Artificial Neural Networks

Lecture Slides for textbook

Machine Learning

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Topics covered

- Threshold Units
- Gradient descents
- Multilayer networks
- Backpropagation
- Hidden layer representation
- Example: Face Recognition
- Advanced topics

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When to Consider Neural Networks

- Input is high-dimensional discrete or real-valued (e.g., raw sensor input)
- Output is discrete or real valued or a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant
- Examples
  - Speech phoneme recognition
  - Image classification
  - Financial prediction

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Artificial Neural Networks to learn f: X → Y

- f might be non-linear function
- X (vector of) continuous and/or discrete vars
- Y (vector of) continuous and/or discrete vars

- Represent f by ***network*** of logistic units
- Each unit is a logistic function

$$unit\ output = \frac{1}{1 + exp(w_0 + \sum_i w_i x_i)}$$

- MLE: train weights of all units to minimize sum of squared errors of predicted network outputs
- MAP: train to minimize sum of squared errors plus weight magnitudes

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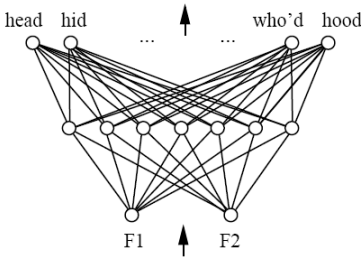
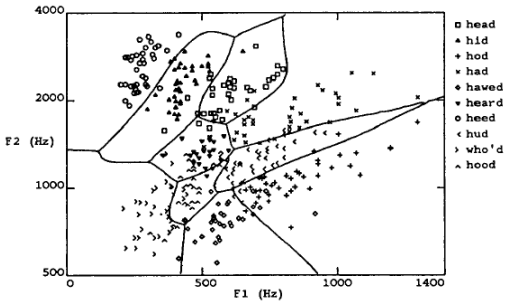
Multilayer Networks of Sigmoid Units





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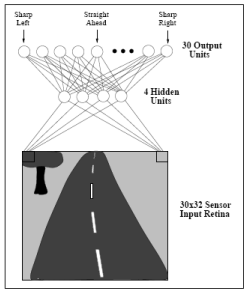
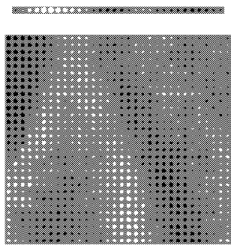
ALVINN drives 70 mph on highways





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Connectionist Model

Consider humans:

- Neuron switching time ~ .001 second
- Number of neurons ~ 10^{10}
- Connections per neuron ~ 10^{4-5}
- Scene recognition time ~ .1 second
- 100 inference steps doesn't seem like enough

→ much parallel computation

Properties of artificial neural nets (ANN's):

- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed process

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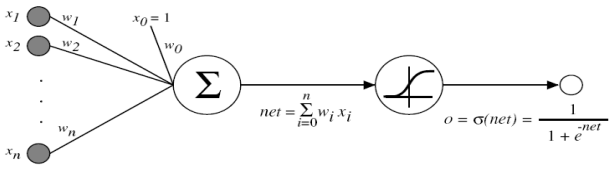
Sigmoid Unit



$\sigma(x)$ is the sigmoid function

$$\frac{1}{1 + e^{-x}}$$

Nice property: $\frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x))$

We can derive gradient decent rules to train

- One sigmoid unit
- *Multilayer networks* of sigmoid units → Backpropagation

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M(C)LE Training for Neural Networks

