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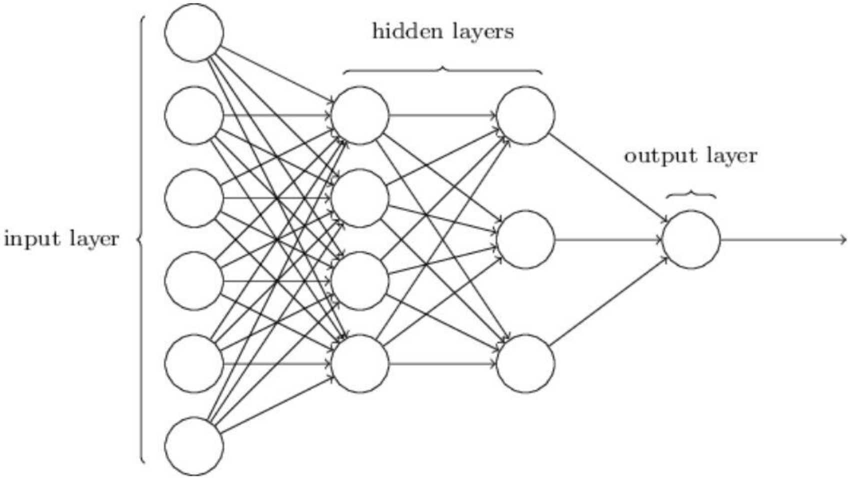
Data Mining and Machine Learning
January–April 2024

Neural networks

- 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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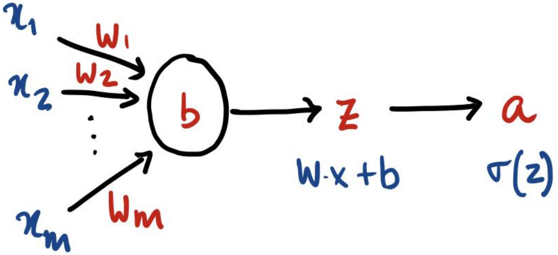
- Structure of an individual neuron
  - Input weights $w_1, \ldots, w_m$, bias b, output z, activation value a



Notation

- Layers $\ell \in \{1, 2, \ldots, L\}$
  - Inputs are connected first hidden layer, layer 1
  - Layer L is the output layer
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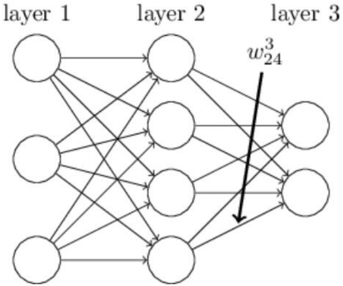
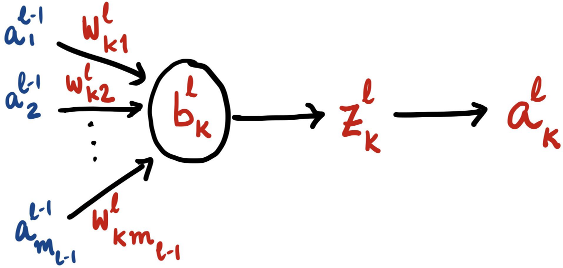
- Layer ℓ has m_ℓ nodes $1, 2, \ldots, m_\ell$
- Node k in layer ℓ has bias b_k^ℓ, output z_k^ℓ and activation value a_k^ℓ
- Weight on edge from node j in level $\ell-1$ to node k in level ℓ is w_{kj}^ℓ





Notation

- Why the inversion of indices in the subscript w^ℓ_{kj}?
  - $z^\ell_k = w^\ell_{k1} a^{\ell-1}_1 + w^\ell_{k2} a^{\ell-1}_2 + \cdots + w^\ell_{km_{\ell-1}} a^{\ell-1}_{m_{\ell-1}}$
  - Let $\overline{w}^\ell_k = (w^\ell_{k1}, w^\ell_{k2}, \ldots, w^\ell_{km_{\ell-1}})$
    and $\overline{a}^{\ell-1} = (a^{\ell-1}_1, a^{\ell-1}_2, \ldots, a^{\ell-1}_{m_{\ell-1}})$
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  - Then $z^{\ell}_k = \overline{w}^{\ell}_k \cdot \overline{a}^{\ell-1}$
- Assume all layers have same number of nodes
  - Let $m = \max_{\ell \in \{1.2,\ldots,L\}} m_\ell$
  - For any layer i, for $k > m_i$, we set all of $w^{\ell}_{kj}, b^{\ell}_k, z^{\ell}_k, a^{\ell}_k$ to 0
- Matrix formulation

