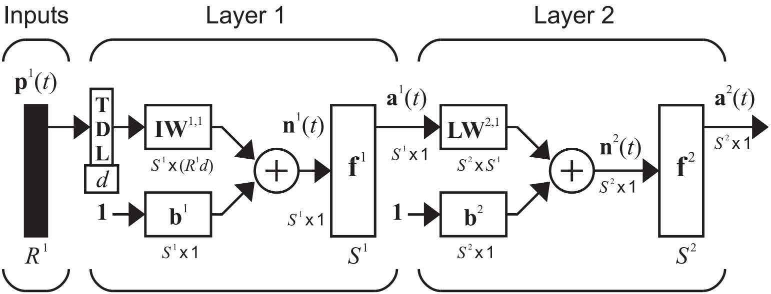
Nonlinear Sequence Processing

Deep Learning

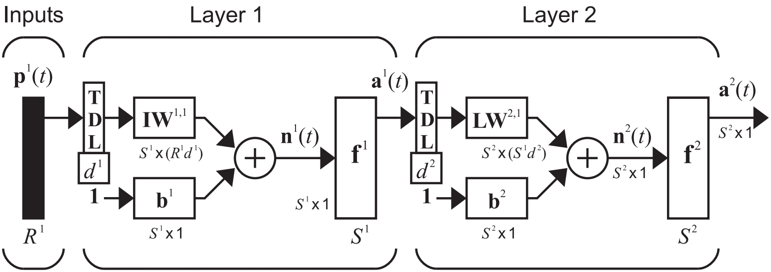
Objective

- The linear sequence processing concepts from the previous chapter lead into the nonlinear networks of this chapter.
- These networks are also dynamic – they have memory in terms of tapped delay lines.
- Some of these networks are strictly feedforward, and some have feedback – recurrent networks.
- Some networks are of the input-output type and use tapped delay lines.
- Other networks are of the state space type, and use single delays.

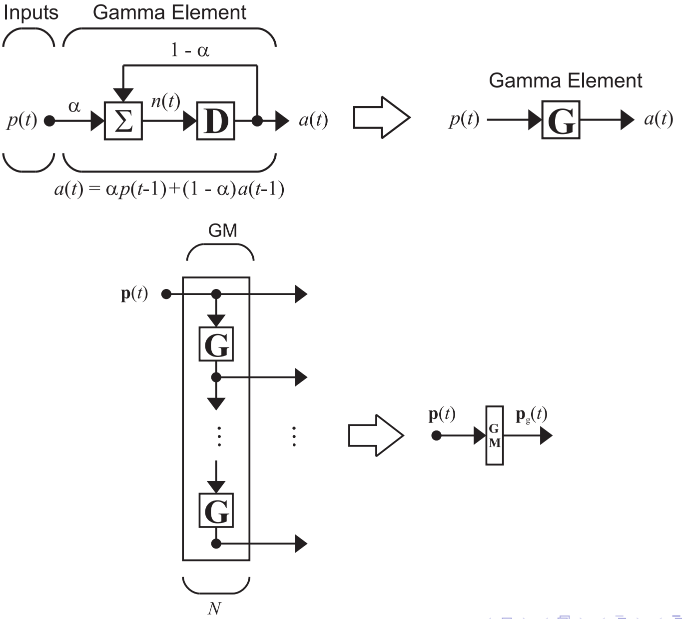
Focused time delay neural network

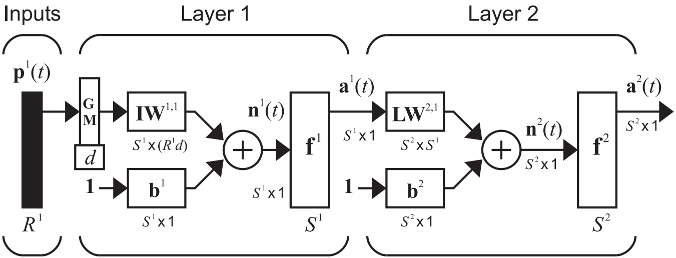


- The TDL is focused at the input to the network.
- An advantage of this dynamic network, because there is no feedback, is that computations can be done in parallel.
- Also, standard backpropagation can be used to compute the gradient.