- Consider regression problem f:X→Y , for scalar Y

$y = f(x) + \varepsilon$ ← assume noise $N(0,\sigma_\varepsilon)$, iid

deterministic

- Let's maximize the conditional data likelihood

$$W \leftarrow \arg\max_W \ln \prod_l P(Y^l|X^l, W)$$

$$W \leftarrow \arg\min_W \sum_l (y^l - \hat{f}(x^l))^2$$

Learned neural network

MAP Training for Neural Networks

- Consider regression problem f:X→Y , for scalar Y

$y = f(x) + \varepsilon$ ← noise $N(0,\sigma_\varepsilon)$

deterministic

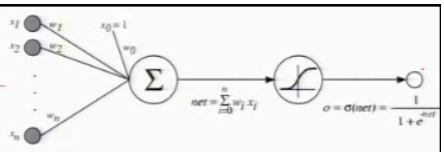
Gaussian P(W) = N(0,σI)

$$W \leftarrow \arg\max_W \ln P(W) \prod_l P(Y^l|X^l, W)$$

$$W \leftarrow \arg\min_W \left[c \sum_i w_i^2\right] + \left[\sum_l (y^l - \hat{f}(x^l))^2\right]$$

ln P(W) ↔ c $\sum_i w_i^2$

Error Gradient for a Sigmoid Unit



$$\begin{aligned}\frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i}\frac{1}{2}\sum_{d\in D}(t_d - o_d)^2 \\ &= \frac{1}{2}\sum_d \frac{\partial}{\partial w_i}(t_d - o_d)^2 \\ &= \frac{1}{2}\sum_d 2(t_d - o_d)\frac{\partial}{\partial w_i}(t_d - o_d) \\ &= \sum_d (t_d - o_d)\left(-\frac{\partial o_d}{\partial w_i}\right) \\ &= -\sum_d (t_d - o_d)\frac{\partial o_d}{\partial net_d}\frac{\partial net_d}{\partial w_i}\end{aligned}$$

x_d = input

t_d = target output

o_d = observed unit output

w_i = weight i

But we know:

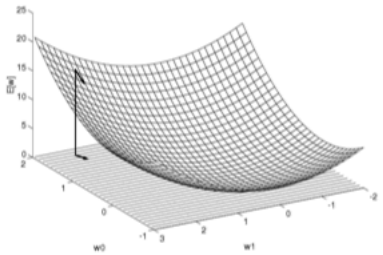
$$\frac{\partial o_d}{\partial net_d} = \frac{\partial \sigma(net_d)}{\partial net_d} = o_d(1 - o_d)$$

$$\frac{\partial net_d}{\partial w_i} = \frac{\partial(\vec{w}\cdot\vec{x}_d)}{\partial w_i} = x_{i,d}$$

So:

$$\frac{\partial E}{\partial w_i} = -\sum_{d\in D}(t_d - o_d)o_d(1 - o_d)x_{i,d}$$

Gradient Descent



Gradient

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots \frac{\partial E}{\partial w_n}\right]$$

Training rule:

$$\Delta\vec{w} = -\eta\nabla E[\vec{w}]$$

i.e.,

$$\Delta w_i = -\eta\frac{\partial E}{\partial w_i}$$

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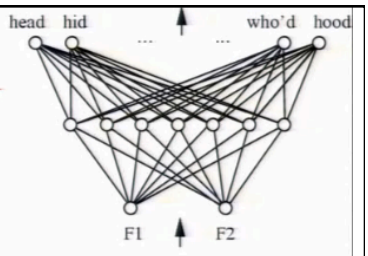
Backpropagation Algorithm (MLE)



Initialize all weights to small random numbers.
Until satisfied, Do

- For each training example, Do
  1. Input the training example to the network and compute the network outputs
  2. For each output unit k

$$\delta_k \leftarrow o_k(1-o_k)(t_k-o_k)$$

  3. For each hidden unit h

$$\delta_h \leftarrow o_h(1-o_h)\sum_{k\in outputs} w_{h,k}\delta_k$$

  4. Update each network weight $w_{i,j}$

$$w_{i,j} \leftarrow w_{i,j} + \Delta w_{i,j}$$

  where

$$\Delta w_{i,j} = \eta \delta_j x_i$$

x_d = input

t_d = target output

o_d = observed unit output

w_{ij} = wt from i to j

More on Backpropagation

- Gradient descent over entire *network* weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)
- Often include weight *momentum* α

$$\Delta w_{i,j}(n) = \eta \delta_j x_{i,j} + \alpha \Delta w_{i,j}(n-1)$$

- Minimizes error over *training* examples
  - Will it generalize well to subsequent examples?
- Training can take thousands of iterations → slow!
- Using network after training is very fast

