ECE 20875

Python for Data Science

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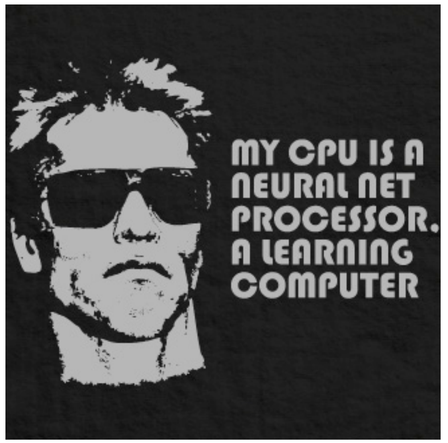
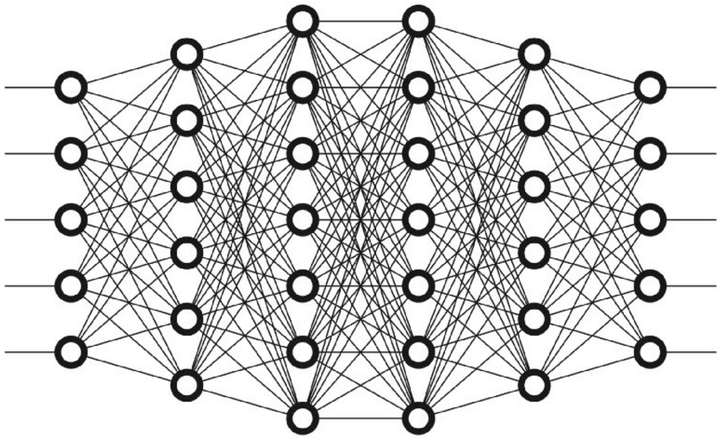
(Adapted from material developed by Profs. Milind Kulkarni, Stanley Chan, Chris Brinton, David Inouye)

introduction to neural networks

neural networks

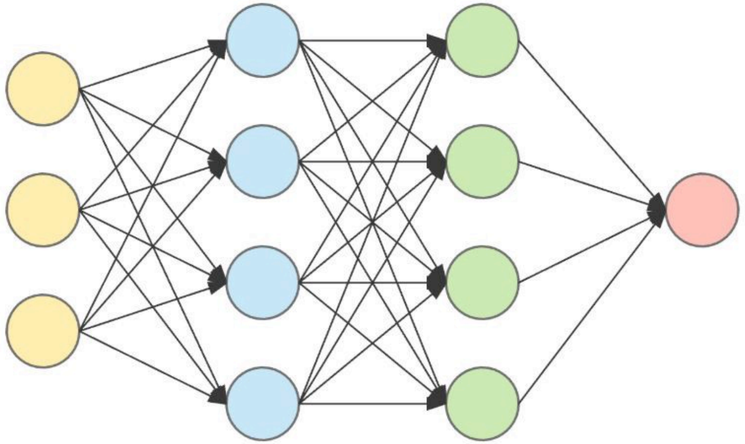


- Show up everywhere (including in pop culture)
  - Machine translation
  - Image recognition
  - Video generation
  - …
- Form the basis of the **deep learning** field
- Too many use cases for us to cover in this class
  - We will focus on neural networks used as **classifiers**



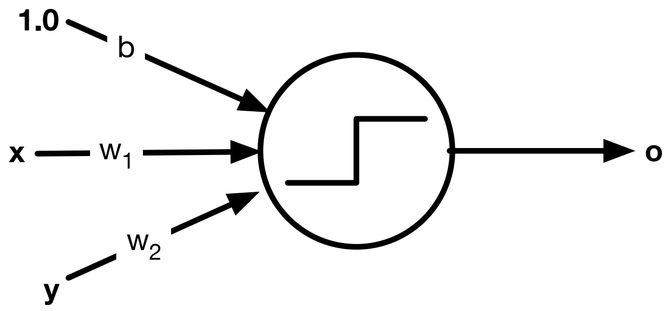
neurons

- The fundamental building blocks of neural networks are called **neurons**
  - Each has an **activation function**, modeled loosely after neurons in the brain, which “activate” when given enough stimulus
  - The human brain is estimated to have more than 10 billion neurons, to give you an idea
- Can view a neuron graphically as a “node” with inputs, and weights
  - The input to the activation function is the dot product of the input and weights



