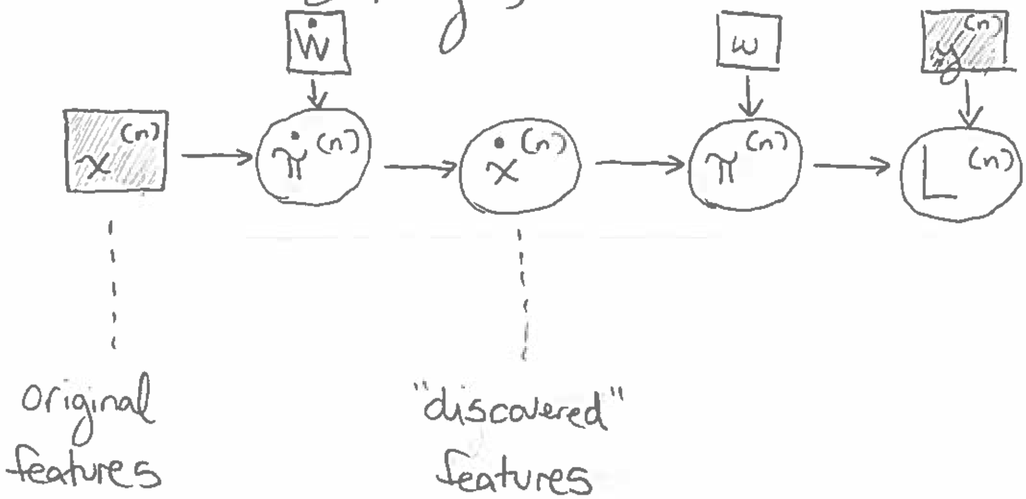
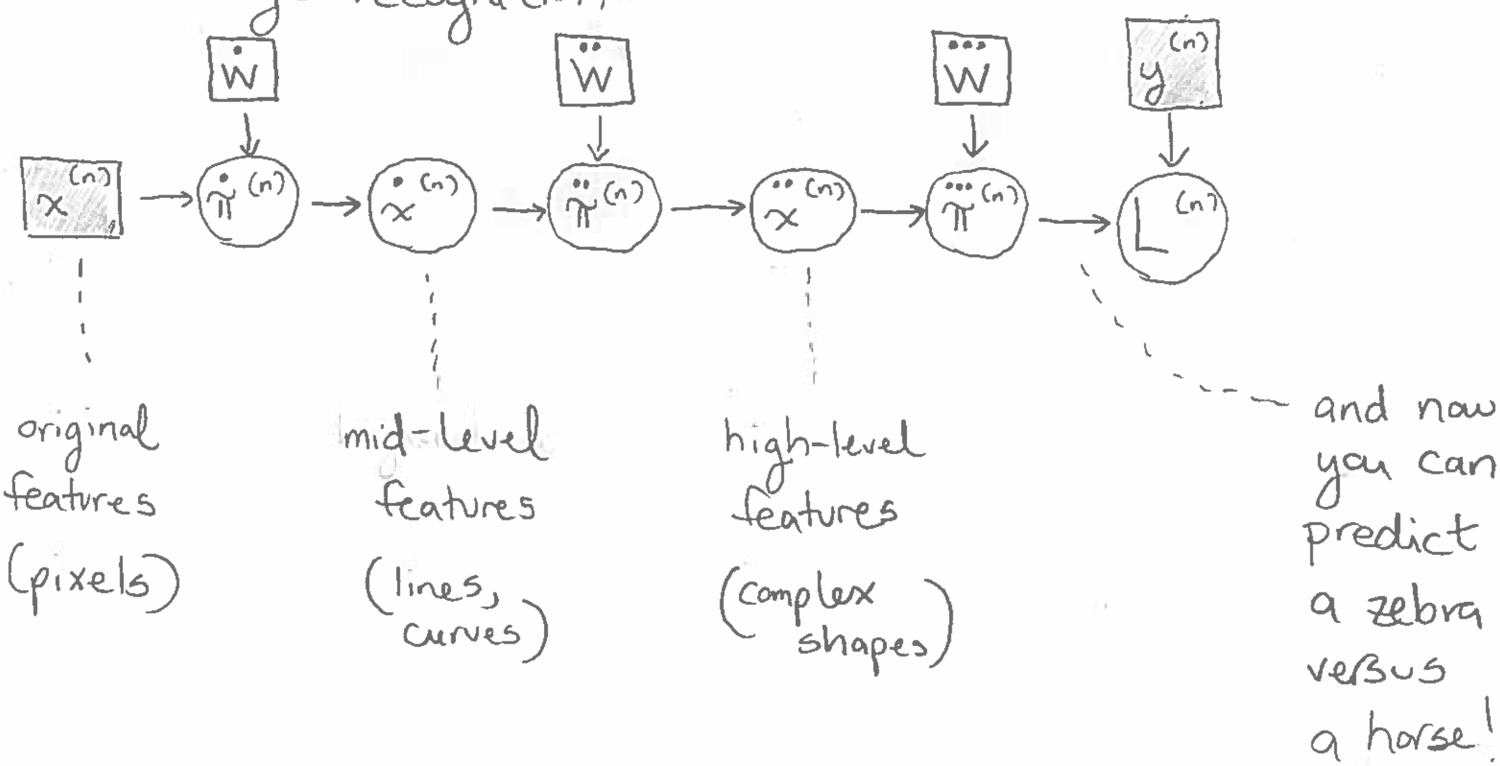
Neural Networks and Backpropagation