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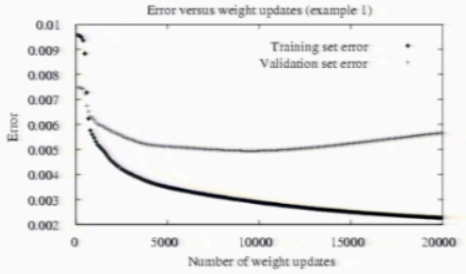
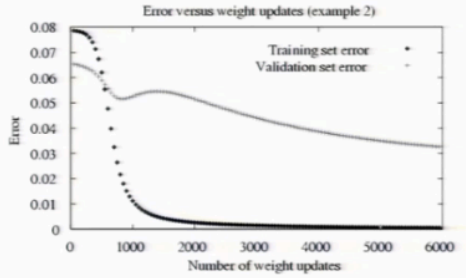
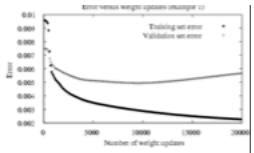
Overfitting in ANNs





Dealing with Overfitting



Our learning algorithm involves a parameter
n=number of gradient descent iterations
How do we choose n to optimize future error?
(note: similar issue for logistic regression, decision trees, …)

e.g. the n that minimizes error rate of neural net over future data

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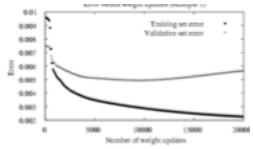
Dealing with Overfitting



Our learning algorithm involves a parameter
n=number of gradient descent iterations
How do we choose n to optimize future error?

- Separate available data into training and validation set
- Use training to perform gradient descent
- n ← number of iterations that optimizes validation set error

→ *gives unbiased estimate of optimal n*
(but a biased estimate of true error)

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K-Fold Cross Validation

Idea: train multiple times, leaving out a disjoint subset of data each time for test. Average the test set accuracies.

Partition data into K disjoint subsets
For k=1 to K
    testData = kth subset
    h ← classifier trained* on all data except for testData
    accuracy(k) = accuracy of h on testData
end
FinalAccuracy = mean of the K recorded testset accuracies

* might withhold some of this to choose number of gradient decent steps

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K-Fold Cross Validation

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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 arbitrarily 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].

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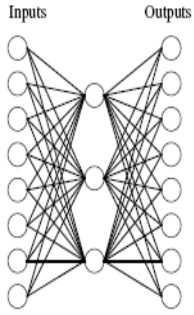
Learning Hidden Layer Representation



A target function:

Input		Output
10000000	→	10000000
01000000	→	01000000
00100000	→	00100000
00010000	→	00010000
00001000	→	00001000
00000100	→	00000100
00000010	→	00000010
00000001	→	00000001

Can this be learned??

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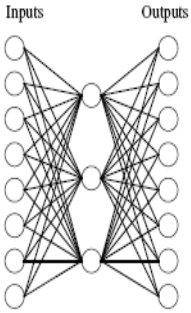
Learning Hidden Layer Representation



Learned hidden layer representation:

Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

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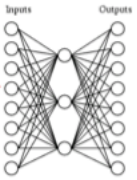
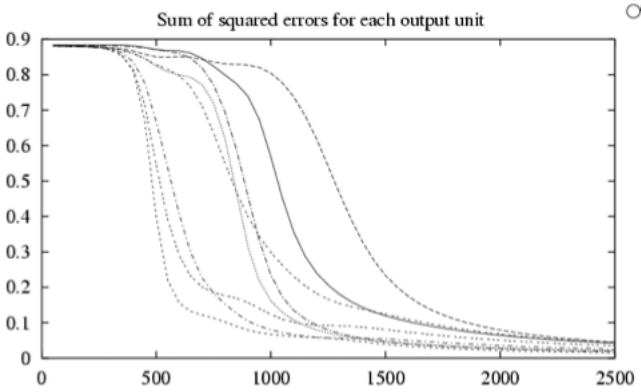
Training