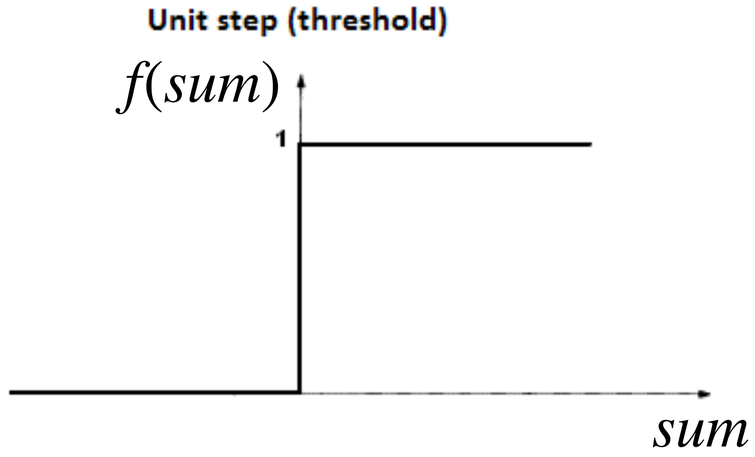
perceptrons

- A **perceptron** is the simplest form of a neuron
  - Activation function is the (Heaviside) **unit step function**: either “on” or “off”
- It uses the following **linear decision boundary**:



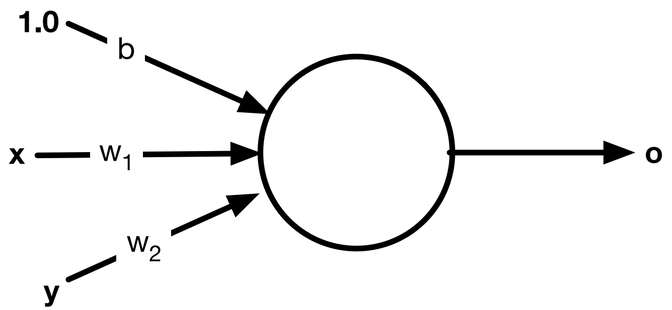
$$sum = \begin{bmatrix} b & w_1 & w_2 \end{bmatrix} \begin{bmatrix} 1.0 \\ x \\ y \end{bmatrix}$$

$$o = f(sum) = \begin{cases} 0, & sum \leq 0 \\ 1, & sum > 0 \end{cases}$$

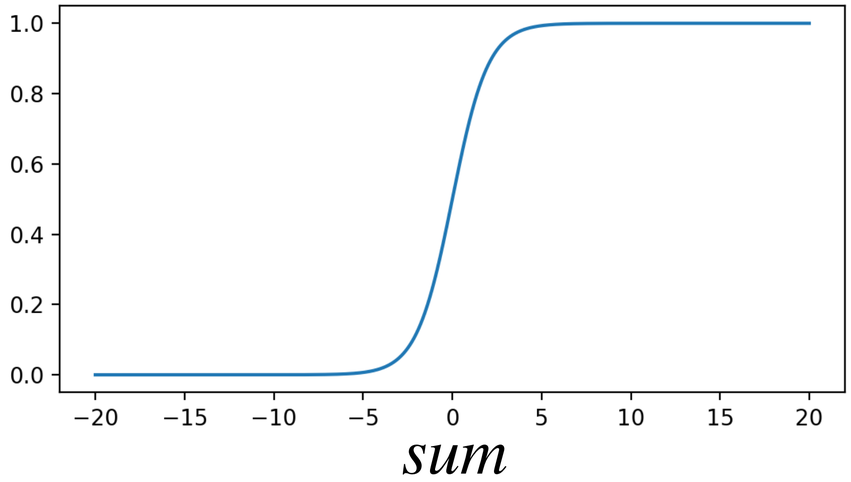


logistic regression: single layer NN

- Learning becomes a problem, because the unit step function cannot be differentiated
  - We need to somehow “smoothen” the transition at $sum = 0$
- One common activation function that does this is the **sigmoidal activation**, shown to the right
  - We can readily calculate the derivative
- This is just logistic regression!
  - A neural network with a single layer and sigmoidal activation is equivalent to logistic regression