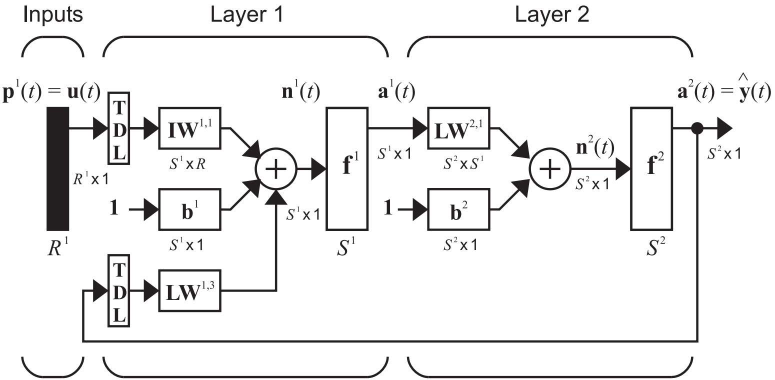
- Because tapped delay lines are distributed throughout the network, the backpropagation algorithm must be adjusted.


Inputs
Gamma Element
1 - α
α
n(t)
p(t)
Σ
D
a(t)
a(t) = αp(t-1)+(1 - α)a(t-1)
Gamma Element
p(t)
G
a(t)
GM
p(t)
G
G
N
p(t)
G
M
p_g(t)

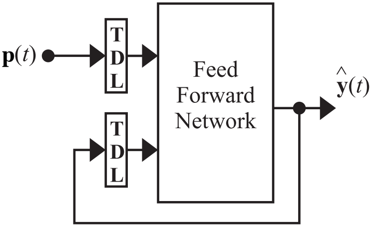


- This network does have some limited feedback, which gives it longer memory.
- Although the feedback is limited, the backpropagation algorithm does have to be somewhat modified.

Nonlinear Autoregressive Network with Exogenous Input

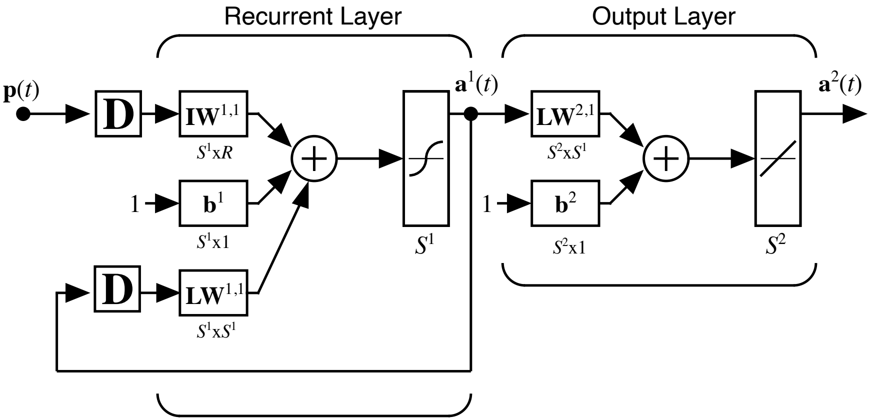


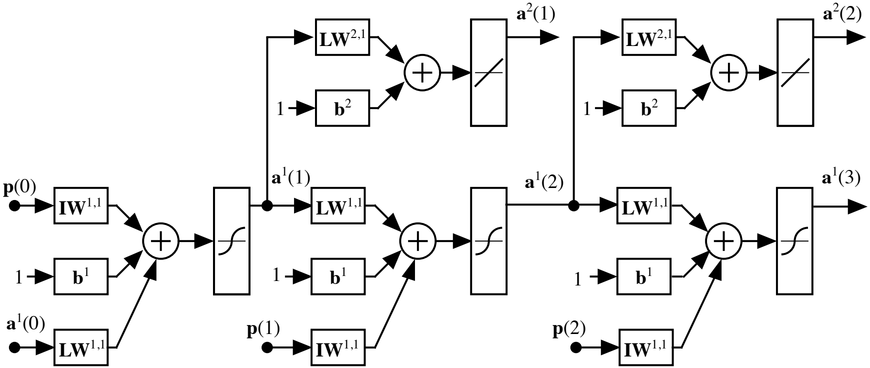
NARX can be trained with standard backprop



