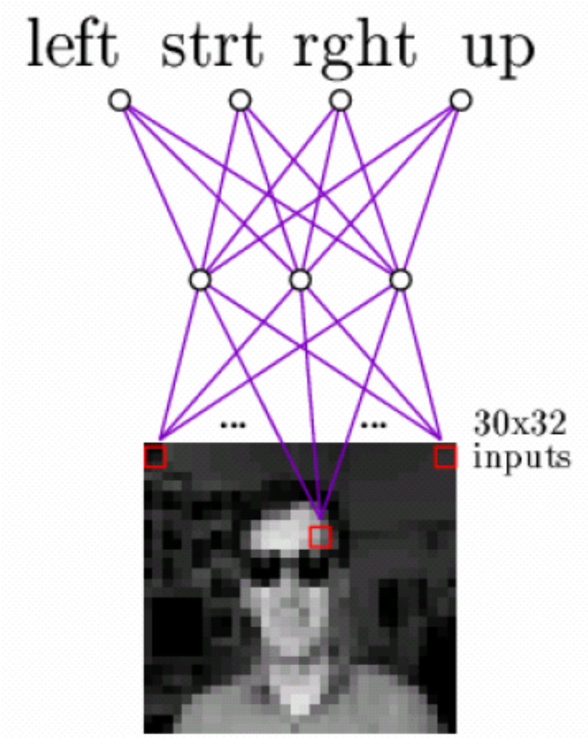
Handwritten Digit Dataset MNIST: 60,000 training samples, 10,000 test samples

Results on MNIST Handwritten Digits

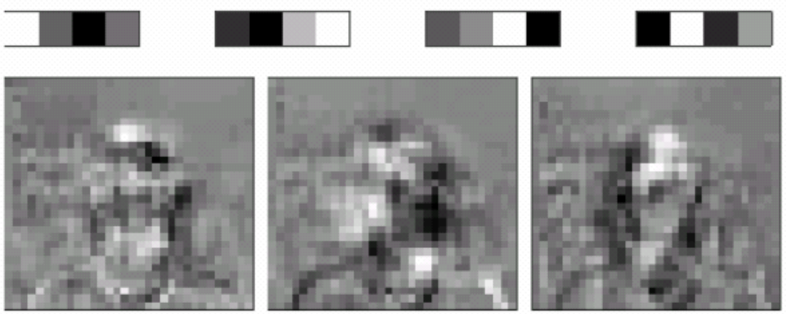
CLASSIFIER	DEFORMATION	PREPROCESSING	ERROR (%)	Reference
linear classifier (1-layer NN)		none	12.00	LeCun et al. 1998
linear classifier (1-layer NN)		deskewing	8.40	LeCun et al. 1998
pairwise linear classifier		deskewing	7.60	LeCun et al. 1998
K-nearest-neighbors, (L2)		none	3.09	Kenneth Wilder, U. Chicago
K-nearest-neighbors, (L2)		deskewing	2.40	LeCun et al. 1998
K-nearest-neighbors, (L2)		deskew, clean, blur	1.80	Kenneth Wilder, U. Chicago
K-NN L3, 2 pixel jitter		deskew, clean, blur	1.22	Kenneth Wilder, U. Chicago
K-NN, shape context matching		shape context feature	0.63	Belongie et al. IEEE PAMI 2002
40 PCA + quadratic classifier		none	3.30	LeCun et al. 1998
1000 RBF + linear classifier		none	3.60	LeCun et al. 1998
K-NN, Tangent Distance		subsamp 16x16 pixels	1.10	LeCun et al. 1998
SVM, Gaussian Kernel		none	1.40	
SVM deg 4 polynomial		deskewing	1.10	LeCun et al. 1998
Reduced Set SVM deg 5 poly		deskewing	1.00	LeCun et al. 1998
Virtual SVM deg-9 poly	Affine	none	0.80	LeCun et al. 1998
V-SVM, 2-pixel jittered		none	0.68	DeCoste and Scholkopf, MLJ 2002
V-SVM, 2-pixel jittered		deskewing	0.56	DeCoste and Scholkopf, MLJ 2002
2-layer NN, 300 HU, MSE		none	4.70	LeCun et al. 1998
2-layer NN, 300 HU, MSE,	Affine	none	3.60	LeCun et al. 1998
2-layer NN, 300 HU		deskewing	1.60	LeCun et al. 1998
3-layer NN, 500+150 HU		none	2.95	LeCun et al. 1998
3-layer NN, 500+150 HU	Affine	none	2.45	LeCun et al. 1998
3-layer NN, 500+300 HU, CE, reg		none	1.53	Hinton, unpublished, 2005
2-layer NN, 800 HU, CE		none	1.60	Simard et al., ICDAR 2003
2-layer NN, 800 HU, CE	Affine	none	1.10	Simard et al., ICDAR 2003
2-layer NN, 800 HU, MSE	Elastic	none	0.90	Simard et al., ICDAR 2003
2-layer NN, 800 HU, CE	Elastic	none	0.70	Simard et al., ICDAR 2003
Convolutional net LeNet-1		subsamp 16x16 pixels	1.70	LeCun et al. 1998
Convolutional net LeNet-4		none	1.10	LeCun et al. 1998
Convolutional net LeNet-5,		none	0.95	LeCun et al. 1998
Conv. net LeNet-5,	Affine	none	0.80	LeCun et al. 1998
Boosted LeNet-4	Affine	none	0.70	LeCun et al. 1998
Conv. net, CE	Affine	none	0.60	Simard et al., ICDAR 2003
Comv net, CE	Elastic	none	0.40	Simard et al., ICDAR 2003