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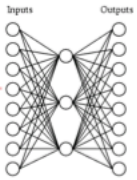
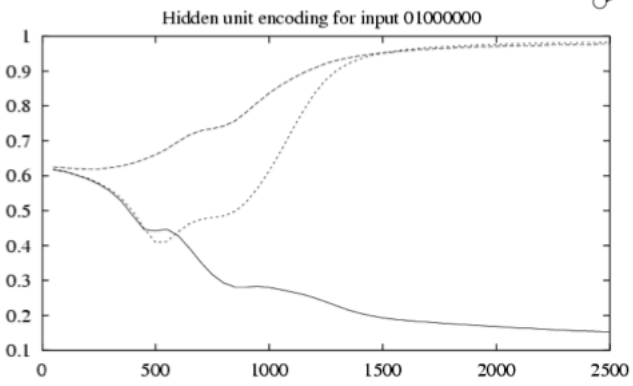
Training





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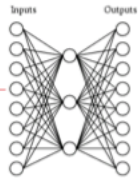
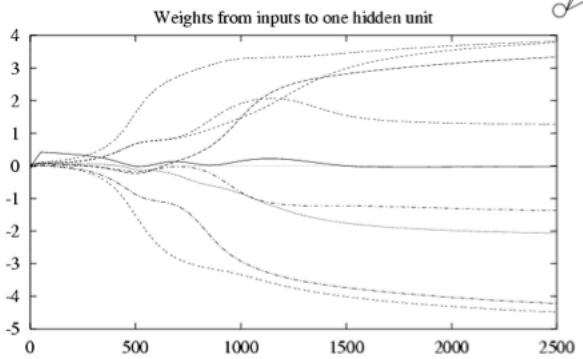
Training





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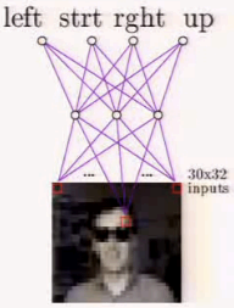
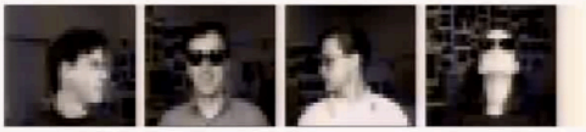
Neural Nets for Face Recognition