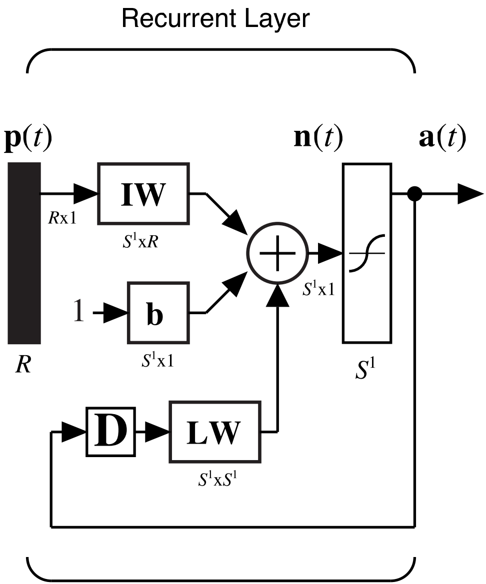
Parallel Architecture

Series-Parallel Architecture


Recurrent Layer
Output Layer
p(t)
D
IW1,1
S1xR
1
b1
S1x1
D
LW1,1
S1xS1
S1
a1(t)
LW2,1
S2xS1
1
b2
S2x1
S2
a2(t)



a²(1)
a²(2)
LW2,1
LW2,1
1
b²
1
b²
p(0)
a¹(1)
a¹(2)
a¹(3)
IW1,1
LW1,1
LW1,1
1
b¹
1
b¹
1
b¹
a¹(0)
LW1,1
p(1)
IW1,1
p(2)
IW1,1


Recurrent Layer
p(t)
n(t)
a(t)
IW
Rx1
S1xR
1
b
S1x1
S1x1
R
S1
D
LW
S1xS1

Real Time Recurrent Learning (RTRL)

$$\frac{\partial F}{\partial \mathbf{x}} = \sum_{t=1}^{Q} \left[\frac{\partial \mathbf{a}(t)}{\partial \mathbf{x}^T} \right]^T \times \frac{\partial^e F}{\partial \mathbf{a}(t)}$$

$$\frac{\partial \mathbf{a}(t)}{\partial \mathbf{x}^T} = \frac{\partial^e \mathbf{a}(t)}{\partial \mathbf{x}^T} + \frac{\partial^e \mathbf{a}(t)}{\partial \mathbf{a}(t-1)^T} \frac{\partial \mathbf{a}(t-1)}{\partial \mathbf{x}^T}$$

Backpropagation Through Time (BTT)

$$\frac{\partial F}{\partial \mathbf{x}} = \sum_{t=1}^{Q} \left[\frac{\partial^e \mathbf{a}(t)}{\partial \mathbf{x}^T} \right]^T \times \frac{\partial F}{\partial \mathbf{a}(t)}$$

$$\frac{\partial F}{\partial \mathbf{a}(t)} = \frac{\partial^e F}{\partial \mathbf{a}(t)} + \frac{\partial^e \mathbf{a}(t+1)}{\partial \mathbf{a}(t)^T} \times \frac{\partial F}{\partial \mathbf{a}(t+1)}$$

