

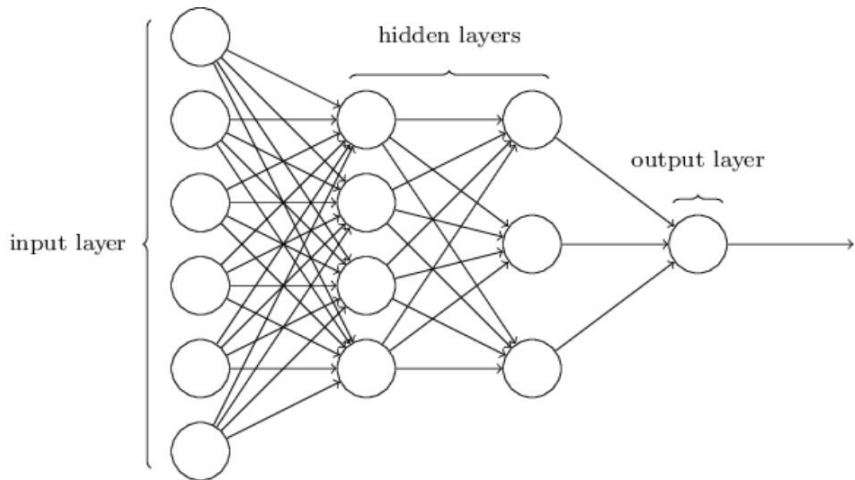
Lecture 20: 28 March, 2023

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Data Mining and Machine Learning
January–April 2023

- Acyclic network of perceptrons with non-linear activation functions

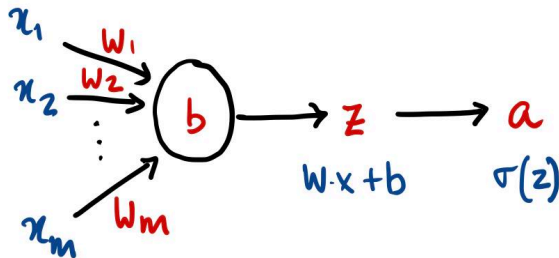


Neural networks

- Without loss of generality,
 - Assume the network is layered
 - All paths from input to output have the same length
 - Each layer is fully connected to the previous one
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 - Assume the network is layered
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- Structure of an individual neuron
 - Input weights w_1, \dots, w_m , bias b , output z , activation value a

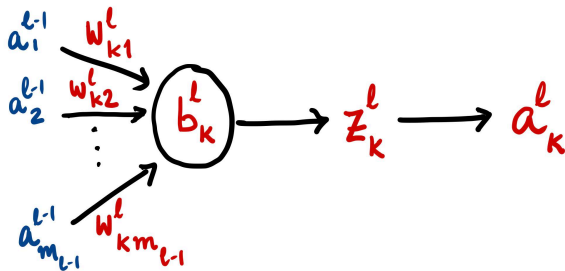
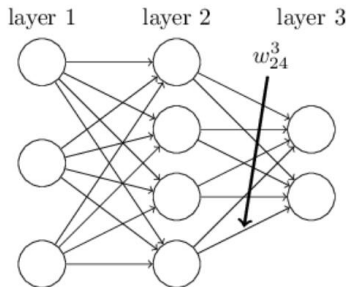


Notation

- Layers $\ell \in \{1, 2, \dots, L\}$
 - Inputs are connected first hidden layer, layer 1
 - Layer L is the output layer
- Layer ℓ has m_ℓ nodes $1, 2, \dots, m_\ell$

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- Layer l has m_l nodes $1, 2, \dots, m_l$
- Node k in layer l has bias b_k^l , output z_k^l and activation value a_k^l
- Weight on edge from node j in level $l-1$ to node k in level l is w_{kj}^l



- Why the inversion of indices in the subscript w_{kj}^l ?

- $z_k^l = w_{k1}^l a_1^{l-1} + w_{k2}^l a_2^{l-1} + \dots + w_{km_{l-1}}^l a_{m_{l-1}}^{l-1}$

- Let $\bar{w}_k^l = (w_{k1}^l, w_{k2}^l, \dots, w_{km_{l-1}}^l)$
and $\bar{a}^{l-1} = (a_1^{l-1}, a_2^{l-1}, \dots, a_{m_{l-1}}^{l-1})$

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- Assume all layers have same number of nodes

- Let $m = \max_{\ell \in \{1, 2, \dots, L\}} m_\ell$

- For any layer i , for $k > m_i$, we set all of $w_{kj}^l, b_k^l, z_k^l, a_k^l$ to 0

