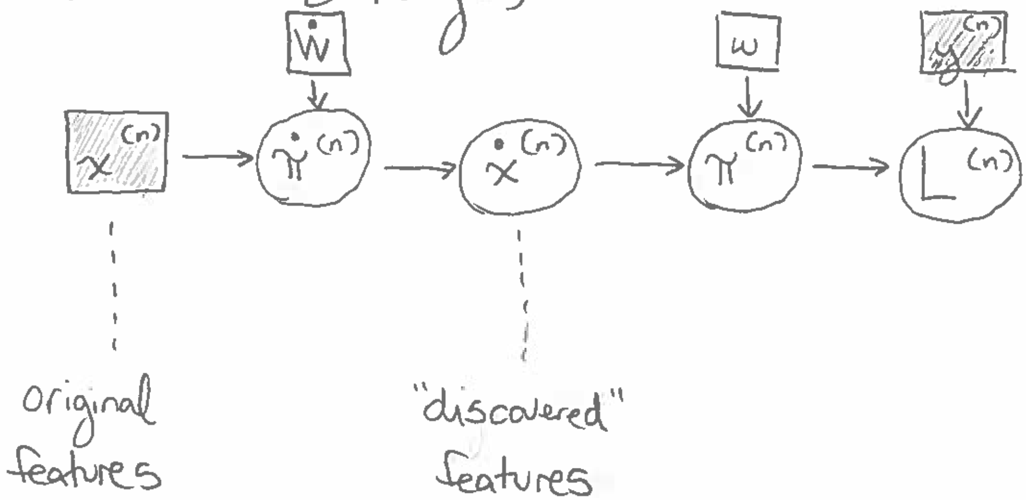
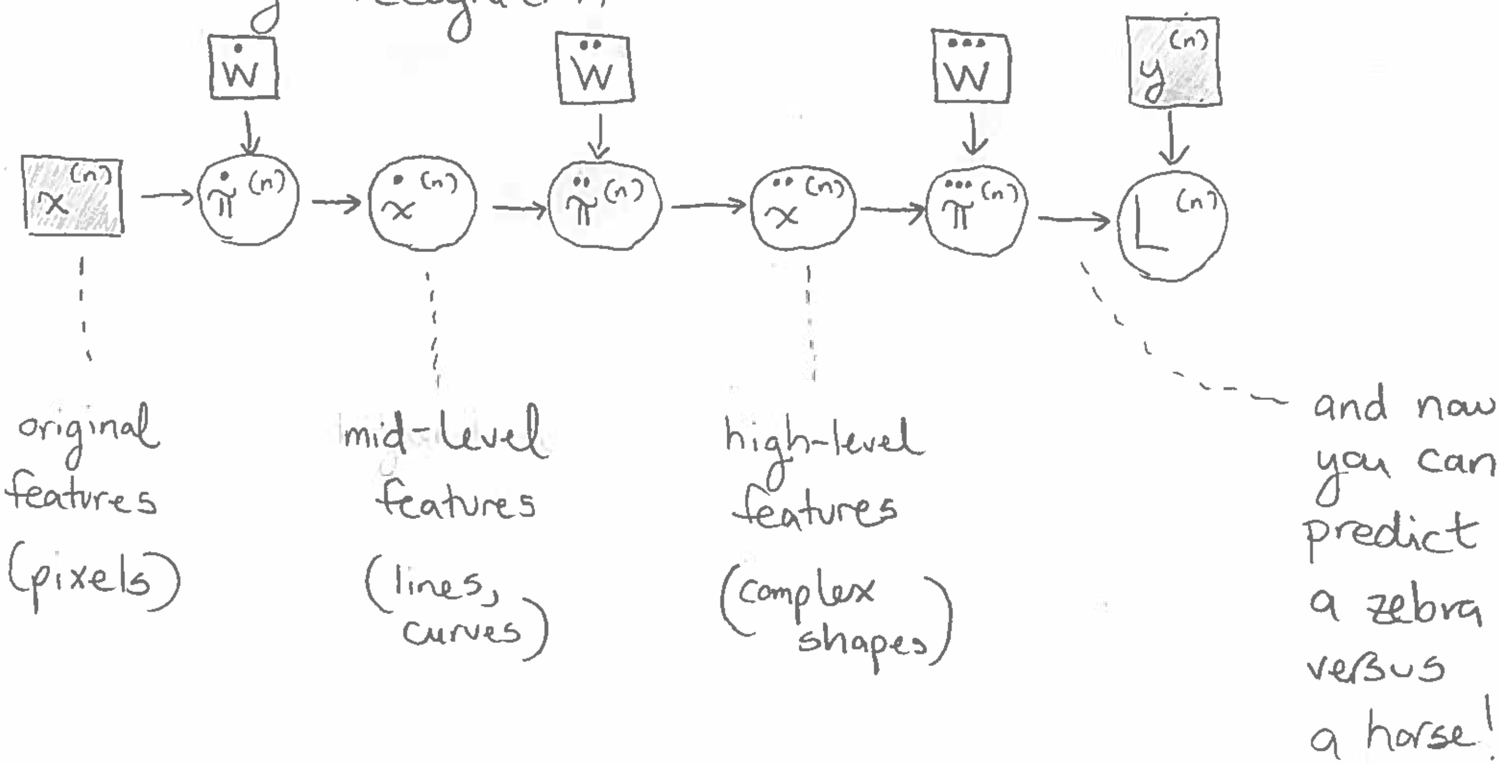
NEURAL NETWORKS AND BACKPROPAGATION

