General Notation

Deep Learning

Importance of notation

- Neural network notation is widely divergent.
- It was developed in fits and starts over many years.
- New architectures are often developed by different disciplines.
- This makes it difficult to see connections between models.
- We will extend the notation of NND2, and use the same notation to represent all architectures.
- The notation is based on the concept of a layer.

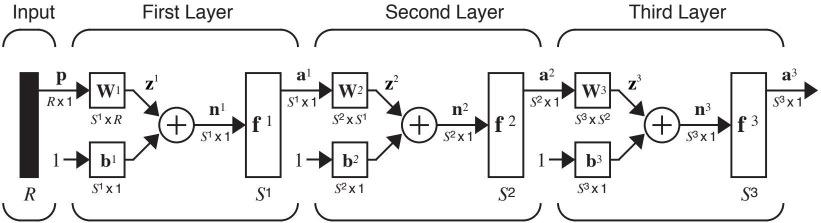
A layer consists of the following parts:

- A set of weight matrices, and associated weight functions, that come into that layer (which may connect from other layers or from external inputs),
- Any tapped delay lines that appear at the input of a weight matrix
- A bias vector,
- A net input function (e.g., a summing junction), and
- An activation function.

MLP Layer Equations

$$
\begin{aligned}
\mathbf{a}^0 &= \mathbf{p} \\
\mathbf{n}^{m+1} &= \mathbf{W}^{m+1}\mathbf{a}^m + \mathbf{b}^{m+1}, m = 0, 1, ..., M-1 \\
\mathbf{a}^m &= \mathbf{f}^m(\mathbf{n}^m)
\end{aligned}
$$

Three layer example



$\mathbf{a}^1 = \mathbf{f}^1(\mathbf{W}^1\mathbf{p}+\mathbf{b}^1)$ $\mathbf{a}^2 = \mathbf{f}^2(\mathbf{W}^2\mathbf{a}^1+\mathbf{b}^2)$ $\mathbf{a}^3 = \mathbf{f}^3(\mathbf{W}^3\mathbf{a}^2+\mathbf{b}^3)$

$$\mathbf{a}^3 = \mathbf{f}^3(\mathbf{W}^3\mathbf{f}^2(\mathbf{W}^2\mathbf{f}^1(\mathbf{W}^1\mathbf{p}+\mathbf{b}^1)+\mathbf{b}^2)+\mathbf{b}^3)$$

Layered Feedforward Neural Network (LFNN)

LFNN Layer Equations

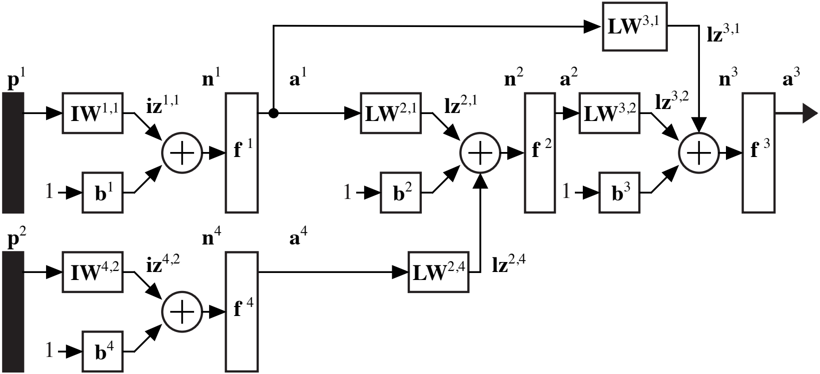
$$\mathbf{n}^m = \sum_{l \in I_m} \mathbf{IW}^{m,l}\mathbf{p}^l + \sum_{l \in L_f^m} \mathbf{LW}^{m,l}\mathbf{a}^l + \mathbf{b}^m$$