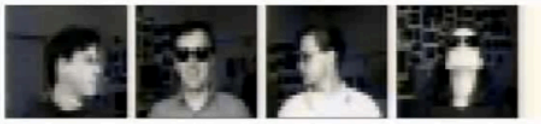




Typical input images

90% accurate learning head pose, and recognizing 1-of-20 faces

Learned Hidden Unit Weights

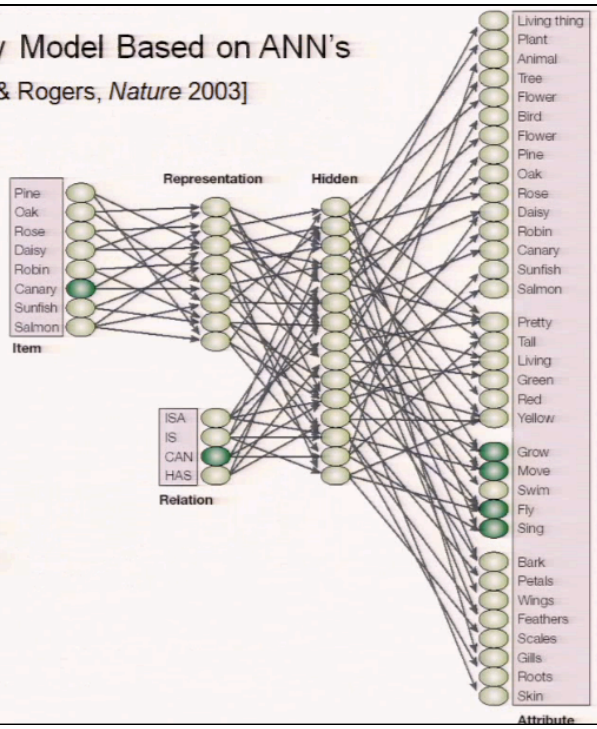


Typical input images

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

Semantic Memory Model Based on ANN's

[McClelland & Rogers, *Nature* 2003]

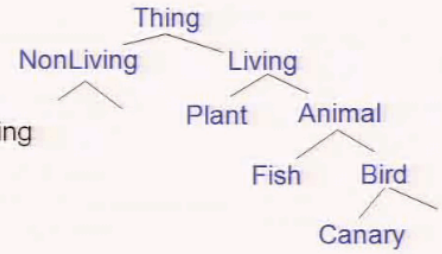


Train with assertions,
e.g., Can(Canary,Fly)

Humans act as though they have a hierarchical memory organization

1. Victims of Semantic Dementia progressively lose knowledge of objects
   But they lose specific details first, general properties later, suggesting hierarchical memory organization

2. Children appear to learn general categories and properties first, following the same hierarchy, top down*.



* some debate remains on this.

Memory deterioration follows semantic hierarchy

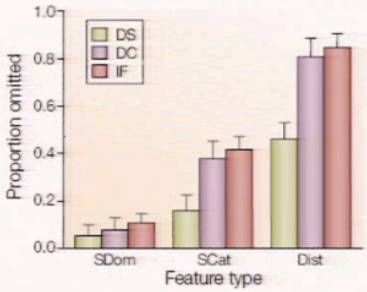
[McClelland & Rogers, *Nature* 2003]

a

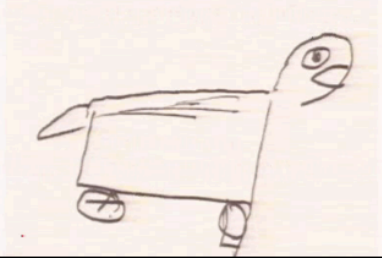
Picture naming responses for JL

Item	Sept. 91	March 92	March 93
Bird	+	+	Animal
Chicken	+	+	Animal
Duck	+	Bird	Dog
Swan	+	Bird	Animal
Eagle	Duck	Bird	Horse
Ostrich	Swan	Bird	Animal
Peacock	Duck	Bird	Vehicle
Penguin	Duck	Bird	Part of animal
Rooster	Chicken	Chicken	Dog