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:



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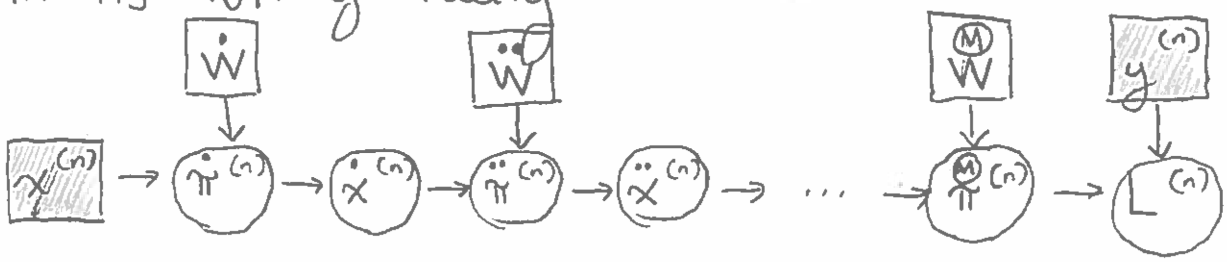
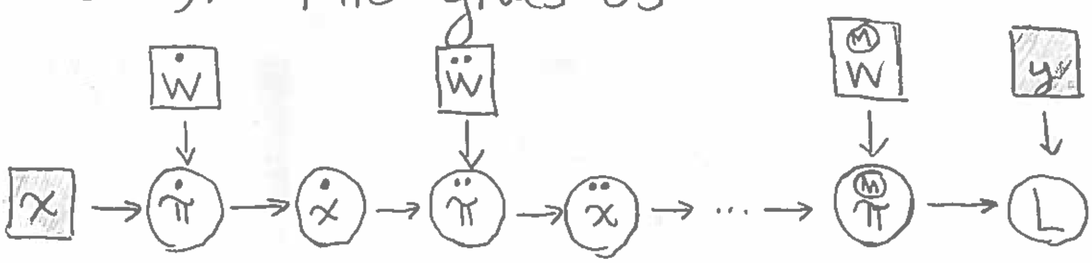
3) In its full generality:

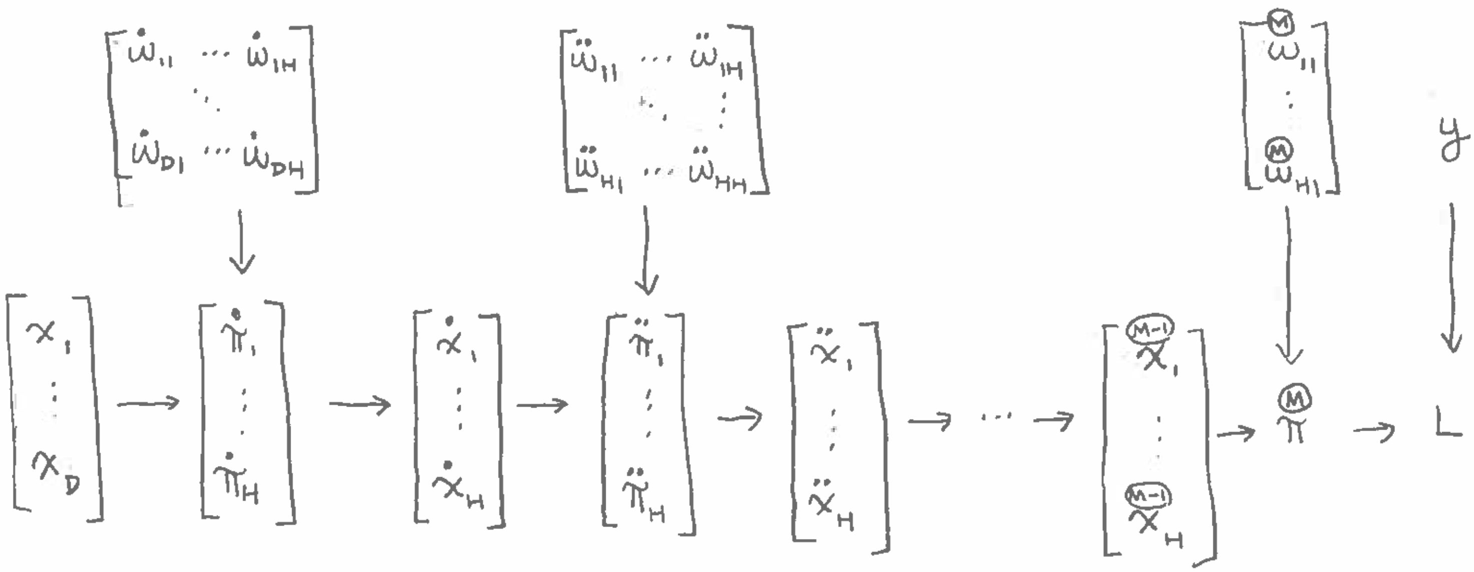


this is called an <u>M-layer feedforward neural network</u>.

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:



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

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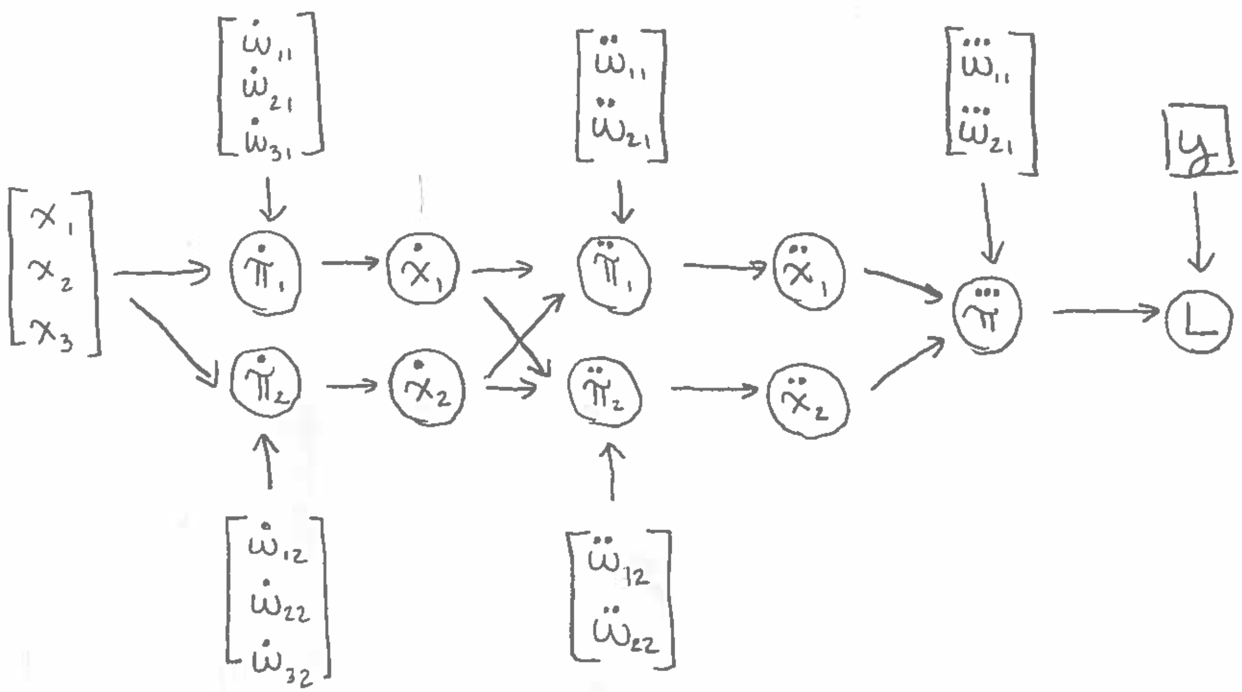
④ To train this model using gradient descent, we need to be able to compute $\dfrac{\partial L}{\partial \overset{(m)}{w}_{ij}}$ for each weight $\overset{(m)}{w}_{ij}$.

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 $D=3$.

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

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):

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

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

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

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:

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

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

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

For the general case:

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

so how do we compute this term?

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(11) Consider $\dfrac{\partial \dddot{\pi}}{\partial \dot{\pi}_j}$ 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]

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

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

but this can be computed recursively in the same way!

(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:

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

$$\frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m)}{\pi}_j} = \boxed{} \quad \leftarrow \text{recursive step}$$

(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 range($\boxed{}$) and j in range($\boxed{}$):

compute $\frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m)}{\pi}_j} = \boxed{}$

(b) $\frac{\partial L}{\partial \overset{(m)}{\omega}_{ij}} = \boxed{} \cdot \frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m)}{\pi}_j}$

Because we compute the partial derivatives $\frac{\partial \overset{(M)}{\pi}}{\partial \overset{(m)}{\pi}_j}$ starting from the final layer M and moving back, we call it backpropagation.