Application: ANN for Face Reco.

- The model



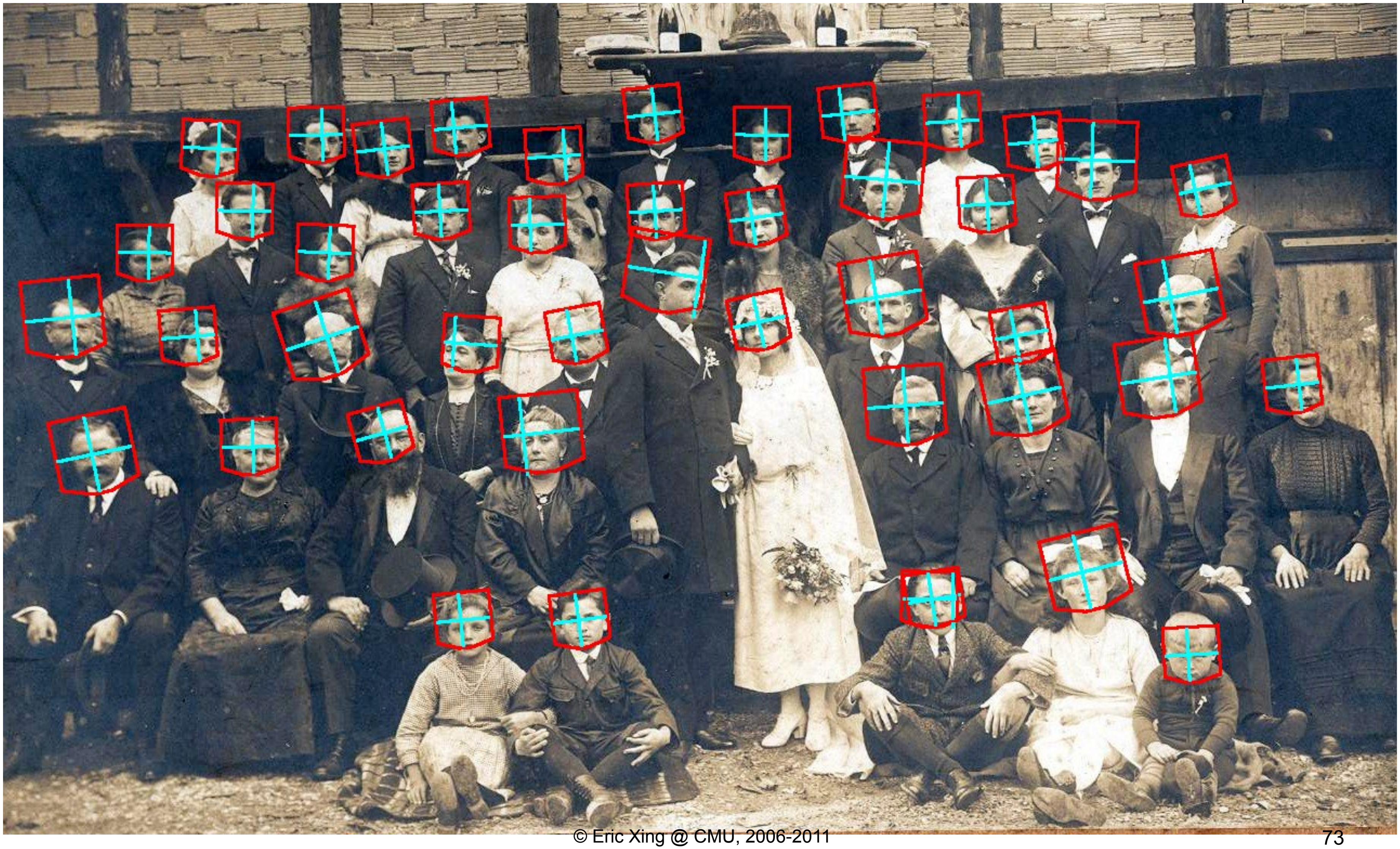
- The learned hidden unit weights



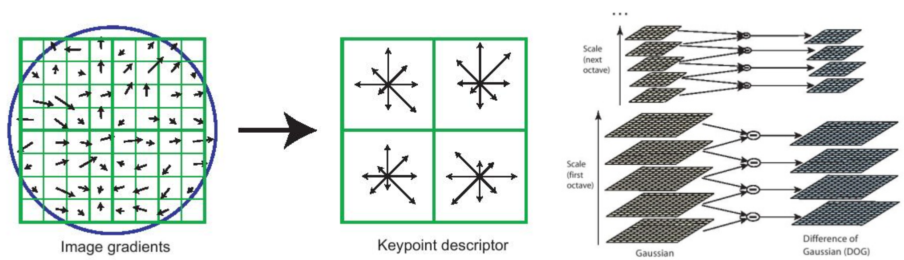
Typical input images

http://www.cs.cmu.edu/~tom/faces.html

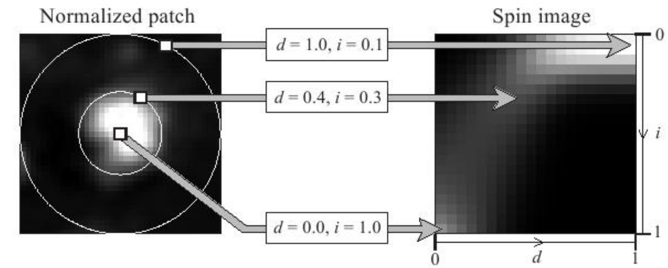
Face Detection with a Convolutional Net



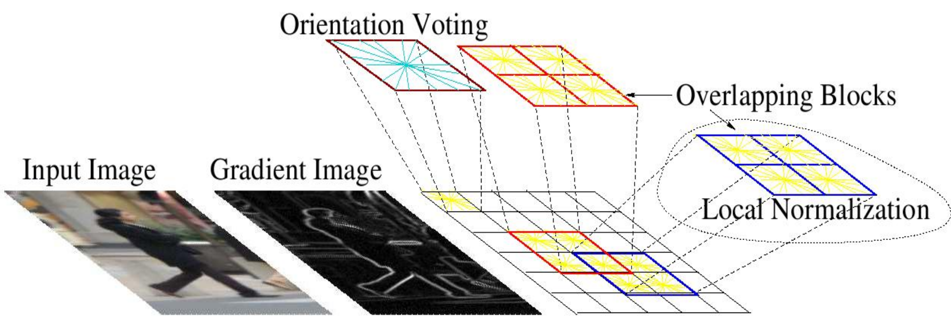
Computer vision features