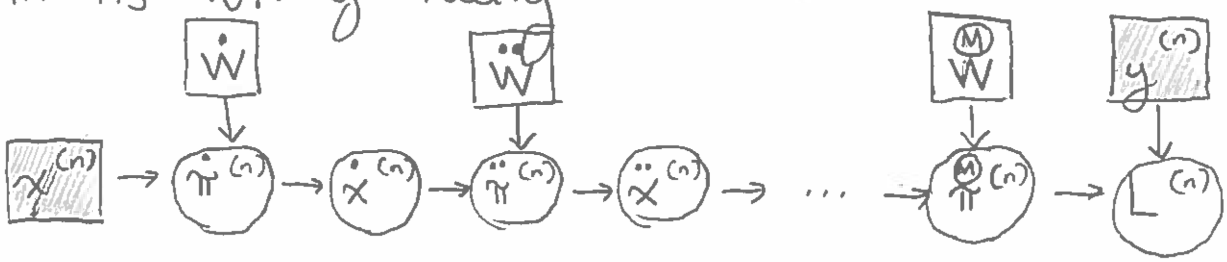
① Consider again our feature discovery network (now drawn horizontally!):



② We could consider generalizing this model to provide multiple layers of feature discovery, e.g. for image recognition:

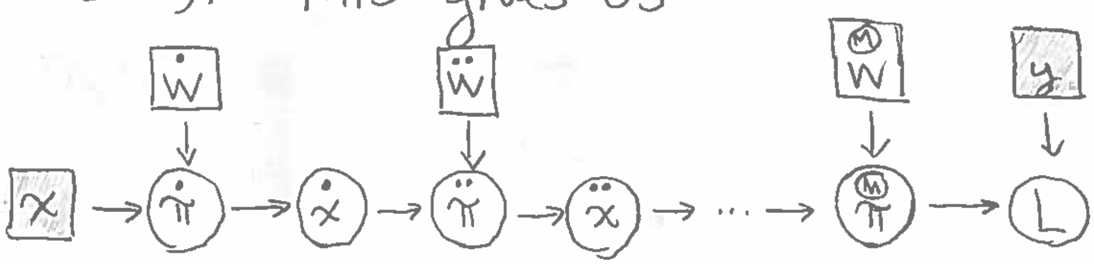


3. In its full generality:



this is called an <u>M-layer feedforward neural network</u>.