- Matrix formulation

$$\begin{bmatrix} \bar{z}_1^l \\ \bar{z}_2^l \\ \dots \\ \bar{z}_m^l \end{bmatrix} = \begin{bmatrix} \bar{w}_1^l \\ \bar{w}_2^l \\ \dots \\ \bar{w}_m^l \end{bmatrix} \begin{bmatrix} a_1^{l-1} \\ a_2^{l-1} \\ \dots \\ a_m^{l-1} \end{bmatrix}$$

Learning the parameters

- Need to find optimum values for all weights w_{kj}^l
- Use gradient descent
 - Cost function C , partial derivatives $\frac{\partial C}{\partial w_{kj}^l}$, $\frac{\partial C}{\partial b_k^l}$

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 - 1 For input \mathbf{x} , $C(\mathbf{x})$ is a function of only the output layer activation, a^L
 - For instance, for training input (\mathbf{x}_i, y_i) , sum-squared error is $(y_i - a_i^L)^2$
 - Note that \mathbf{x}_i, y_i are fixed values, only a_i^L is a variable

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- 2 Total cost is average of individual input costs

- Each input \mathbf{x}_i incurs cost $C(\mathbf{x}_i)$, total cost is $\frac{1}{n} \sum_{i=1}^n C(\mathbf{x}_i)$
- For instance, mean sum-squared error $\frac{1}{n} \sum_{i=1}^n (y_i - a_i^L)^2$

Learning the parameters

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- With these assumptions:

- We can write $\frac{\partial C}{\partial w_{kj}^l}$, $\frac{\partial C}{\partial b_k^l}$ in terms of individual $\frac{\partial a_i^l}{\partial w_{kj}^l}$, $\frac{\partial a_i^l}{\partial b_k^l}$
- Can extrapolate change in individual cost $C(\mathbf{x})$ to change in overall cost C — **stochastic gradient descent**

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- Can extrapolate change in individual cost $C(x)$ to change in overall cost C — **stochastic gradient descent**

- Complex dependency of C on w_{kj}^l , b_k^l

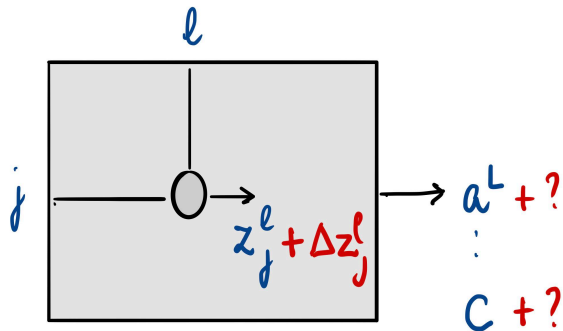
- Many intermediate layers
- Many paths through these layers

- Use **chain rule** to decompose into local dependencies

- $y = g(f(x)) \Rightarrow \frac{\partial g}{\partial x} = \frac{\partial g}{\partial f} \frac{\partial f}{\partial x}$

Calculating dependencies

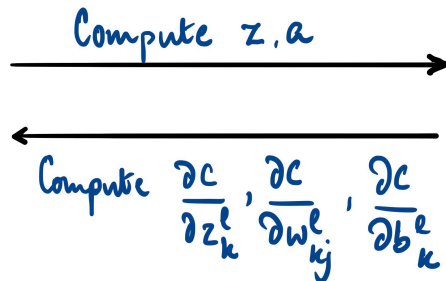
- If we perturb the output z_j^l at node j in layer l , what is the impact on final output, overall cost?



- Focus on $\frac{\partial C}{\partial z_j^l}$ — from these, we can compute $\frac{\partial C}{\partial w_{jk}^l}$, $\frac{\partial C}{\partial b_j^l}$

Computing partial derivatives

- Use chain rule to run **backpropagation algorithm**
 - Given an input, execute the network from left to right to compute all outputs
 - Using the chain rule, work backwards from right to left to compute all values of $\frac{\partial C}{\partial z_j^l}$



Applying the chain rule

Let δ_j^ℓ denote $\frac{\partial C}{\partial z_j^\ell}$

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Layers 1, 2, ..., L

Base Case

$\ell = L, \delta_j^L$

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■ For instance, if $C = \frac{1}{n} \sum_{i=1}^n (y_i - a_i^L)^2$, then $\frac{\partial C}{\partial a_j^L} = 2(y_j - a_j^L)(-1) = \underline{\underline{2(a_j^L - y_j)}}$

Handwritten notes:
- A green circle highlights $\frac{\partial C}{\partial a_j^L}$ in the chain rule equation.
- A green arrow points from the circled term to the corresponding term in the derivative calculation.
- A green arrow points from (-1) to $(a_j^L - y_j)$.
- The final result $2(a_j^L - y_j)$ is underlined twice.
- The text "jth term" is written below the summation index $i=1$.