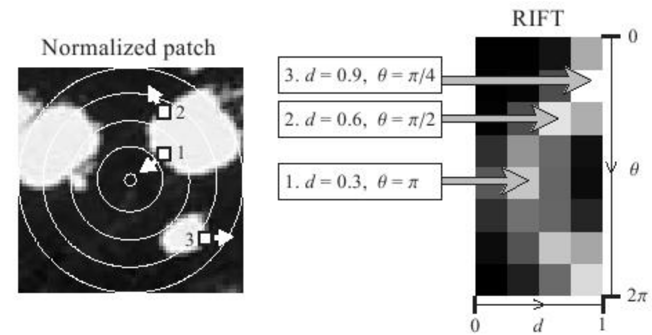


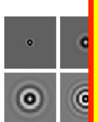
SIFT



Spin image

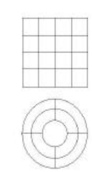






Drawbacks of feature engineering

1. Needs expert knowledge
2. Time consuming hand-tuning



(e)

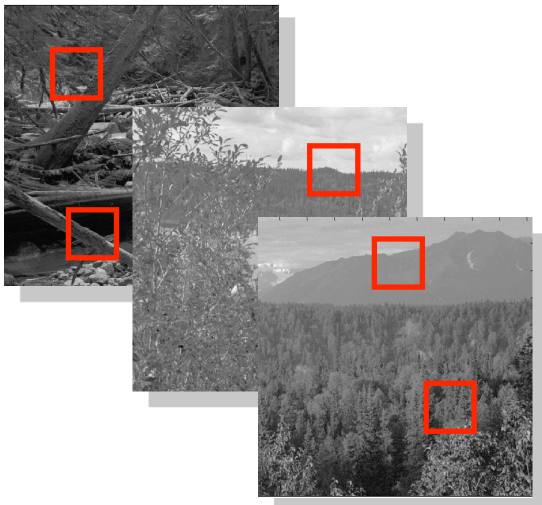
Textons

GLOH

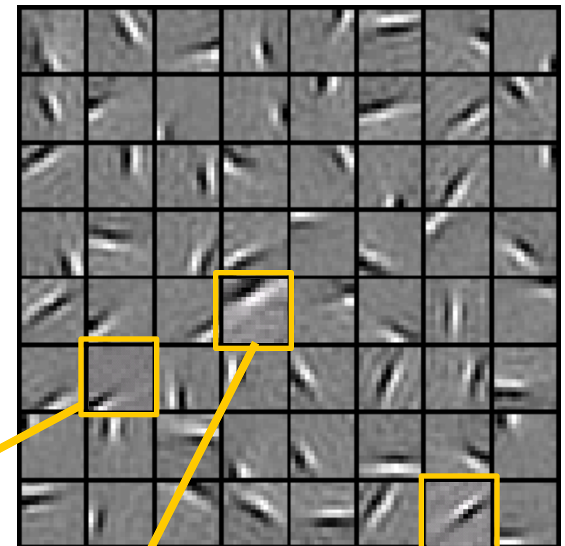
and Ng

Sparse coding on images

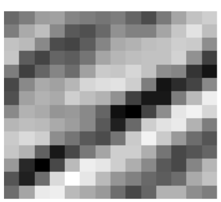
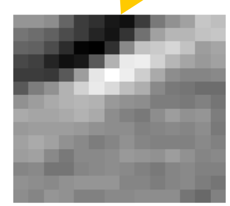
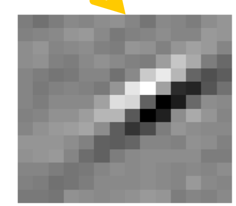
Natural Images



Learned bases: "Edges"



New example

 $= 0.8 *$  $+ 0.3 *$  $+ 0.5 *$ 

$$x = 0.8 * b_{36} + 0.3 * b_{42} + 0.5 * b_{65}$$

[0, 0, … **0.8**, …, **0.3**, …, **0.5**, …] = coefficients (feature representation)