- Let $Q = 2$, and let $F(\mathbf{x}) = (\mathbf{t} - \mathbf{a}(2))^T(\mathbf{t} - \mathbf{a}(2)) = \mathbf{e}^T\mathbf{e}$

$$\frac{\partial F}{\partial \mathbf{a}(t)} = \frac{\partial^e F}{\partial \mathbf{a}(t)} + \frac{\partial^e \mathbf{a}(t+1)}{\partial \mathbf{a}(t)^T} \times \frac{\partial F}{\partial \mathbf{a}(t+1)}$$

$$\frac{\partial F}{\partial \mathbf{a}(t)} = \mathbf{0}, t > Q$$

$$\frac{\partial F}{\partial \mathbf{a}(2)} = \cancelto{-2\mathbf{e}}{\frac{\partial^e F}{\partial \mathbf{a}(2)}} + \frac{\partial^e \mathbf{a}(3)}{\partial \mathbf{a}(2)^T} \times \cancelto{0}{\frac{\partial F}{\partial \mathbf{a}(3)}} = -2\mathbf{e}$$

$$\frac{\partial F}{\partial \mathbf{a}(1)} = \cancelto{0}{\frac{\partial^e F}{\partial \mathbf{a}(1)}} + \frac{\partial^e \mathbf{a}(2)}{\partial \mathbf{a}(1)^T} \times \cancelto{-2\mathbf{e}}{\frac{\partial F}{\partial \mathbf{a}(2)}} = [\mathbf{LW}]^T \dot{\mathbf{F}}(\mathbf{n}(2))^T [-2\mathbf{e}]$$

$$\frac{\partial F}{\partial \mathbf{x}} = \sum_{t=1}^{Q} \left[\frac{\partial^e \mathbf{a}(t)}{\partial \mathbf{x}^T}\right]^T \times \frac{\partial F}{\partial \mathbf{a}(t)}$$

$$\frac{\partial F}{\partial lw_{i,j}} = \sum_{t=1}^{2} \left[\frac{\partial^e \mathbf{a}(t)}{\partial lw_{i,j}}\right]^T \times \frac{\partial F}{\partial \mathbf{a}(t)}$$

$$\frac{\partial^e \mathbf{a}^T(t)}{\partial lw_{i,j}} \frac{\partial F}{\partial \mathbf{a}(t)} = \frac{\partial^e \mathbf{n}^T(t)}{\partial lw_{i,j}} \frac{\partial^e \mathbf{a}^T(t)}{\partial \mathbf{n}(t)} \frac{\partial F}{\partial \mathbf{a}(t)}$$

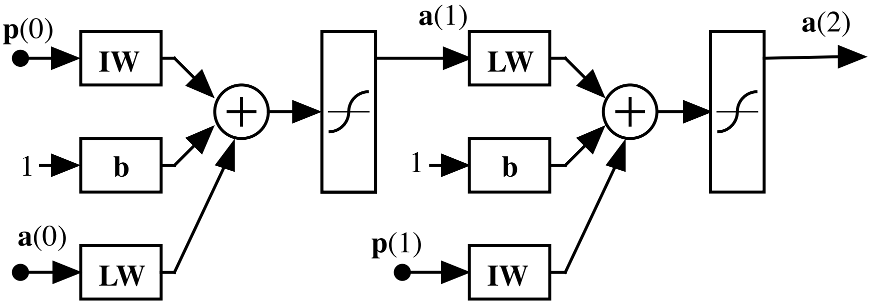
$$\frac{\partial^e \mathbf{n}(t)}{\partial lw_{i,j}} = \boldsymbol{\epsilon}_i a_j(t-1)$$

$$\frac{\partial^e \mathbf{a}^T(t)}{\partial \mathbf{n}(t)} = \dot{\mathbf{F}}^T(\mathbf{n}(t))$$

