Neural Network

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Neural Network — idea

If our linear model is underfitting training data, what should we do?

- Approach (1) – feature engineering:
  $\mathbf{x} \longrightarrow$ hand-crafted $\Phi \rightarrow \mathbf{z} \rightarrow$ linear model $\rightarrow y$
- Approach (2) – Neural Network:
  $\mathbf{x} \longrightarrow$ learned $\Phi \rightarrow \mathbf{z} \rightarrow$ linear model $\rightarrow y$

Q: Which approach requires less human brain work?

A: (2)

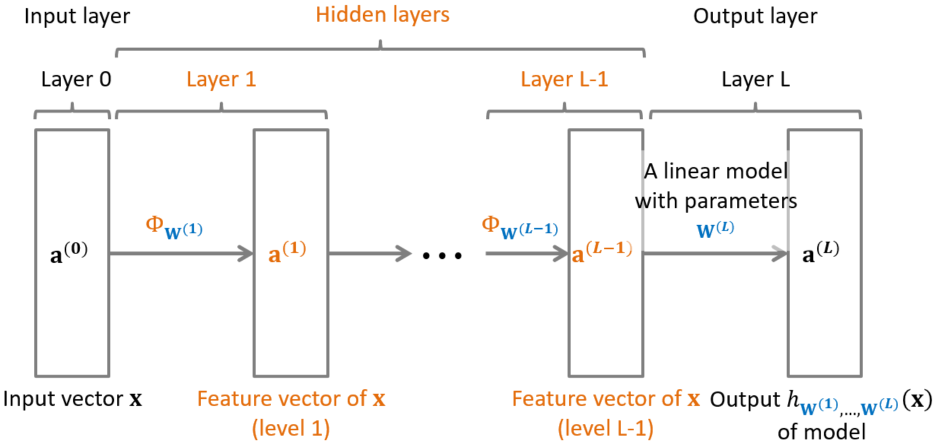
Q: Which approach produces $\mathbf{z}$ less interpretable?

A: (2)

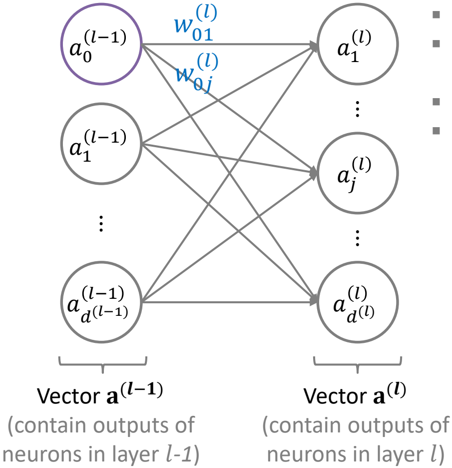
Q: Which approach requires more training data?

A: (2)

Neural Network — model form


Input layer
Hidden layers
Output layer
Layer 0
Layer 1
Layer L-1
Layer L
$\mathbf{a}^{(0)}$
$\Phi_{\mathbf{W}^{(1)}}$
$\mathbf{a}^{(1)}$
$\Phi_{\mathbf{W}^{(L-1)}}$
$\mathbf{a}^{(L-1)}$
A linear model with parameters $\mathbf{W}^{(L)}$
$\mathbf{a}^{(L)}$
Input vector $\mathbf{x}$
Feature vector of $\mathbf{x}$ (level 1)
Feature vector of $\mathbf{x}$ (level L-1)
Output $h_{\mathbf{W}^{(1)},\dots,\mathbf{W}^{(L)}}(\mathbf{x})$ of model

How is $a^{(l)}$ computed from $a^{(l-1)}$?



- Each node is a neuron
- Value inside a node is the output of this neuron
- Each edge is a weight (parameter)
- **The output of a neuron is computed as follows**: (1) compute the weighted sum of neurons' outputs in the previous layer, (2) pass the result through a nonlinear function – called activation function (e.g. logistic)
  - $w_{ij}^{(l)}$: the weight corresponding to the edge from neuron i in layer $l-1$ to neuron j in layer l
    $(1 \leq l \leq L,\ 0 \leq i \leq d^{(l-1)},\ 1 \leq j \leq d^{(l)})$
  - $a_j^{(l)} = \theta\left(s_j^{(l)}\right)$ with $s_j^{(l)} = \sum_{i=0}^{d^{(l-1)}} w_{ij}^{(l)} a_i^{(l-1)}$ and θ is some activation function

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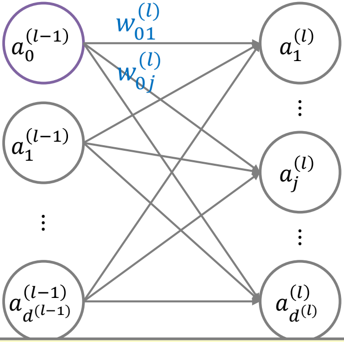

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Common activation functions:

- Logistic: $\theta(s) = \frac{1}{1+e^{-s}} \in [0, 1]$
- Tanh: $\theta(s) = 2\text{logistic}(2s) - 1 \in [-1, 1]$
- Relu: $\theta(s) = \max(0, s) \in [0, \infty)$
- ...