$$\begin{bmatrix} \overline{z}^{\ell}_1 \\ \overline{z}^{\ell}_2 \\ \cdots \\ \overline{z}^{\ell}_m \end{bmatrix} = \begin{bmatrix} \overline{w}^{\ell}_1 \\ \overline{w}^{\ell}_2 \\ \cdots \\ \overline{w}^{\ell}_m \end{bmatrix} \begin{bmatrix} a^{\ell-1}_1 \\ a^{\ell-1}_2 \\ \cdots \\ a^{\ell-1}_m \end{bmatrix}$$

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

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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 $(y_i - a^L_i)^2$
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  2. Total cost is average of individual input costs
     - Each input $\boldsymbol{x}_i$ incurs cost $C(\boldsymbol{x}_i)$, total cost is $\dfrac{1}{n}\sum_{i=1}^{n} C(\boldsymbol{x}_i)$
     - For instance, mean sum-squared error $\dfrac{1}{n}\sum_{i=1}^{n}(y_i - a_i^L)^2$

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- With these assumptions:
  - We can write $\frac{\partial C}{\partial w_{kj}^{\ell}}$, $\frac{\partial C}{\partial b_k^{\ell}}$ in terms of individual $\frac{\partial a_i^L}{\partial w_{kj}^{\ell}}$, $\frac{\partial a_i^L}{\partial b_k^{\ell}}$
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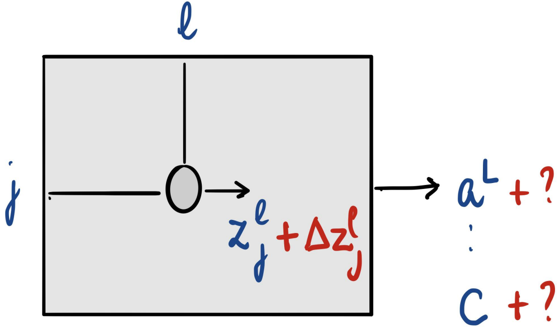
  - Can extrapolate change in individual cost $C(x)$ to change in overall cost C — stochastic gradient descent
- Complex dependency of C on w^{ℓ}_{kj}, b^{ℓ}_{k}
  - Many intermediate layers
  - Many paths through these layers
- Use chain rule to decompose into local dependencies
  - $y = g(f(x)) \Rightarrow \frac{\partial g}{\partial x} = \frac{\partial g}{\partial f}\frac{\partial f}{\partial x}$

Calculating dependencies

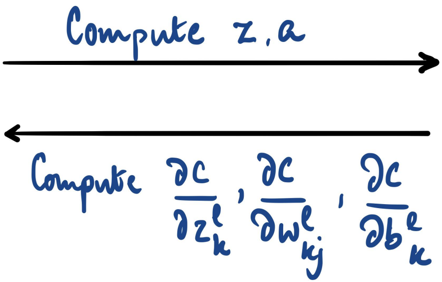
- If we perturb the output z_j^ℓ at node j in layer ℓ, what is the impact on final output, overall cost?



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

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



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- $a_j^L = \sigma(z_j^L)$, so $\dfrac{\partial a_j^L}{\partial z_j^L} = \sigma'(z_j^L)$
  - $\sigma(u) = \dfrac{1}{1+e^{-u}}$, $\sigma'(u) = \dfrac{\partial \sigma(u)}{\partial u} = \sigma(u)(1-\sigma(u))$ Work this out!

Applying the chain rule

Induction step

From $\delta_j^{\ell+1}$ to δ_j^{ℓ}

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

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

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  - $\dfrac{\partial z_k^{\ell}}{\partial w_{kj}^{\ell}} = a_j^{\ell-1}$ — terms with $i \neq j$ vanish
  - $\dfrac{\partial z_k^{\ell}}{\partial b_k^{\ell}} = 1$ — 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 $\dfrac{\partial C}{\partial w_{kj}^\ell}$, $\dfrac{\partial C}{\partial b_k^\ell}$
- 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

Challenges

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