$$\mathbf{a}^m = \mathbf{f}^m((n)^m)$$

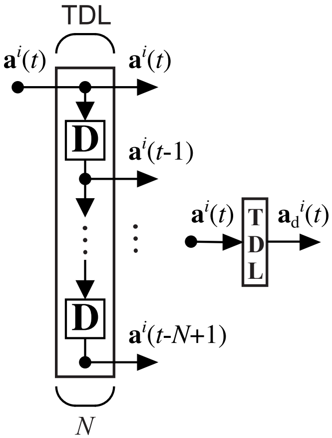
- $\mathbf{p}^l$ - lth input to the network
- $\mathbf{IW}^{m,l}$ - input weight between input l and layer m
- $\mathbf{LW}^{m,l}$ - layer weight between layer l and layer m
- I_m - indices of input vectors that connect to layer m
- L_m^f - layers connecting directly forward to layer m

Simulation Order

- For an MLP the output is computed starting at Layer 1 and proceeding in order to Layer M.
- For an LFNN, Layer 1 is not necessarily connected to Layer 2.
- No loops are allowed in an LFNN.
- We need to proceed in the proper layer order, so that the necessary inputs at each layer will be available.
- This ordering (which need not be unique) is called the Simulation Order.
- In the network on the next slide, one possible Simulation Order is 1-2-4-3.


LW3,1
lz3,1
p1
n1
a1
n2
a2
n3
a3
IW1,1
iz1,1
LW2,1
lz2,1
LW3,2
lz3,2
f 1
f 2
f 3
1
b1
1
b2
1
b3
p2
n4
a4
IW4,2
iz4,2
LW2,4
lz2,4
f 4
1
b4

- Feedforward networks have no memory
- Outputs are computed only from the current inputs
- To include memory we add tapped delay lines to the input of layers



Layered Digital Dynamic Network (LDDN)

$$\mathbf{n}^m(t) = \sum_{l \in L_m^f} \sum_{d \in DL_{m,l}} \mathbf{LW}^{m,l}(d)\mathbf{a}^l(t-d)$$

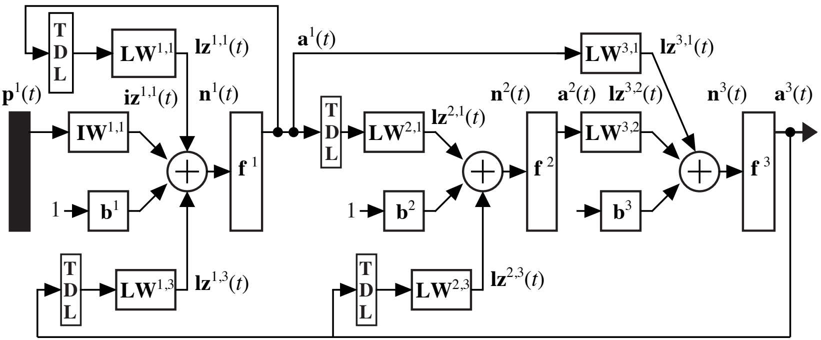
$$+ \sum_{l \in I_m} \sum_{d \in DI_{m,l}} \mathbf{IW}^{m,l}(d)\mathbf{p}^l(t-d) + \mathbf{b}^m$$

$$\mathbf{a}^m(t) = \mathbf{f}^m(\mathbf{n}^m(t))$$

- $\mathbf{p}^l(t)$ - lth input to the network at time t
- $\mathbf{IW}^{m,l}(d)$ - weight between input l and layer m at delay d
- $\mathbf{LW}^{m,l}(d)$ - weight between layer l and layer m at delay d
- $DL_{m,l}$ - delays between layers l and m
- $DI_{m,l}$ - delays between input l and layer m

LDDN properties

- An LDDN can have arbitrary connections between layers, but every feedback loop must contain at least one delay.
- Forward computations must be performed forward in time and forward in the simulation order for layers.
- LDDNs can have multiple input vectors and multiple output layers.