Q: Does layer L (last layer) need neuron 0 (whose output value is always 1)?

A: No

hidden layers, # neurons / hidden layer, and activation function are hyper-parameters (we must choose them before training)

Q: If we $\uparrow$ # hidden layers as well as # neurons / hidden layer, training error $\uparrow$/$\downarrow$?
A: $\downarrow$ (this is good or bad?)
But it can $\uparrow$ if difficulties of minimizing E_{train} kick in:
The deeper (having more hidden layer) the network, the more complex the surface of E_{train}

Neural Network — training

Given training data: $\{(\mathbf{x}^{(1)}, y^{(1)}), ..., (\mathbf{x}^{(N)}, y^{(N)})\}$
where:

- $\mathbf{x}^{(n)} \in \mathbb{R}^{d+1}$
- $y^{(n)} \in \mathbb{R}$ (regression) or $\{1, 2, ..., K\}$ (classification)

We should choose model $h_{\mathbf{W}^{(1)},...,\mathbf{W}^{(L)}}(\mathbf{x})$
with $\mathbf{W}^{(1)}, ..., \mathbf{W}^{(L)} = ?$

Steps to find W's

Step 1. Define error function on training data

$$E_{\text{train}}(\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L)}) = \frac{1}{N} \sum_{n=1}^{N} e\left(h_{\mathbf{W}^{(1)},\ldots}(\mathbf{x}^{(n)}), y^{(n)}\right)$$

Step 2. $\min_{\mathbf{W}^{(1)},\ldots,\mathbf{W}^{(L)}} E_{\text{train}}(\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L)})$

Can use iterative gradient-based algorithms such as SGD

$$w_{ij}^{(l)} \leftarrow w_{ij}^{(l)} - \alpha \frac{1}{\text{mini-batch size}} \sum_{(\mathbf{x},y)\in\text{mini-batch}} \frac{\partial e\left(h_{\mathbf{w}^{(1)},\ldots}(\mathbf{x}),y\right)}{\partial w_{ij}^{(l)}}$$

Inside SGD, can use **back-prop**agation algorithm to compute $\frac{\partial e}{\partial w_{ij}^{(l)}} \forall l, i, j$ efficiently

Review of chain rule

1 path

$$x \rightarrow y = f_1(x) \rightarrow z = f_2(y)$$

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}$$

More than 1 path

$$\begin{aligned} x \rightarrow\ & y_1 = f_1(x) \rightarrow z = f_3(y_1, y_2) \\ \searrow\ & y_2 = f_2(x) \nearrow \end{aligned}$$

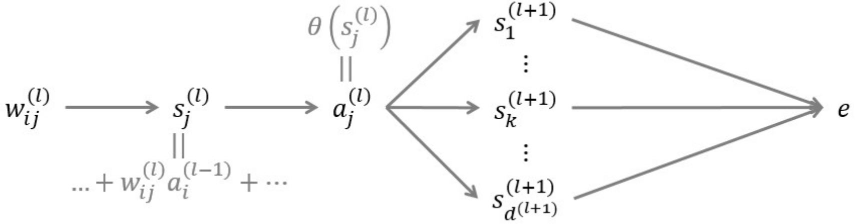
$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x}$$

$$\begin{tikzcd}
 & & & s_1^{(l+1)} \arrow[ddr] & \\
 & & \theta\left(s_j^{(l)}\right) \arrow[d, equal] & \vdots & \\
w_{ij}^{(l)} \arrow[r] & s_j^{(l)} \arrow[r] \arrow[d, equal] & a_j^{(l)} \arrow[uur] \arrow[r] \arrow[ddr] & s_k^{(l+1)} \arrow[r] & e \\
 & \ldots + w_{ij}^{(l)} a_i^{(l-1)} + \cdots & & \vdots & \\
 & & & s_{d^{(l+1)}}^{(l+1)} \arrow[uur] &
\end{tikzcd}$$

$$\frac{\partial e}{\partial w_{ij}^{(l)}} = \underbrace{\frac{\partial e}{\partial s_j^{(l)}}}_{\delta_j^{(l)}} \underbrace{\frac{\partial s_j^{(l)}}{\partial w_{ij}^{(l)}}}_{a_i^{(l-1)}}$$