$$o = f(sum) = \frac{1}{1 + e^{-sum}}$$

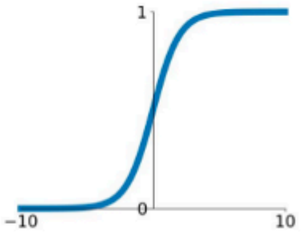


choices of activation functions

- The sigmoid function is computationally expensive, though (recall its derivative is complicated)
- There are many other activation functions we can use too. For example:
  - `tanh`: Hyperbolic tangent, has steeper derivatives than sigmoid
  - `ReLU`: Much easier to compute, but the outputs can be very large, and outputs below $x = 0$ suffer from the **vanishing gradient** problem
  - `Leaky ReLU`: Allows the output of `ReLU` below 0 to be slightly negative, which helps prevent neurons from falling into "dead states" from the vanishing gradient

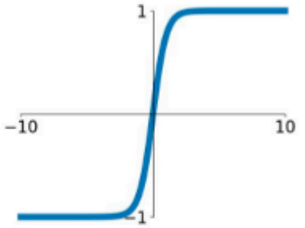
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



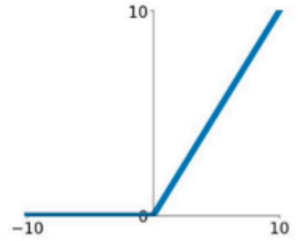
tanh

$$\tanh(x)$$



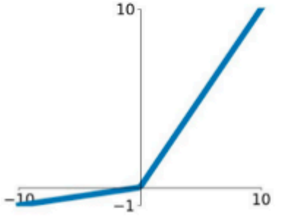
ReLU

$$\max(0, x)$$



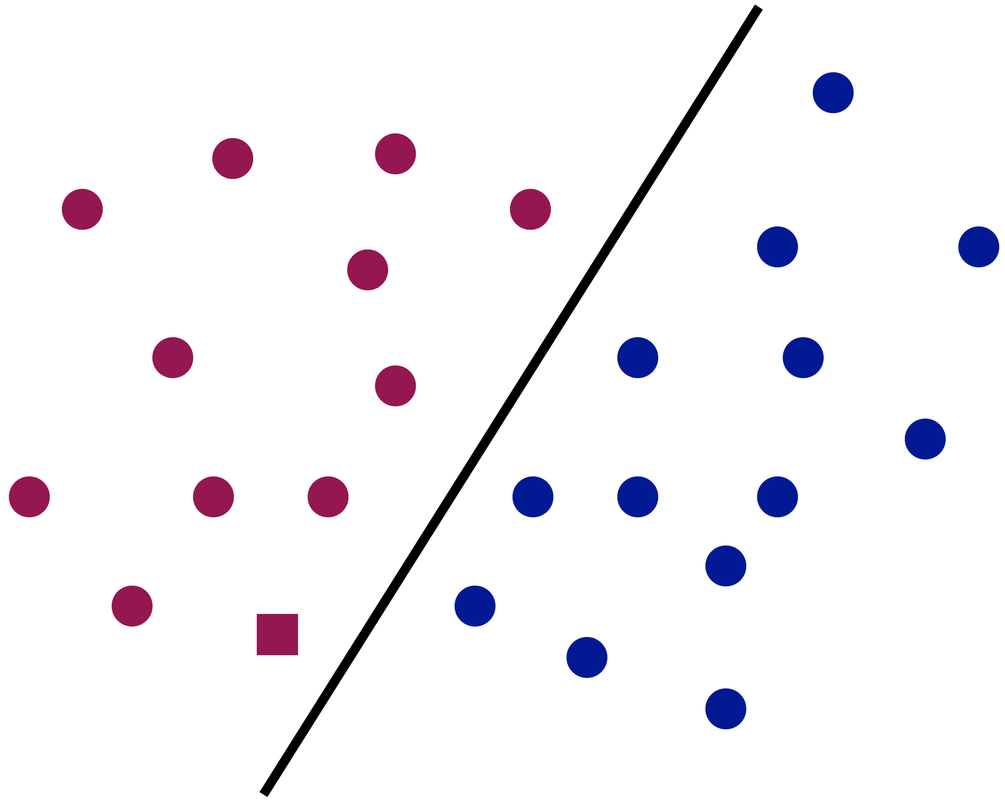
Leaky ReLU

$$\max(0.1x, x)$$



decision boundaries

- Basic classification problem for neural networks:
  - I have a set of labeled **training data**
  - Learn a **decision boundary** that separates the two classes of data
- Given a **new point**
  - Classify it using the decision boundary you learned
  - Similar to other classifiers we looked at!