T D L
LW1,1
lz1,1(t)
a1(t)
LW3,1
lz3,1(t)
p1(t)
iz1,1(t)
n1(t)
n2(t)
a2(t)
lz3,2(t)
n3(t)
a3(t)
IW1,1
T D L
LW2,1
lz2,1(t)
LW3,2
f 1
f 2
f 3
1
b1
1
b2
b3
T D L
LW1,3
lz1,3(t)
T D L
LW2,3
lz2,3(t)

Generalized LDDN (GLDDN)

- For the LDDN (and LFNN) the weight function is a standard matrix multiplication (dot product) between the weight matrix and the input to the layer.
- The net input function for an LDDN (or an LFNN) is a sum of the weight function outputs and the bias.
- The GLDDN (and GLFNN) can have arbitrary weight functions and net input functions.
- Forward computations for a GLDDN are performed in the same order as those for an LDDN with the same structure.

Weight Functions

$$\mathbf{iz}^{m,l}(t,d) = \mathbf{ih}^{m,l}(\mathbf{IW}^{m,l}(d), \mathbf{p}^{l}(t-d))$$

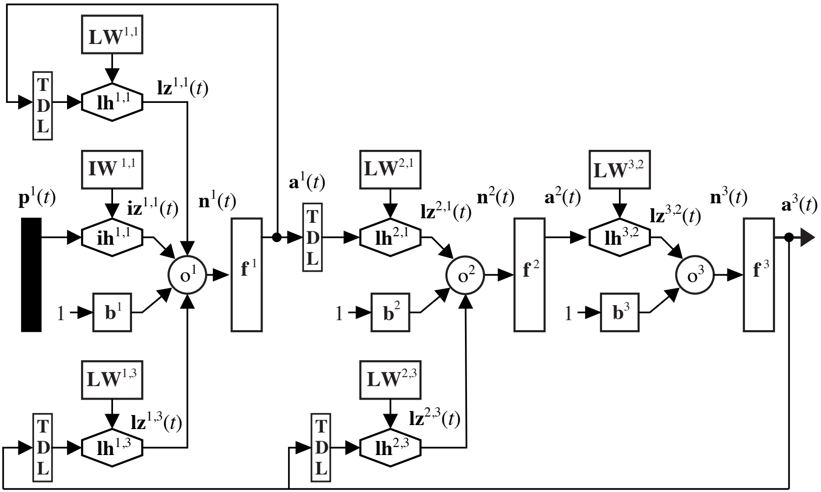
$$\mathbf{lz}^{m,l}(t,d) = \mathbf{lh}^{m,l}(\mathbf{LW}^{m,l}(d), \mathbf{a}^{l}(t-d))$$

Net Input Function

$$\mathbf{n}^{m}(t) = \mathbf{o}^{m}(\mathbf{iz}^{m,l}(t,d)|_{d\in DI_{m,l}}^{l\in I_m}, \mathbf{lz}^{m,l}(t,d)|_{d\in DL_{m,l}}^{l\in L_m^f}, \mathbf{b}^{m})$$

Transfer Function

$$\mathbf{a}^{m}(t) = \mathbf{f}^{m}(\mathbf{n}^{m}(t))$$


LW1,1
T
D
L
lh1,1
lz1,1(t)
IW 1,1
p1(t)
iz1,1(t)
ih1,1
n1(t)
a1(t)
o1
1
b1
f 1
LW1,3
lz1,3(t)
T
D
L
lh1,3
LW2,1
lz2,1(t)
n2(t)
T
D
L
lh2,1
o2
1
b2
f 2
LW2,3
lz2,3(t)
T
D
L
lh2,3
a2(t)
LW3,2
lz3,2(t)
n3(t)
lh3,2
o3
1
b3
f 3
a3(t)

