Error backpropagation

Lecture 12

goal: compute 1st & 2nd derivatives of $E(\vec{w})$ [wrt $\vec{w}$] efficiently.

Consider a general NN with arbitrary feed-forward topology, arbitrary activation f's and a general error f'n:

$$E(\vec{w}) = \sum_{n=1}^{N} E_n(\vec{w})$$

Consider first a linear model:

$$\begin{cases} y_k = \sum_i w_{ki} x_i, \\ E_n = \frac{1}{2} \sum_k (y_{nk} - t_{nk})^2 \end{cases}$$

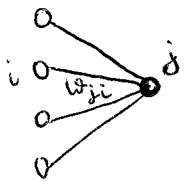
$$y_k(\vec{x}_n, \vec{w})$$

Then $$\frac{\partial E_n}{\partial w_{ji}} = \sum_k (y_{nk} - t_{nk}) \underbrace{\frac{\partial y_{nk}}{\partial w_{ji}}}_{\delta_{kj} x_{ni}} =$$

$$= \underbrace{(y_{nj} - t_{nj})}_{\text{"error signal"}} \underbrace{x_{ni}}_{\text{"input"}}$$

More generally,

$$a_j = \sum_i w_{ji} \underbrace{z_i}_{\text{activation of unit } i \text{ connected to unit } j}$$



Then $z_j = h(a_j)$

↑ activation of unit j

Now consider $\frac{\partial E_n}{\partial w_{ji}} = \underbrace{\frac{\partial E_n}{\partial a_j}}_{\equiv \delta_j} \underbrace{\frac{\partial a_j}{\partial w_{ji}}}_{= z_i} \equiv$ (no sum!)

$\equiv \delta_j z_i$.

($z_i = 1$ if we are dealing with bias)

If j is an output unit,

$$\delta_j = \frac{\partial E_n}{\partial a_j} = \underbrace{y_j - t_j}_{n \text{ index omitted for simplicity}}$$ for regression OR classification

Indeed, for regression

$y_k = a_k$ (unit activation function)

$$\hookrightarrow \frac{\partial E}{\partial a_k} = y_k - t_k .$$

For $K=2$ classification,

$$\frac{\partial E_n}{\partial a_j} = -\left[\frac{t_j}{y_j} \underbrace{\frac{\partial y_j}{\partial a_j}}_{\nearrow y_j(1-y_j)} + (1-t_j)(-1)\frac{1}{1-y_j}\frac{\partial y_j}{\partial a_j} \right] \equiv$$

$y_j = \sigma(a_j)$, sigmoid

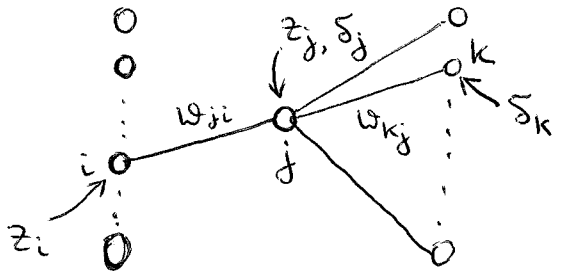
$$\equiv -\left[t_j(1-y_j) - (1-t_j)y_j \right] = y_j - t_j .$$

Same for $K=2$ classif's and $K>2$ classif'n.

If j is a hidden unit,

$$\delta_j = \frac{\partial E_n}{\partial a_j} = \sum_k \frac{\partial E_n}{\partial a_k}\frac{\partial a_k}{\partial a_j} \Diamond$$

$\uparrow$ over all "future" units, hidden or output, to which j is connected



$$\Diamond \sum_k \delta_k \frac{\partial}{\partial a_j}\left(\sum_i w_{ki} h(a_i)\right) = \sum_{k,i} \delta_k w_{ki} \underbrace{\frac{\partial h(a_i)}{\partial a_j}}_{h'(a_j)\delta_{ij}} =$$

$$= h'(a_j) \sum_k w_{kj}\delta_k. \qquad (*)$$

We can use $(*)$ by starting from output units (for which δ_j is easily computed) and computing δ_j's for hidden units in a <u>backpropagation pass</u>.