creating decisions with neurons

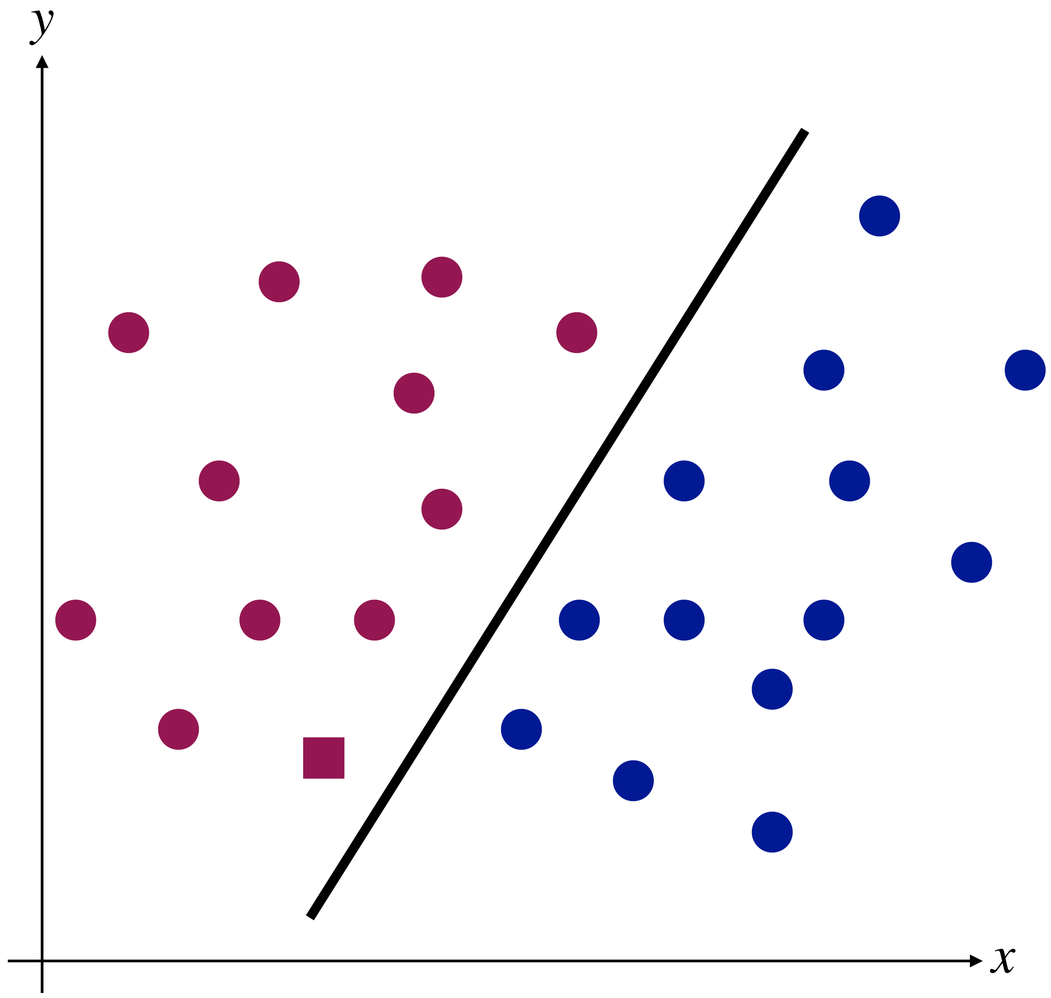
- The basic idea of neural networks is to add layers of complexity on how decision boundaries are defined

- A perceptron will induce a decision boundary that is a straight line, i.e.,

$$f(x, y) = \begin{cases} 0, & b + w_1 x + w_2 y \leq 0 \\ 1, & b + w_1 x + w_2 y > 0 \end{cases}$$