Gradient calculation 2

$$\frac{\partial^e \mathbf{a}^T(t)}{\partial lw_{i,j}} \frac{\partial F}{\partial \mathbf{a}(t)} = a_j(t-1)\dot{f}(n_i(t))\frac{\partial F}{\partial a_i(t)}$$

$$\begin{aligned}\frac{\partial F}{\partial \mathbf{LW}} =& \sum_{t=1}^{2} \dot{\mathbf{F}}^T(\mathbf{n}(t))\frac{\partial F}{\partial \mathbf{a}(t)}\mathbf{a}^T(t-1) \\ =& \dot{\mathbf{F}}^T(\mathbf{n}(1))\frac{\partial F}{\partial \mathbf{a}(1)}\mathbf{a}^T(0) + \dot{\mathbf{F}}^T(\mathbf{n}(2))\frac{\partial F}{\partial \mathbf{a}(2)}\mathbf{a}^T(1) \\ =& \dot{\mathbf{F}}^T(\mathbf{n}(1))\mathbf{LW}^T\dot{\mathbf{F}}^T(\mathbf{n}(2))\left[-2\mathbf{e}\right]\mathbf{a}^T(0) \\ & + \dot{\mathbf{F}}^T(\mathbf{n}(2))\left[-2\mathbf{e}\right]\mathbf{a}^T(1)\end{aligned}$$


p(0)
IW
1
b
a(0)
LW
a(1)
LW
1
b
p(1)
IW
a(2)

Standard Backpropagation for Multilayer Networks

$$
\begin{aligned}
\mathbf{s}^M &= \dot{\mathbf{F}}^{\mathbf{M}} \left(\mathbf{n}^M\right)^T [-2\mathbf{e}] \\
\mathbf{s}^m &= \dot{\mathbf{F}}^m (\mathbf{n}^m)^T (\mathbf{W}^{m+1})^T \mathbf{s}^{m+1} \\
\frac{\partial \hat{F}(\mathbf{x})}{\partial w_{i,j}^m} &= s_i^m a_j^{m-1} \\
\frac{\partial F(\mathbf{x})}{\partial \mathbf{W}^m} &= \mathbf{s}^m \left(\mathbf{a}^{m-1}\right)^T
\end{aligned}
$$

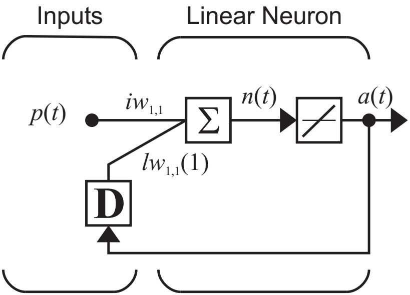
Static backpropagation for unrolled network

$$
\begin{aligned}
\mathbf{s}(2) &= \dot{\mathbf{F}}\left(\mathbf{n}(2)\right)^T \left[-2\mathbf{e}\right] \\
\mathbf{s}(1) &= \dot{\mathbf{F}}(\mathbf{n}(1))^T \mathbf{LW}^T \mathbf{s}(2) \\
&= \dot{\mathbf{F}}(\mathbf{n}(1))^T \mathbf{LW}^T \dot{\mathbf{F}}\left(\mathbf{n}(2)\right)^T \left[-2\mathbf{e}\right] \\
\left.\frac{\partial F(\mathbf{x})}{\partial \mathbf{LW}}\right|_{t=2} &= \mathbf{s}(2)\mathbf{a}(1)^T = \dot{\mathbf{F}}\left(\mathbf{n}(2)\right)^T \left[-2\mathbf{e}\right]\mathbf{a}(1)^T \\
\left.\frac{\partial F(\mathbf{x})}{\partial \mathbf{LW}}\right|_{t=1} &= \mathbf{s}(1)\mathbf{a}(0)^T = \dot{\mathbf{F}}(\mathbf{n}(1))^T \mathbf{LW}^T \dot{\mathbf{F}}\left(\mathbf{n}(2)\right)^T \left[-2\mathbf{e}\right]\mathbf{a}(0)^T \\
\left.\frac{\partial F(\mathbf{x})}{\partial \mathbf{LW}}\right|_{total} &= \dot{\mathbf{F}}(\mathbf{n}(1))^T \mathbf{LW}^T \dot{\mathbf{F}}\left(\mathbf{n}(2)\right)^T \left[-2\mathbf{e}\right]\mathbf{a}(0)^T \\
&+ \dot{\mathbf{F}}\left(\mathbf{n}(2)\right)^T \left[-2\mathbf{e}\right]\mathbf{a}(1)^T
\end{aligned}
$$