Courtesy: Lee and Ng

Basis (or features) can be learned by Optimization

Given input data $\{x^{(1)}, \ldots, x^{(m)}\}$, we want to find good bases $\{b_1, \ldots, b_n\}$:

$$\min_{b,a} \sum_i \| x^{(i)} - \sum_j a_j^{(i)} b_j \|_2^2 + \beta \sum_i \| a^{(i)} \|_1$$

Reconstruction error — Sparsity penalty

$$\forall j: \ \| b_j \| \le 1$$

Normalization constraint

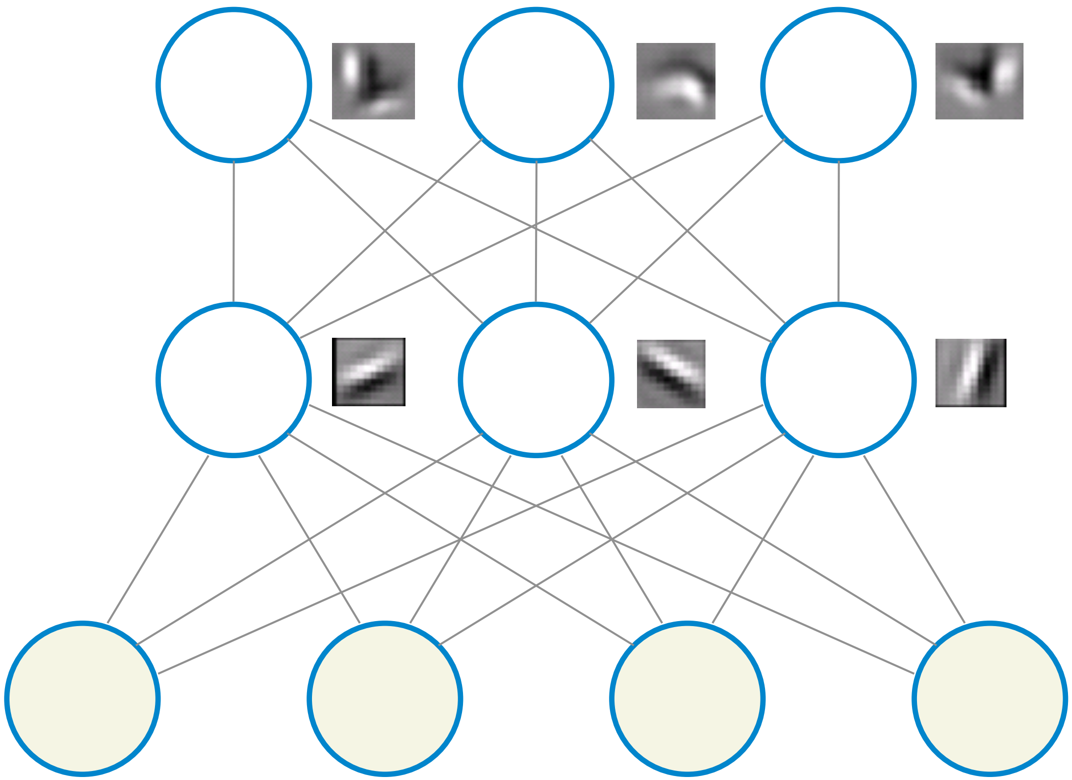
Solve by alternating minimization:

-- Keep *b* fixed, find optimal *a*.

-- Keep *a* fixed, find optimal *b*.