Finally, use $\frac{\partial E_n}{\partial w_{ji}} = \delta_j z_i$ to compute all gradients.

If needed, finish with

$$\frac{\partial E}{\partial w_{ji}} = \sum_n \frac{\partial E_n}{\partial w_{ji}}.$$

The above derivation can be easily generalized to several types of activation functions $h(\cdot)$.

Ex. Consider a two-layer network as before, and focus on regression:

output units $\Rightarrow y_k = a_k$

hidden units $\Rightarrow h(a_k) = \tanh(a_k)$

Note that $\frac{d\tanh(a)}{da} = 1 - \tanh^2(a)$

For pattern n, $E_n = \frac{1}{2}\sum_{k=1}^{K} (y_k - t_k)^2$ (K ← # output units)

Forward pass:

$$\begin{cases} a_j = \sum_{i=0}^{D} w_{ji}^{(1)} x_i & (D \leftarrow \text{\# input units};\ x_i \uparrow \text{inputs}) \\ z_j = \tanh(a_j) & \\ y_k = \sum_{j=0}^{M} w_{kj}^{(2)} z_j & (M \leftarrow \text{\# hidden units}) \end{cases}$$

Next, compute $\delta_k = y_k - t_k$

Use (*) to find

$$\delta_j = (1 - z_j^2) \sum_{k=1}^{K} w_{kj}\, \delta_k \quad \text{for hidden units}$$

Finally, compute

$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \delta_j x_i \quad , \quad \frac{\partial E_n}{\partial w_{kj}^{(2)}} = \delta_k z_j$$

and sum over n.

Note that backpropagation is $O(W)$, where W is the total # weights & biases. Most effort goes into evaluating

$$a_j = \sum_i w_{ji} z_i$$

Forward propagation (computing E_n) is $O(W)$ as well. Note that finite difference:

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{E_n(w_{ji} + \xi) - E_n(w_{ji} - \xi)}{2\xi} + O(\xi^2)$$

is $O(W^2)$ since each E_n computation is $O(W)$ & one needs W of those. However, it can be used for checks. (numerical)

Jacobian matrix

$J_{ki} = \frac{\partial y_k}{\partial x_i}$ local sensitivity of outputs to changes in inputs

$$\Delta y_k \simeq \sum_i \underbrace{\frac{\partial y_k}{\partial x_i}}_{J_{ki}} \underbrace{\Delta x_i}_{\text{small input perturbations}} \qquad \left|\frac{\Delta x_i}{x_i}\right| \ll 1$$

J_{ki} can be evaluated using backpropagation:

$$J_{ki} = \frac{\partial y_k}{\partial x_i} = \sum_j \frac{\partial y_k}{\partial a_j} \underbrace{\frac{\partial a_j}{\partial x_i}}_{w_{ji}} \qquad (*)$$

j: over all "future" units j connected to unit i

Further, $\frac{\partial y_k}{\partial a_j} = \sum_\ell \frac{\partial y_k}{\partial a_\ell} \frac{\partial a_\ell}{\partial a_j}$ (=)

ℓ: over all "future" units ℓ connected to unit j

$$(=) \sum_\ell \frac{\partial y_k}{\partial a_\ell} \frac{\partial}{\partial a_j} \sum_i w_{\ell i} \underbrace{h(a_i)}_{z_i} =$$

$$= \sum_{\ell,i} \frac{\partial y_k}{\partial a_\ell} w_{\ell i} h'(a_i) \delta_{ij} = h'(a_j) \sum_\ell w_{\ell j} \frac{\partial y_k}{\partial a_\ell} .$$

Start from output units, e.g. with sigmoid activation functions:

$$\frac{\partial y_k}{\partial a_j} = \sigma'(a_k) \underbrace{\frac{\partial a_k}{\partial a_j}}_{\delta_{kj}} = \sigma(a_j)(1-\sigma(a_j))\,\delta_{kj}.$$