Gradient Calculation for a GLFNN

- A generalized LFNN can have multiple input vectors and multiple output layers.
- Let U be the set of output layer indices. (Output layers will be compared to targets.)
- The gradient of the performance function with respect to a weight would be

$$\frac{\partial F(\mathbf{x})}{\partial iw_{i,j}^{m,l}} = \left(\frac{\partial F(\mathbf{x})}{\partial \mathbf{n}^m}\right)^T \frac{\partial \mathbf{n}^m}{\partial iw_{i,j}^{m,l}} = (\mathbf{s}^m)^T \frac{\partial \mathbf{n}^m}{\partial iw_{i,j}^{m,l}}$$

$$\mathbf{s}^m \triangleq \frac{\partial F(\mathbf{x})}{\partial \mathbf{n}^m}$$

Weight and bias derivatives

$$\frac{\partial \mathbf{n}^m}{\partial iw_{i,j}^{m,l}} = \frac{\partial \mathbf{n}^m}{\partial (\mathbf{iz}^{m,l})^T} \frac{\partial \mathbf{iz}^{m,l}}{\partial iw_{i,j}^{m,l}}$$

$$\frac{\partial \mathbf{n}^m}{\partial lw_{i,j}^{m,l}} = \frac{\partial \mathbf{n}^m}{\partial (\mathbf{lz}^{m,l})^T} \frac{\partial \mathbf{lz}^{m,l}}{\partial lw_{i,j}^{m,l}}$$

$$\frac{\partial \mathbf{n}^m}{\partial b_i^m} = \frac{\partial \mathbf{n}^m}{\partial b_i^m}$$

MLP case

The previous equations simplify for the standard MLP network.

$$
\begin{aligned}
\frac{\partial \mathbf{n}^m}{\partial (\mathbf{iz}^{m,l})^T} &= \mathbf{I}, &\qquad \frac{\partial \mathbf{n}^m}{\partial (\mathbf{lz}^{m,l})^T} &= \mathbf{I} \\
\frac{\partial \mathbf{iz}^{m,l}}{\partial iw_{i,j}^{m,l}} &= p_j^l \mathbf{e}_i, &\qquad \frac{\partial \mathbf{lz}^{m,l}}{\partial lw_{i,j}^{m,l}} &= a_j^l \mathbf{e}_i \\
\frac{\partial \mathbf{n}^m}{\partial b_i^m} &= \mathbf{e}_i
\end{aligned}
$$

Where $\mathbf{e}_i$ is a vector whose i^{th} element is 1, and the rest of the elements are zero.

Backpropagation for a GLFNN

The sensistivity $\mathbf{s}^m$ is computed by starting at all $\mathbf{s}^u$, $u \in U$. The performance function $F(\mathbf{x})$ will be an explicit function of these output layers.

$$\mathbf{s}^u = \frac{\partial F(\mathbf{x})}{\partial \mathbf{n}^u} = \left(\frac{\partial \mathbf{a}^u}{\partial \left(\mathbf{n}^u\right)^T} \right)^T \frac{\partial F(\mathbf{x})}{\partial \mathbf{a}^u} = \dot{\mathbf{F}}^u(\mathbf{n}^u)^T \frac{\partial F(\mathbf{x})}{\partial \mathbf{a}^u}$$

The remaining sensitivities $\mathbf{s}^m$ for $m \notin U$ are computed by following the backpropagation order (inverse of the simulation order), where L_m^b contains the indices of layers directly connected backward to layer m.

$$\mathbf{s}^m = \sum_{l \in L_m^b} \left(\frac{\partial \mathbf{a}^m}{\partial \left(\mathbf{n}^m\right)^T} \right)^T \left(\frac{\partial \mathbf{lz}^{l,m}}{\partial \left(\mathbf{a}^m\right)^T} \right)^T \left(\frac{\partial \mathbf{n}^l}{\partial \left(\mathbf{lz}^{m,l}\right)^T} \right)^T \mathbf{s}^l$$

The previous equations simplify for the standard MLP network.

$$\frac{\partial \mathbf{n}^{l}}{\partial(\mathbf{lz}^{l,m})^{T}} = \mathbf{I}$$

$$\frac{\partial \mathbf{lz}^{l,m}}{\partial(\mathbf{a}^{m})^{T}} = \mathbf{LW}^{l,m}$$

$$\frac{\partial \mathbf{a}^{m}}{\partial\left(\mathbf{n}^{m}\right)^{T}} = \dot{\mathbf{F}}^{m}(\mathbf{n}^{m})$$

$$\mathbf{s}^{m} = \dot{\mathbf{F}}^{m}(\mathbf{n}^{m})^{T}\left(\mathbf{LW}^{m+1,m}\right)^{T}\mathbf{s}^{m+1}$$