Let's drop all those (n) superscripts for convenience (we'll bring them back when needed to avoid confusion). This gives us:



Just in case we've forgotten which of these are vectors and which are matrices, here it is explicitly:

$$
\begin{tikzcd}
& \begin{bmatrix} \dot{w}_{11} & \cdots & \dot{w}_{1H} \\ & \ddots & \\ \dot{w}_{D1} & \cdots & \dot{w}_{DH}\end{bmatrix} \arrow[d] & & \begin{bmatrix}\ddot{w}_{11} & \cdots & \ddot{w}_{1H}\\ & \ddots & \vdots \\ \ddot{w}_{H1} & \cdots & \ddot{w}_{HH}\end{bmatrix} \arrow[d] & & & & \begin{bmatrix}\overset{M}{w}_{11}\\ \vdots \\ \overset{M}{w}_{H1}\end{bmatrix}\arrow[d] & y \arrow[d]\\
\begin{bmatrix}x_1\\ \vdots\\ x_D\end{bmatrix} \arrow[r] & \begin{bmatrix}\dot{\pi}_1\\ \vdots\\ \dot{\pi}_H\end{bmatrix} \arrow[r] & \begin{bmatrix}\dot{x}_1\\ \vdots \\ \dot{x}_H\end{bmatrix}\arrow[r] & \begin{bmatrix}\ddot{\pi}_1\\ \vdots\\ \ddot{\pi}_H\end{bmatrix}\arrow[r] & \begin{bmatrix}\ddot{x}_1\\ \vdots\\ \ddot{x}_H\end{bmatrix}\arrow[r] & \cdots \arrow[r] & \begin{bmatrix}\overset{M-1}{x}_1\\ \vdots\\ \overset{M-1}{x}_H\end{bmatrix}\arrow[r] & \overset{M}{\pi} \arrow[r] & L
\end{tikzcd}
$$

We assume each "feature discovery" layer discovers H features.

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(4) To train this model using gradient descent, we need to be able to compute $\dfrac{\partial L}{\partial \overset{(m)}{w}_{ij}}$ for each weight $\overset{(m)}{w}_{ij}$.

Before doing this in its full generality, let's see how we can compute these derivatives for a 3-layer network where $H=2$ and $D=3$.

$$
\begin{tikzcd}
 & \begin{bmatrix} \dot{w}_{11} & \dot{w}_{12} \\ \dot{w}_{21} & \dot{w}_{22} \\ \dot{w}_{31} & \dot{w}_{32} \end{bmatrix} \arrow[d] & & \begin{bmatrix} \ddot{w}_{11} & \ddot{w}_{12} \\ \ddot{w}_{21} & \ddot{w}_{22} \end{bmatrix} \arrow[d] & & \begin{bmatrix} \dddot{w}_{11} \\ \dddot{w}_{21} \end{bmatrix} \arrow[d] & y \arrow[d] \\
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \arrow[r] & \begin{bmatrix} \dot{\pi}_1 \\ \dot{\pi}_2 \end{bmatrix} \arrow[r] & \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} \arrow[r] & \begin{bmatrix} \ddot{\pi}_1 \\ \ddot{\pi}_2 \end{bmatrix} \arrow[r] & \begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{bmatrix} \arrow[r] & \dddot{\pi} \arrow[r] & L
\end{tikzcd}
$$

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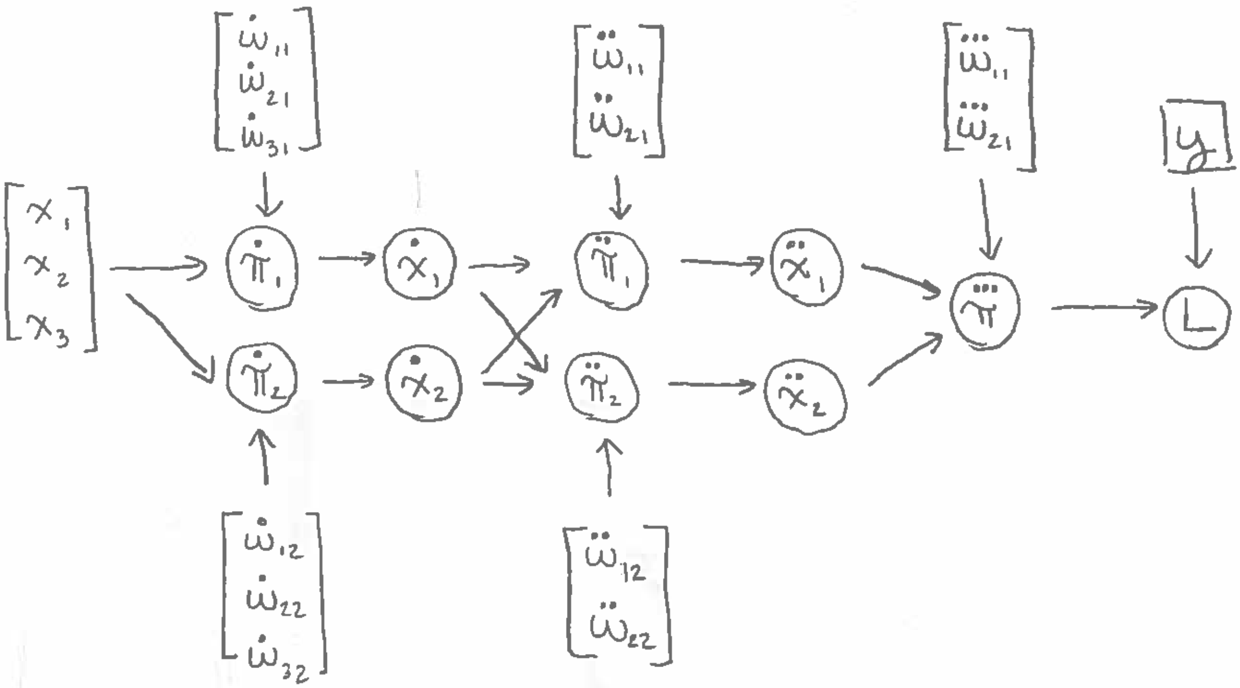
(5) As we did before for the feature discovery network, let's break down the endogenous variables into scalars to make it easier to apply the Chain Rule of Partial Derivatives:



(6) Our goal is to compute (for all relevant i, j):

$$\frac{\partial L}{\partial \dot{\omega}_{ij}} \quad \text{and} \quad \frac{\partial L}{\partial \ddot{\omega}_{ij}} \quad \text{and} \quad \frac{\partial L}{\partial \dddot{\omega}_{ij}}$$

First, we can observe that $\dddot{\pi}$ separates L from all $\overset{(m)}{\omega}_{ij}$, so:

$$\frac{\partial L}{\partial \overset{(m)}{\omega}_{ij}} = \underbrace{\frac{\partial L}{\partial \dddot{\pi}}} \cdot \frac{\partial \dddot{\pi}}{\partial \overset{(m)}{\omega}_{ij}}$$

This is the just the standard derivative of the loss function.

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7) So the challenge is to compute $\dfrac{\partial \dddot{\pi}}{\partial \overset{(m)}{\omega}_{ij}}$ for any layer m.

It's straightforward for $m=3$:

$$\frac{\partial \dddot{\pi}}{\partial \dddot{\omega}_{ij}} = \frac{\partial}{\partial \dddot{\omega}_{ij}}\left(\begin{bmatrix} \dddot{\omega}_{11} \\ \dddot{\omega}_{21}\end{bmatrix}^T \begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{bmatrix}\right) = \ddot{x}_i$$

8) What about $m=2$?

$$\frac{\partial \dddot{\pi}}{\partial \ddot{\omega}_{ij}} = \frac{\partial \dddot{\pi}}{\partial \ddot{\pi}_j} \cdot \frac{\partial \ddot{\pi}_j}{\partial \ddot{\omega}_{ij}}$$

[$\ddot{\pi}_j$ separates $\dddot{\pi}$ from $\ddot{\omega}_{ij}$, so Chain Rule applies]

$$= \frac{\partial \dddot{\pi}}{\partial \ddot{\pi}_j} \cdot \dot{x}_i$$

$$\left[\frac{\partial \ddot{\pi}_j}{\partial \ddot{\omega}_{ij}} = \dot{x}_i \right]$$

9) What about $m=1$?

$$\frac{\partial \dddot{\pi}}{\partial \dot{\omega}_{ij}} = \frac{\partial \dddot{\pi}}{\partial \dot{\pi}_j} \frac{\partial \dot{\pi}_j}{\partial \dot{\omega}_{ij}}$$