Algorithm:

1. Choose $\vec{x}_n$ and forward-propagate
2. For each k, start with output units and backpropagate $\Rightarrow$ find $\frac{\partial y_k}{\partial a_j}$, $\forall j$
3. Find J_{ki} using (*)

Can be checked against finite difference:

$$\frac{\partial y_k}{\partial x_i} = \frac{y_k(x_i+\xi) - y_k(x_i-\xi)}{2\xi} + O(\xi^2)$$

needs $2D$ forward propagations (D = # inputs)

Hessian matrix

$$H_{ij} = \frac{\partial^2 E}{\partial w_i \partial w_j}$$

$i, j = 1, \ldots, W$ ← total # weights & biases

all weights / biases relabeled using one consecutive index.

(1) H_{ij} used in some non-linear optimization algorithms

(2) H_{ij} is used in Bayesian neural networks

Exact evaluation:

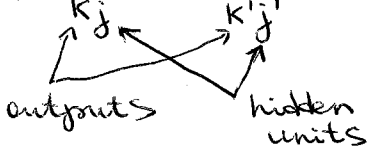
Consider a two-layer network for simplicity.

Define $\delta_k = \underbrace{\frac{\partial E_n}{\partial a_k}}_{\text{as before}}$, $M_{kk'} = \frac{\partial^2 E_n}{\partial a_k \partial a_{k'}}$

here, k & k' can be hidden or output nodes (hidden)

(a) Both weights in the second layer:

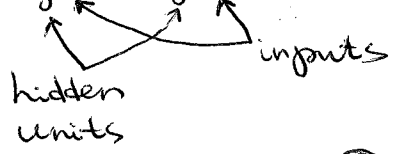
$$\frac{\partial^2 E_n}{\partial w^{(2)}_{kj} \partial w^{(2)}_{k'j'}} = \frac{\partial^2 E_n}{\partial a_k \partial a_{k'}} \frac{\partial a_k}{\partial w^{(2)}_{kj}} \frac{\partial a_{k'}}{\partial w^{(2)}_{k'j'}} =$$



$$= M_{kk'} z_j z_{j'}.$$

(b) Both weights in the first (input) layer:

$$\frac{\partial^2 E_n}{\partial w^{(1)}_{ji} \partial w^{(1)}_{j'i'}} = \frac{\partial^2 E_n}{\partial a_j \partial a_{j'}} \underbrace{\frac{\partial a_j}{\partial w^{(1)}_{ji}}}_{x_i} \underbrace{\frac{\partial a_{j'}}{\partial w^{(1)}_{j'i'}}}_{x_{i'}} \equiv$$



$$\equiv M_{jj'} x_i x_{i'}.$$

(c) One weight in each layer:

$$\frac{\partial^2 E_n}{\partial w^{(1)}_{ji} \partial w^{(2)}_{kj'}} = \frac{\partial}{\partial w^{(1)}_{ji}} \left[\frac{\partial E_n}{\partial a_k} \underbrace{\frac{\partial a_k}{\partial w^{(2)}_{kj'}}}_{z_{j'}} \right] =$$

$$= \underbrace{\frac{\partial^2 E_n}{\partial a_j \partial a_k}}_{M_{jk} = M_{kj}} x_i z_{j'} + \underbrace{\frac{\partial E_n}{\partial a_k}}_{\delta_k} \frac{\partial z_{j'}}{\partial w^{(1)}_{ji}} \equiv$$

$$\equiv M_{jk} x_i z_{j'} + \delta_k h'(a_j) \delta_{jj'} x_i.$$

Thus, we need to backpropagate $M_{kk'}$.