Summary GLFNN gradient calculations

$$\mathbf{s}^u = \dot{\mathbf{F}}^u(\mathbf{n}^u)^T \frac{\partial F(\mathbf{x})}{\partial \mathbf{a}^u}$$

$$\mathbf{s}^m = \sum_{l \in L_m^b} \dot{\mathbf{F}}^m(\mathbf{n}^m)^T \left(\frac{\partial \mathbf{lz}^{l,m}}{\partial \left(\mathbf{a}^m\right)^T} \right)^T \left(\frac{\partial \mathbf{n}^l}{\partial \left(\mathbf{lz}^{m,l}\right)^T} \right)^T \mathbf{s}^l$$

$$\frac{\partial F(\mathbf{x})}{\partial iw_{i,j}^{m,l}} = (\mathbf{s}^m)^T \frac{\partial \mathbf{n}^m}{\partial (\mathbf{iz}^{m,l})^T} \frac{\partial \mathbf{iz}^{m,l}}{\partial iw_{i,j}^{m,l}}$$

$$\frac{\partial F(\mathbf{x})}{\partial lw_{i,j}^{m,l}} = (\mathbf{s}^m)^T \frac{\partial \mathbf{n}^m}{\partial (\mathbf{lz}^{m,l})^T} \frac{\partial \mathbf{lz}^{m,l}}{\partial lw_{i,j}^{m,l}}$$

$$\frac{\partial F(\mathbf{x})}{\partial b_i^m} = (\mathbf{s}^m)^T \frac{\partial \mathbf{n}^m}{\partial b_i^m}$$

$$
\begin{aligned}
\mathbf{s}^u &= -2\dot{\mathbf{F}}^u(\mathbf{n}^u)^T\left(\mathbf{t}^u - \mathbf{a}^u\right) \\
\mathbf{s}^m &= \sum_{l \in L_m^b} \left(\dot{\mathbf{F}}^m(\mathbf{n}^m)\right)^T \left(\mathbf{LW}^{l,m}\right)^T \mathbf{s}^l \\
\frac{\partial F(\mathbf{x})}{\partial iw_{i,j}^{m,l}} &= \left(\mathbf{s}^m\right)^T p_j^l \mathbf{e}_i = s_i^m p_j^l \\
\frac{\partial F(\mathbf{x})}{\partial lw_{i,j}^{m,l}} &= \left(\mathbf{s}^m\right)^T a_j^l \mathbf{e}_i = s_i^m a_j^l \\
\frac{\partial F(\mathbf{x})}{\partial b_i^m} &= \left(\mathbf{s}^m\right)^T \mathbf{e}_i = s_i^m
\end{aligned}
$$

Key concept – modularity

- Network outputs are computed one layer at a time in the simulation order (modular).
- Layer: weight function $\rightarrow$ net input function $\rightarrow$ transfer function.
- Gradient of performance is computed one layer at a time in the backpropagation order (modular).
- To compute the gradient, for each layer, you need only
  - $\dot{\mathbf{F}}^m(\mathbf{n}^m)$ – derivative of transfer function
  - $\frac{\partial \mathbf{lz}^{l,m}}{\partial (\mathbf{a}^m)}$ – derivative of weight function w.r.t. layer input
  - $\frac{\partial \mathbf{lz}^{m,l}}{\partial lw^{m,l}_{i,j}}$ – derivative of weight function w.r.t. the weight
  - $\frac{\partial \mathbf{n}^m}{\partial (\mathbf{lz}^{m,l})^T}$ – derivative of net function w.r.t. weight output
  - $\frac{\partial \mathbf{n}^m}{\partial b^m_i}$ – derivative of net function w.r.t. bias