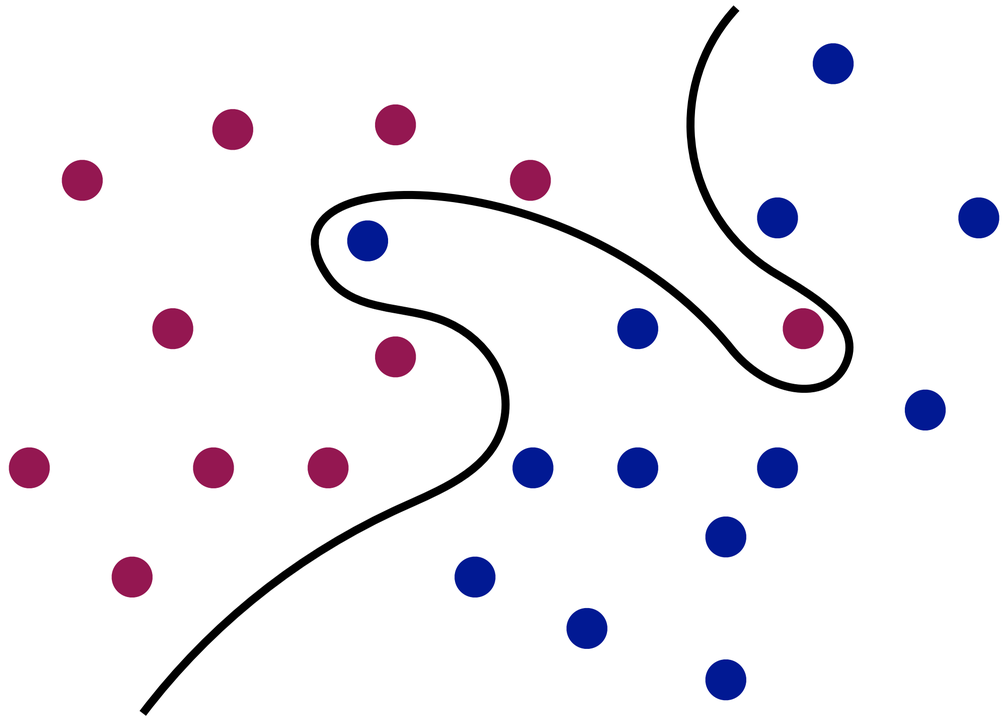
  - How do we learn the parameters w_1, w_2, and b of this model?

  - Instead of gradient descent, there is a "special" algorithm for perceptrons



non-linear decision boundaries

- The special **perceptron training algorithm** is guaranteed to converge if a **linear decision boundary** exists
- But if no linear boundary exists, the algorithm will not converge, not even to an imperfect solution
- Perceptrons cannot learn non-linear decision boundaries!
- To learn them with neural networks, we need two things:
  - Multiple layers of neurons
  - Smoother activation functions



multi-layer NN structure and intuition

(a) The building block of neural networks (a single **neuron**) is like a little logistic regression model:

1. Weighted summation of n inputs: $z = \sum_{i=1}^{n} w_i x_i$
2. Activation function: $y = f(z) = f\left(\sum_{i=1}^{n} w_i x_i \right)$

(b) We can put many of these neurons together to form a **feed-forward neural network** (or sometimes simply **deep NN** or **multilayer NN**)

1. Each neuron computes weighted summation and activation function
2. Stacking the neurons vertically forms a NN **layer**
3. Feeding the output of one layer as the input to the next layer creates a deep NN **(DNN)**