Courtesy: Lee and Ng

Learning Feature Hierarchy

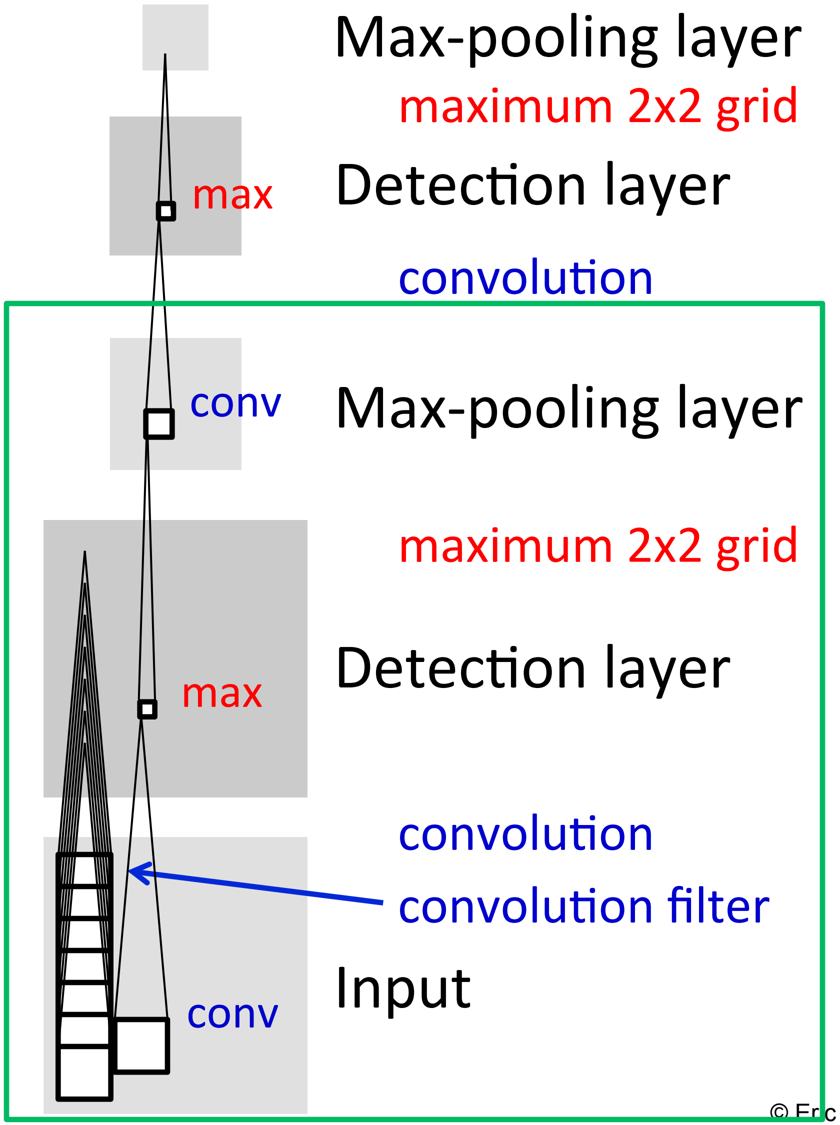


DBN (Hinton et al., 2006) with additional sparseness constraint.

[Related work: Hinton, Bengio, LeCun, and others.]

Courtesy: Lee and Ng

Convolutional architectures



- Weight sharing by convolution (e.g., [Lecun et al., 1989])
- "Max-pooling"
  Invariance
  Computational efficiency
  Deterministic and feed-forward
- One can develop convolutional Restricted Boltzmann machine (CRBM).
- One can define *probabilistic max-pooling* that *combine bottom-up and top-down information*.