Indeed, $\frac{\partial E_n}{\partial a_j} = \sum_k \frac{\partial E_n}{\partial a_k} \underbrace{\frac{\partial a_k}{\partial a_j}}$ $\quad a_k = \sum_\ell w_{k\ell} h(a_\ell)$

$= h'(a_j) \sum_k \frac{\partial E_n}{\partial a_k} w_{kj}$.

k: hidden / downstream of & connected to j

$\sum_\ell w_{k\ell} h'(a_\ell) \underbrace{\frac{\partial a_\ell}{\partial a_j}}_{\delta_{\ell j}} =$

$= w_{kj} h'(a_j)$.

Now, $\frac{\partial^2 E_n}{\partial a_i \partial a_j} = h''(a_i) \delta_{ij} \sum_k \frac{\partial E_n}{\partial a_k} w_{kj} +$

i: hidden

$+ h'(a_j) \sum_{k,k'} \frac{\partial^2 E_n}{\partial a_k \partial a_{k'}} w_{kj} \underbrace{\frac{\partial a_{k'}}{\partial a_i}}$ $\quad a_{k'} = \sum_\ell w_{k'\ell} h(a_\ell)$ (=)

k: downstream of j; k': downstream of i

$\sum_\ell h'(a_\ell) \delta_{\ell i} w_{k'\ell} =$

$= h'(a_i) w_{k'i}$

(=) $h''(a_i) \delta_{ij} \sum_k \underbrace{\frac{\partial E_n}{\partial a_k}}_{\delta_k} w_{kj} + h'(a_i) h'(a_j) \sum_{k,k'} \underbrace{\frac{\partial^2 E_n}{\partial a_k \partial a_{k'}}}_{M_{kk'}} w_{kj} w_{k'i}$ $\quad (**)$

Compute M_{ij} recursively starting from output nodes. For ex., for regression we get:

output nodes $\begin{cases} \frac{\partial E_n}{\partial a_j} = \frac{\partial E_n}{\partial y_j} = y_j - t_j, \\ \frac{\partial^2 E_n}{\partial a_i \partial a_j} = \delta_{ij}. \end{cases}$

$a_i = y_i$ here

Then we can compute M_{ij} for hidden nodes using (**).

Finally, in the "mixed" case:

$$\frac{\partial}{\partial a_i}\frac{\partial E_n}{\partial y_j} = \frac{\partial}{\partial a_i}(y_j - t_j) = \sum_k \frac{\partial (y_j - t_j)}{\partial a_k}\frac{\partial a_k}{\partial a_i} \quad (=)$$

(j: output, i: hidden; k: output; $\frac{\partial a_k}{\partial a_i} = w_{ki}\, h'(a_i)$)

$$(=) \sum_k \delta_{jk}\, w_{ki}\, h'(a_i) = h'(a_i)\, w_{ji}.$$

Thus we can compute all M_{ij} & therefore all H_{ij}. This is an $O(W^2)$ computation.

This can be checked against finite differences:

$$\frac{\partial^2 E}{\partial w_{ji}\,\partial w_{lk}} = \frac{1}{4\varepsilon^2}\Big[E(w_{ji}+\varepsilon, w_{lk}+\varepsilon) - E(w_{ji}+\varepsilon, w_{lk}-\varepsilon) - E(w_{ji}-\varepsilon, w_{lk}+\varepsilon) + E(w_{ji}-\varepsilon, w_{lk}-\varepsilon)\Big] + O(\varepsilon^2)$$

↑ 4 forward propagations with $O(W)$ operations each × W^2 Hessian elements (⇒)

(⇒) $O(W^3)$ computation.

However, we can use a mixed approach:

$$\frac{\partial^2 E}{\partial w_{ji}\,\partial w_{lk}} = \frac{1}{2\varepsilon}\left[\left.\frac{\partial E}{\partial w_{ji}}\right|_{w_{lk}+\varepsilon} - \left.\frac{\partial E}{\partial w_{ji}}\right|_{w_{lk}-\varepsilon}\right] + O(\varepsilon^2)$$

compute using backpropagation in $O(W)$ steps × W weights to perturbed $(w_{lk} \pm \varepsilon)$: $O(W^2)$ computation just as with explicit backpropagation above.