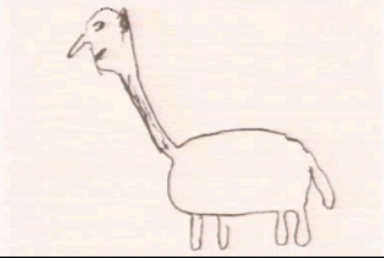
b



c IF's delayed copy of a camel



d DC's delayed copy of a swan



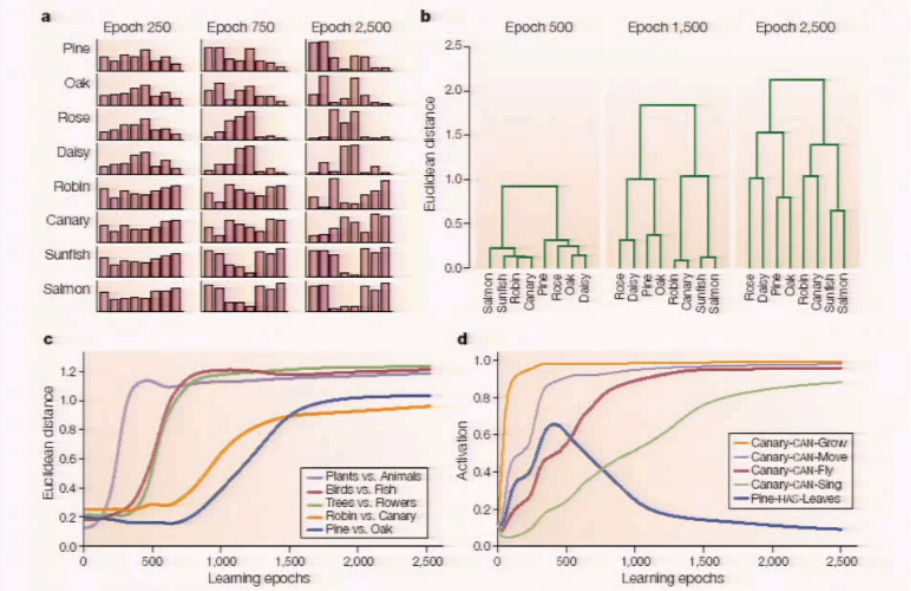


Figure 4 | **The process of differentiation of conceptual representations.** The representations are those seen in the feedforward network model shown in FIG. 3. **a** | Acquired patterns of activation that represent the eight objects in the training set at three points in the learning process (epochs 250, 750 and 2,500). Early in learning, the patterns are undifferentiated; the first difference to appear is between plants and animals. Later, the patterns show clear differentiation at both the superordinate (plant–animal) and intermediate (bird–fish/tree–flower) levels. Finally, the individual concepts are differentiated, but the overall hierarchical organization of the similarity structure remains. **b** | A standard hierarchical clustering analysis program has been used to visualize the similarity structure in the

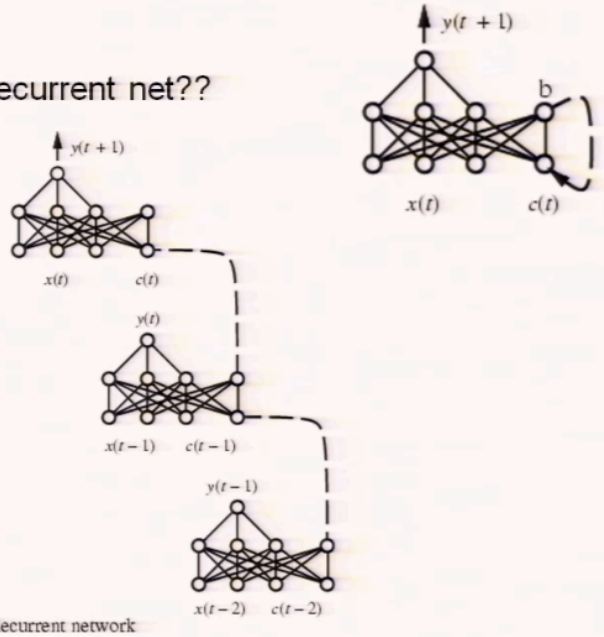
Training Networks on Time Series

- Suppose we want to predict next state of world
  - and it depends on history of unknown length (non-Markovian)
  - e.g., robot with forward-facing sensors trying to predict next sensor reading as it moves and turns
- Idea: use hidden layer in network to capture state history

(a) Feedforward network (b) Recurrent network

Training Networks on Time Series

How can we train recurrent net??



(c) Recurrent network unfolded in time

Summary: Neural Networks

- Represent highly non-linear decision surfaces
- Learn f: X → Y, where Y is vector (e.g., image)
- Hidden layer represents re-representation of input
  - to optimize prediction accuracy (minimize sum sq error)
- Role in modeling human cognition
- Local minimum problems solving for MLE/MAP parameters using gradient descent

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Homework

- Problems 4.5, 4.7 & 4.8

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