[$\dot{\pi}_j$ separates $\dddot{\pi}$ from $\dot{\omega}_{ij}$, so Chain Rule applies]

$$= \frac{\partial \dddot{\pi}}{\partial \dot{\pi}_j} \cdot x_i$$

$$\left[\frac{\partial \dot{\pi}_j}{\partial \dot{\omega}_{ij}} = x_i \right]$$

(10) In summary:

$$\frac{\partial \dddot{\pi}}{\partial \dddot{\omega}_{ij}} = \ddot{x}_i$$

$$\frac{\partial \dddot{\pi}}{\partial \ddot{\omega}_{ij}} = \dot{x}_i \frac{\partial \dddot{\pi}}{\partial \ddot{\pi}_j}$$

$$\frac{\partial \dddot{\pi}}{\partial \dot{\omega}_{ij}} = x_i \frac{\partial \dddot{\pi}}{\partial \dot{\pi}_j}$$

for the general case:

$$\frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m)}{\omega}_{ij}} = \overset{(m-1)}{x}_i \cdot \underbrace{\frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m)}{\pi}_j}}$$

so how do we compute this term?

(11) Consider $\frac{\partial \dddot{\pi}}{\partial \dot{\pi}_j}$ for our 3-layer network.

$$\frac{\partial \dddot{\pi}}{\partial \dot{\pi}_j} = \frac{\partial \dddot{\pi}}{\partial \dot{x}_j} \frac{\partial \dot{x}_j}{\partial \dot{\pi}_j}$$

[$\dot{x}_j$ separates $\dddot{\pi}$ from $\dot{\pi}_j$, so Chain Rule applies]

$$= \left(\sum_{h=1}^{2} \frac{\partial \dddot{\pi}}{\partial \ddot{\pi}_h} \frac{\partial \ddot{\pi}_h}{\partial \dot{x}_j} \right) \frac{\partial \dot{x}_j}{\partial \dot{\pi}_j}$$

[$\{\ddot{\pi}_1, \ddot{\pi}_2\}$ separates $\dddot{\pi}$ from $\dot{x}_j$, so Chain Rule applies]

$$= \frac{\partial \dot{x}_j}{\partial \dot{\pi}_j} \sum_{h=1}^{2} \frac{\partial \ddot{\pi}_h}{\partial \dot{x}_j} \frac{\partial \dddot{\pi}}{\partial \ddot{\pi}_h}$$

$$= a'(\dot{\pi}_j) \sum_{h=1}^{2} \ddot{\omega}_{hj} \underbrace{\frac{\partial \dddot{\pi}}{\partial \ddot{\pi}_h}}$$

but this can be computed recursively in the same way!

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(12) In summary (for our 3-layer example):

$$\frac{\partial \dddot{\pi}}{\partial \dot{\pi}_j} = a'(\dot{\pi}_j) \sum_{h=1}^{2} \ddot{\omega}_{hj} \frac{\partial \dddot{\pi}}{\partial \ddot{\pi}_h}$$

and for the general case:

$$\frac{\partial \overset{(M)}{\pi}}{\partial \overset{(M)}{\pi}} = 1 \qquad \leftarrow \text{ base case}$$

$$\frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m)}{\pi}_j} = a'(\overset{(m)}{\pi}_j) \sum_{h=1}^{H} \overset{(m+1)}{\omega}_{hj} \frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m+1)}{\pi}_h} \qquad \leftarrow \text{ recursive step}$$

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(13) Putting it all together, we have cobbled together a strategy for computing every partial derivative $\frac{\partial L}{\partial \overset{(m)}{\omega}_{ij}}$:

BACKPROPAGATION:

(a) for m in $\{M-1, \ldots, 1\}$ and j in $\{1, \ldots, H\}$:

compute $\frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m)}{\pi}_j} = a'(\overset{(m)}{\pi}_j) \sum_{h=1}^{H} \overset{(m+1)}{\omega}_{hj} \frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m+1)}{\pi}_h}$

computed in an earlier iteration, since we loop backwards from $M-1$

(b) $$\frac{\partial L}{\partial \overset{(m)}{\omega}_{ij}} = \underbrace{\frac{\partial L}{\partial \overset{(M)}{\pi}}}_{\text{just a simple derivative of the loss function}} \cdot \overset{(m-1)}{x}_i \cdot \underbrace{\frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m)}{\pi}_j}}_{\text{computed during (a)}}$$

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(14) Because we compute the partial derivatives $\frac{\partial \pi^{(M)}}{\partial \pi^{(m)}}$ starting from the final layer M and moving backwards, this algorithm is known as <u>backpropagation</u>.