Learning long term dependencies

- For some recurrent network problems, we would like to predict responses that may be significantly delayed from the corresponding stimulus.
  - A chess game can be lost 12 moves after a mistake.
  - Words in a previous paragraph can provide context for a translation.
- A network structure must enable this possibility (have long term memory).
- Even within a structure that allows long term memory, the actual memory depends on the weights.
- Long memory systems can flirt with instability.

Simple recurrent network



$$a(t) = iw_{1,1}p(t) + lw_{1,1}(1)a(t\text{-}1)$$

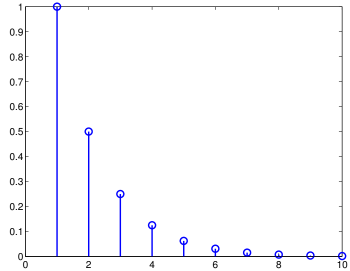
Let $lw_{1,1} = 0.5$ and $iw_{1,1} = 1$. Apply the input sequence of a one followed by 9 zeros, with zero initial condition (impulse response).

$$a(t) = iw_{1,1}p(t) + lw_{1,1}a(t-1) = p(t) + 0.5a(t-1)$$

$$a(1) = p(1) = 1$$

$$a(2) = 0.5a(1) = 0.5$$

$$a(t) = 0.5^{(t-1)}$$



Gradient also decays quickly

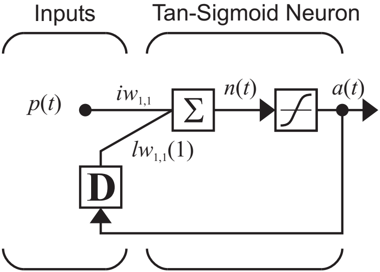
$$\frac{\partial F}{\partial a(t)} = \frac{\partial^e F}{\partial a(t)} + lw_{1,1} \frac{\partial F}{\partial a(t+1)}$$

If the error only occurs at the 10th time point, and $lw_{1,1} = 0.5$, we have

$$\frac{\partial F}{\partial a(t)} = 0.5^{(10-t)} \frac{\partial^e F}{\partial a(10)}$$

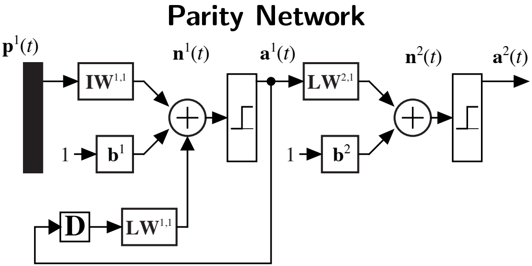
- If the network is stable, derivatives decay as you go back in time.
- Because the derivatives are small, it will take a long time to learn long term dependencies.

Nonlinear transfer function increases decay



$a(t) = tansig(\ iw_{1,1}p(t) + lw_{1,1}(1)a(t\text{-}1)\ )$

$$\frac{\partial F}{\partial a(t)} = \frac{\partial^e F}{\partial a(t)} + \dot{f}(n(t))lw_{1,1}\frac{\partial F}{\partial a(t+1)}, \left|\dot{f}(n(t))\right| \leq 1$$



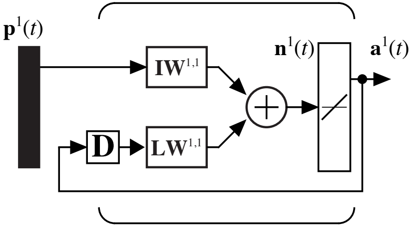
$$\mathbf{IW}^{1,1} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \mathbf{LW}^{1,1} = \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}, \mathbf{LW}^{2,1} = \begin{bmatrix} 1 & -1 \end{bmatrix}, \mathbf{b}^{1} = \begin{bmatrix} -0.5 \\ -1.5 \end{bmatrix}, \mathbf{b}^{2} = [-0.5]$$

- This network computes the parity of a sequence of bits.
- It can remember back as many bits as have been presented.