Courtesy: Lee and Ng

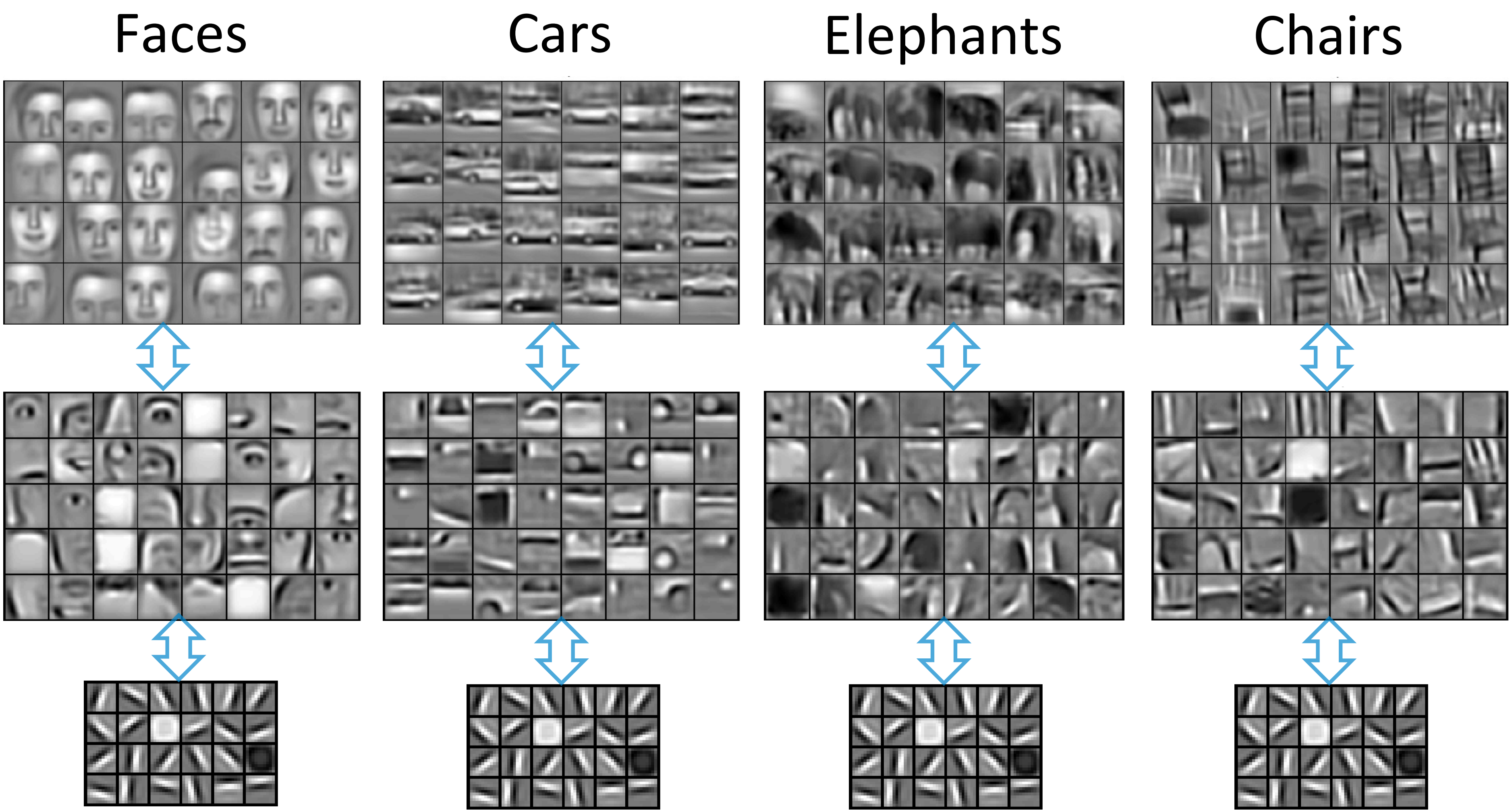
Convolutional Deep Belief Networks

- Bottom-up (greedy), layer-wise training
  - Train one layer (convolutional RBM) at a time.

- Inference (approximate)
  - Undirected connections for all layers (Markov net) [Related work: Salakhutdinov and Hinton, 2009]
  - Block Gibbs sampling or mean-field
  - Hierarchical probabilistic inference

Courtesy: Lee and Ng

Unsupervised learning of object-parts



Courtesy: Lee and Ng

Weaknesses & Criticisms

- Learning everything. Better to encode prior knowledge about structure of images.

  A: Compare with machine learning vs. linguists debate in NLP.

- Results not yet competitive with best engineered systems.

  A: Agreed. True for some domains.

Courtesy: Lee and Ng

Tutorials

- LSTMs
  - Christopher Olah's blog
  - http://colah.github.io/posts/2015-08-Understanding-LSTMs/
- Convolutional Neural Networks
  - Andrej Karpathy, CS231n Notes
  - http://cs231n.github.io/convolutional-networks/