$$\underbrace{\frac{\partial e}{\partial a_j^{(l)}}}\underbrace{\frac{\partial a_j^{(l)}}{\partial s_j^{(l)}}}_{\theta'\left(s_j^{(l)}\right)}$$

$$\sum_{k=1}^{d^{(l+1)}} \underbrace{\frac{\partial e}{\partial s_k^{(l+1)}}}_{\delta_k^{(l+1)}} \underbrace{\frac{\partial s_k^{(l+1)}}{\partial a_j^{(l)}}}_{w_{jk}^{(l+1)}}$$



$$\frac{\partial e}{\partial w_{ij}^{(l)}} = \underbrace{\frac{\partial e}{\partial s_j^{(l)}}}_{\delta_j^{(l)}} \underbrace{\frac{\partial s_j^{(l)}}{\partial w_{ij}^{(l)}}}_{a_i^{(l-1)}}$$

$$\theta'\left(s_j^{(l)}\right) \sum_{k=1}^{d^{(l+1)}} w_{jk}^{(l+1)} \delta_k^{(l+1)}$$

To compute $\frac{\partial e}{\partial w_{ij}^{(l)}}$ $\forall l, i, j$, we need to compute:

1. $a_i^{(l-1)}$ $\forall l, i$: $\boldsymbol{x} = \boldsymbol{a}^{(0)} \to \boldsymbol{a}^{(1)} \to \cdots \to \boldsymbol{a}^{(L)}$
2. $\delta_j^{(l)}$ $\forall l, j$: $\underbrace{\boldsymbol{\delta}^{(1)} \leftarrow \cdots \leftarrow \boldsymbol{\delta}^{(L-1)} \leftarrow \boldsymbol{\delta}^{(L)}}_{\text{Back-prop}}$

Q: Do we need to compute $\delta_0^{(l)}$ (delta of neuron 0 whose output value is always 1)?

A: No

Q: If layer L (last layer) is Softmax Regression (and the error function is cross-entropy), what is the formula to compute $\delta_j^{(L)}$?

Hint: In “HW2-Slide.pdf”, we have this formula for Softmax Regression:

$$\frac{\partial E_{train}}{\partial w_{ij}} = \frac{1}{N} \sum_{n=1}^{N} x_i^{(n)} (h_{\mathbf{w}}(\mathbf{x}^{(n)})_j - onehot(y^{(n)})_j)$$

A: $\delta_j^{(L)} = h_{\mathbf{w}^{(1)},\ldots,\mathbf{w}^{(L)}}(\mathbf{x})_j - onehot(y)_j$

with $h_{\mathbf{w}^{(1)},\ldots,\mathbf{w}^{(L)}}(\mathbf{x})_j \equiv a_j^{(L)}$

Sketch of SGD implementation for Neural Network

1. Initialize $\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L)}$
   (it's important to initialize "properly")
2. Repeat until termination criteria are satisfied:
   A. Shuffle the order of training examples
   B. For mini-batch $b = 1, \ldots, \frac{N}{B}$:
      Do "SGD mini-batch steps" to update $\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L)}$

SGD mini-batch steps

1. Compute output matrices of all layers:
   $\mathbf{A}^{(0)} = mb\_\mathbf{X}$
   $\mathbf{A}^{(l)} = some\_funct\left(\mathbf{A}^{(l-1)}, \mathbf{W}^{(l)}\right) \qquad l = 1, ..., L-1$
   $\mathbf{A}^{(L)} = some\_funct\left(\mathbf{A}^{(L-1)}, \mathbf{W}^{(L)}\right)$
2. Compute delta matrix of layer L:
   $\mathbf{D}^{(L)} = some\_funct\left(\mathbf{A}^{(L)}, mb\_\mathbf{Y}\right)$
3. Compute gradient of layer L:
   $\mathbf{G}^{(L)} = some\_funct\left(\mathbf{A}^{(L-1)}, \mathbf{D}^{(L)}\right)$
4. Update weight matrix of layer L:
   $\mathbf{W}^{(L)} \leftarrow \mathbf{W}^{(L)} - \alpha\mathbf{G}^{(L)}$
5. For layer $l = L-1, ..., 1$:
   A. Compute delta matrix of layer l:
      $\mathbf{D}^{(l)} = some\_funct\left(\mathbf{D}^{(l+1)}, \mathbf{W}^{(l+1)}, \mathbf{A}^{(l)}\right)$
   B. Compute gradient of layer l: similar to step 3
   C. Update weight matrix of layer l: similar to step 4

Neural Network — dealing with overfitting

- Weight decay (L2 regularization)
- Drop-out
- Data augmentation
- ...