Difficulties in learning long term dependencies

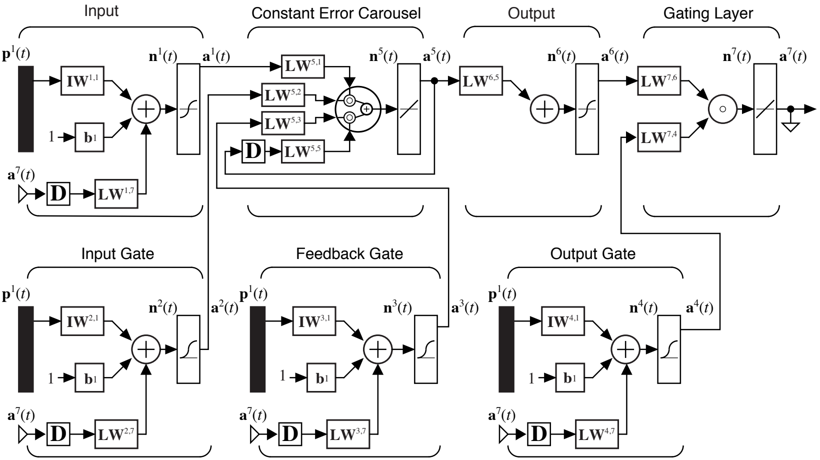
- Long term memories are network weights – short term memories are layer outputs.
- We need a network with long short term memory
- In recurrent networks, as the weights change during training, the length of the short term memory will change.
- If the initial weights produce a network without long short term memory, it will be difficult to increase it.
- This is because the gradient will be small for short short term memory networks.
- If the initial weights produce long short term memory, instabilities can easily occur.

- To maintain a long memory, we would like the feedback matrix $\mathbf{LW}^{1,1}$ to have some eigenvalues very close to one.
- This has to be maintained during training, or the gradients will vanish.
- In addition, to ensure long memories, the derivative of the transfer function should be constant.
- Eigenvalues greater than one $\rightarrow$ unstable.
- Solution: Set $\mathbf{LW}^{1,1} = \mathbf{I}$ and use linear transfer function.



Gating

- We don't want to indiscriminately remember everything.
- To remember selectively, we introduce several gates (switches).
  - An input gate will allow selective inputs into the CEC.
  - A feedback (or forget) gate will clear the CEC.
  - An output gate will allow selective outputs from the CEC.
- Each gate will be a layer with inputs from the gated ouputs and the network inputs.
- The result is called Long Short Term Memory (LSTM).
- With the CEC, short term memories last longer.


Input
Constant Error Carousel
Output
Gating Layer
Input Gate
Feedback Gate
Output Gate
p1(t)
n1(t)
a1(t)
IW1,1
b1
1
a7(t)
D
LW1,7
LW5,1
LW5,2
LW5,3
LW5,5
n5(t)
a5(t)
LW6,5
n6(t)
a6(t)
LW7,6
LW7,4
n7(t)
a7(t)
IW2,1
n2(t)
a2(t)
LW2,7
IW3,1
n3(t)
a3(t)
LW3,7
IW4,1
n4(t)
a4(t)
LW4,7