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■ $a_j^L = \sigma(z_j^L)$, so $\frac{\partial a_j^L}{\partial z_j^L} = \sigma'(z_j^L)$

■ $\sigma(u) = \frac{1}{1 + e^{-u}}, \sigma'(u) = \frac{\partial \sigma(u)}{\partial u} = \sigma(u)(1 - \sigma(u))$ **Work this out!**

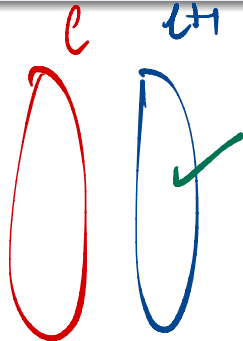
value

Applying the chain rule

Induction step

From $\delta_j^{\ell+1}$ to δ_j^ℓ

$$\frac{\partial C}{\partial z_j^\ell}$$

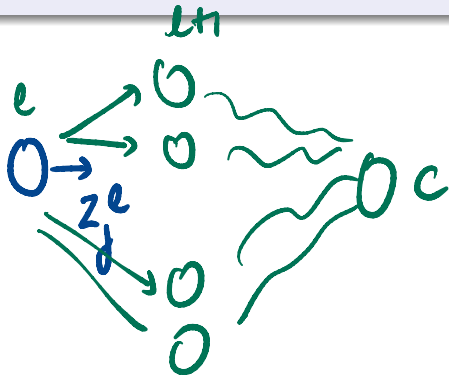


Applying the chain rule

Induction step

From $\delta_j^{\ell+1}$ to δ_j^ℓ

$$\delta_j^\ell = \frac{\partial C}{\partial z_j^\ell} = \sum_{k=1}^m \frac{\partial C}{\partial z_k^{\ell+1}} \frac{\partial z_k^{\ell+1}}{\partial z_j^\ell}$$



Applying the chain rule

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Applying the chain rule

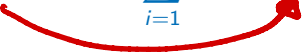
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- Second term:
$$z_k^{\ell+1} = \sum_{i=1}^m w_{ki}^{\ell+1} a_i^\ell + b_k^{\ell+1} = \sum_{i=1}^m w_{ki}^{\ell+1} \sigma(z_i^\ell) + b_k^{\ell+1}$$



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 - For $i = j$, $\frac{\partial}{\partial z_j^\ell} [w_{kj}^{\ell+1} \sigma(z_j^\ell) + b_k^{\ell+1}] = w_{kj}^{\ell+1} \sigma'(z_j^\ell)$

$C \cdot \sigma(z)$

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- So $\frac{\partial z_k^{\ell+1}}{\partial z_j^\ell} = w_{kj}^{\ell+1} \sigma'(z_j^\ell)$

Finishing touches

What we actually need to compute are $\frac{\partial C}{\partial w_{kj}^\ell}$, $\frac{\partial C}{\partial b_k^\ell}$

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- $\frac{\partial z_k^l}{\partial b_k^l} = 1$ — terms with $i \neq j$ vanish

Backpropagation

- In the forward pass, compute all z_k^l, a_k^l
- In the backward pass, compute all δ_k^l , from which we can get all $\frac{\partial C}{\partial w_{kj}^l}, \frac{\partial C}{\partial b_k^l}$
- Increment each parameter by a step Δ in the direction opposite the gradient

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Typically, partition the training data into groups (**mini batches**)

- Update parameters after each mini batch — stochastic gradient descent
- **Epoch** — one pass through the entire training data

- Backpropagation dates from mid-1980's

Learning representations by back-propagating errors

David E. Rumelhart, Geoffrey E. Hinton and Ronald J. Williams

Nature, **323**, 533–536 (1986)

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Challenges

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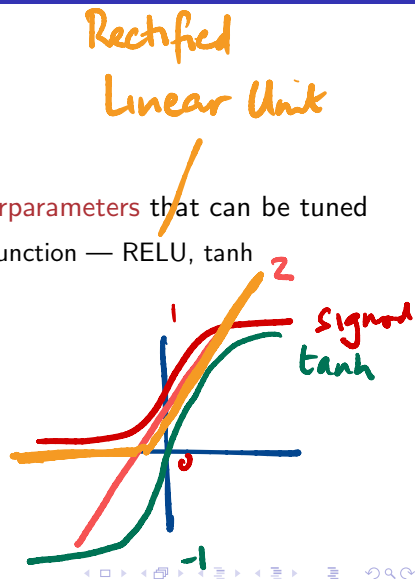
"Deep" learning
- depth of NN

- Computationally infeasible till advent of modern parallel hardware, GPUs for vector (tensor) calculations
- **Vanishing gradient problem** — cascading derivatives make gradients in initial layers very small, convergence is slow
 - In rare cases, **exploding gradient** also occurs

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 - Training: Mini-batch size, number of epochs
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$$\max(0, z)$$



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- Loss functions
 - As we have seen MSE is not a good choice
 - Cross entropy is better — corresponds to finding MLE