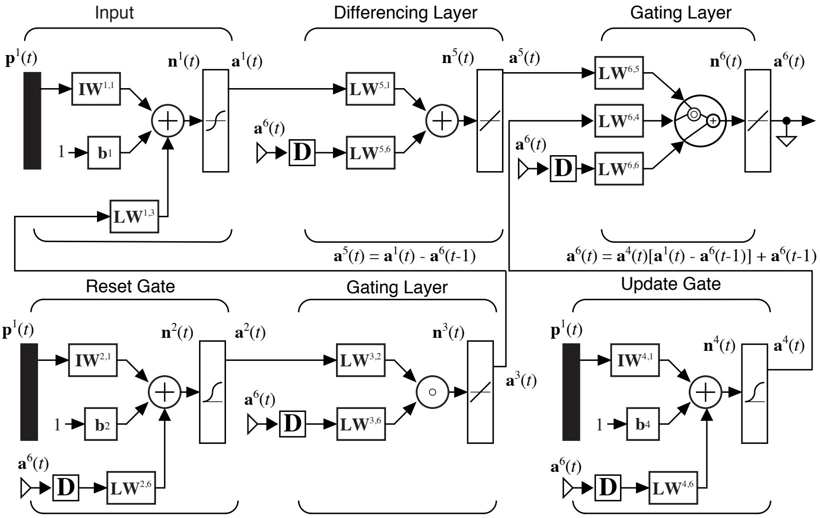
LSTM Details

- The $\circ$ operator is the Hadamard product, which is an element by element matrix multiplication.
- The weights in the CEC are all fixed to the identity matrix. They are not trained.
- The output and gating layer weights are also fixed to the identity matrix.
- It has been shown that the best results are obtained when initializing the feedback (forget) gate bias, $\mathbf{b}^3$, to all ones or larger values. This turns the gate on initially.
- Other weights and biases are set to small random numbers.
- The output of the gating layer generally connects to another layer or a multilayer network with softmax transfer function.
- Multiple LSTMs can be cascaded together.

- LSTM is trained with the standard gradient-based algorithms as with other deep networks.
- The original LSTM paper used RTRL for computing the gradient.
- An approximate gradient is used, in which the derivatives are only propagated in time through the CEC delays. Only static derivatives are computed for the remaining terms.

Variations of the LSTM

- There have been many variations of the LSTM
- In the original LSTM, there was no feedback (forget) gate.
- Some variations feeback the CEC output $\mathbf{a}^5(t)$ to the gate layers. These are called "peephole" connections.
- See `http://jmlr.org/proceedings/papers/v37/jozefowicz15.pdf` for an experimental comparison of various alternatives.
- One of the popular alternatives is the Gated Recurrent Unit (GRU), shown on the following page.


Input
Differencing Layer
Gating Layer
p1(t)
IW1,1
b1
1
n1(t)
a1(t)
LW1,3
LW5,1
a6(t)
D
LW5,6
n5(t)
a5(t)
a5(t) = a1(t) - a6(t-1)
LW6,5
LW6,4
a6(t)
D
LW6,6
n6(t)
a6(t)
a6(t) = a4(t)[a1(t) - a6(t-1)] + a6(t-1)
Reset Gate
Gating Layer
Update Gate
p1(t)
IW2,1
b2
1
n2(t)
a2(t)
a6(t)
D
LW2,6
LW3,2
a6(t)
D
LW3,6
n3(t)
a3(t)
p1(t)
IW4,1
b4
1
n4(t)
a4(t)
a6(t)
D
LW4,6

GRU Details

- The differencing layer subtracts the delayed network output $\mathbf{a}^6(t-1)$ from the processed input $\mathbf{a}^1(t)$.
- $\mathbf{LW}^{5,1} = \mathbf{I}$ and $\mathbf{LW}^{5,6} = -\mathbf{I}$. They are not trained.
- The gating layer weights are fixed to the identity matrix.
- The delayed network output is gated by the reset gate, before it is fed into the input layer. This resets the memory.
- The overall output can be considered a weighted average of a candidate potential output $\mathbf{a}^1(t)$ and the previous output $\mathbf{a}^6(t-1)$.

$$
\begin{aligned}
\mathbf{a}^6(t) &= \mathbf{a}^4(t) \times [\mathbf{a}^1(t) - \mathbf{a}^6(t-1)] + \mathbf{a}^6(t-1) \\
&= \mathbf{a}^4(t) \times \mathbf{a}^1(t) + [1 - \mathbf{a}^4(t)] \times \mathbf{a}^6(t-1)
\end{aligned}
$$