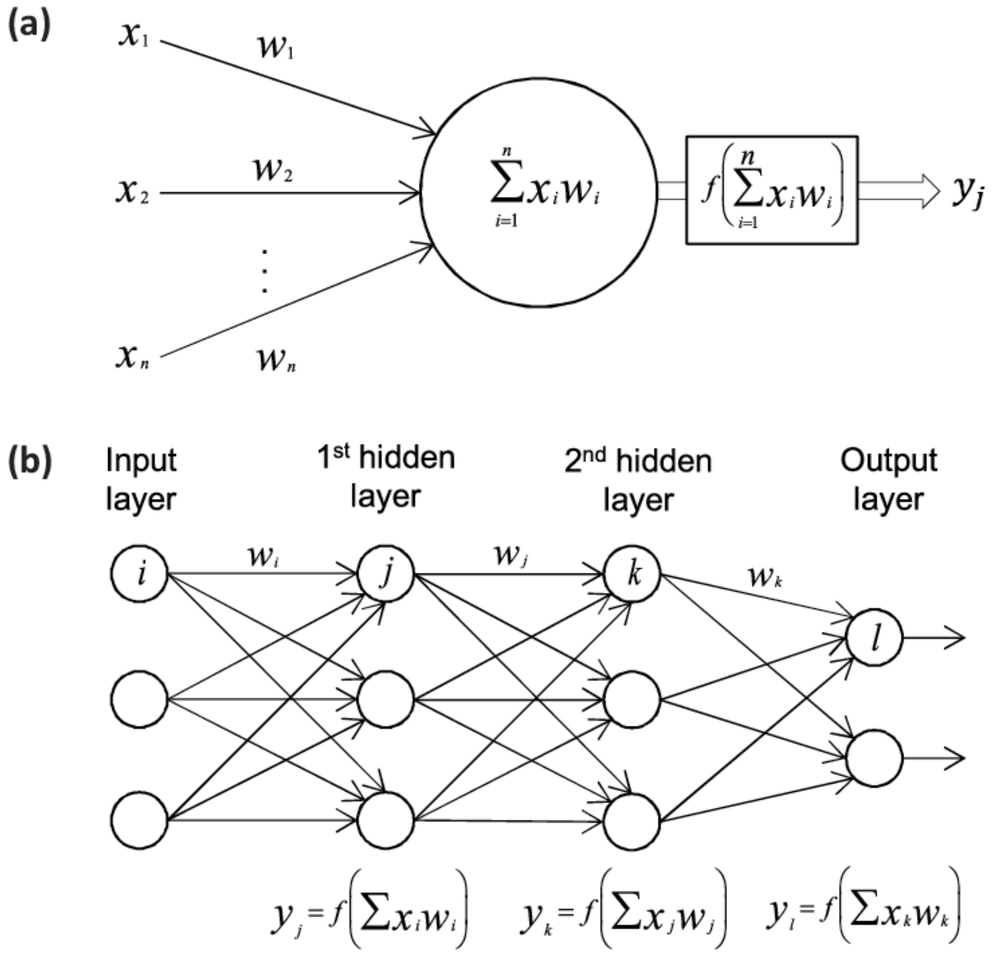


Figure from: Vieira, Sandra & Pinaya, Walter & Mechelli, Andrea. (2017). Using deep learning to investigate the neuroimaging correlates of psychiatric and neurological disorders: Methods and applications. Neuroscience & Biobehavioral Reviews. 74. 10.1016/j.neubiorev.2017.01.002.

multi-layer NN mathematical form

1. Notice that the weighted summation for neuron j can be seen as a dot product:

$$z_j = \sum_{i=1}^{n} w_i x_i = \mathbf{w}_j^T \mathbf{x}$$

2. When stacking neurons vertically the layer outputs can be seen as a matrix multiplication:

$$\begin{aligned} z_1 &= \mathbf{w}_1^T \mathbf{x} \\ z_2 &= \mathbf{w}_2^T \mathbf{x} \\ &\vdots \\ z_n &= \mathbf{w}_n^T \mathbf{x} \end{aligned} \quad , \quad \text{which can be written as } \mathbf{z} = \begin{bmatrix} \mathbf{w}_1^T \\ \mathbf{w}_2^T \\ \vdots \\ \mathbf{w}_n^T \end{bmatrix} \mathbf{x} = W\mathbf{x}$$

3. Now the activation function is applied *independently* to each output:

$$\begin{aligned} y_1 &= f(z_1) \\ y_2 &= f(z_2) \\ &\vdots \\ y_n &= f(z_n) \end{aligned} \quad , \quad \text{which can be written as } \mathbf{y} = \begin{bmatrix} f(z_1) \\ f(z_2) \\ \vdots \\ f(z_n) \end{bmatrix} = f(\mathbf{z})$$

4. Thus we can write a DNN mathematically as function composition:

$$DNN(\mathbf{x}) = \mathbf{f}(W^{(3)}\,\mathbf{f}(W^{(2)}\,\overbrace{\mathbf{f}(W^{(1)}\mathbf{x})}^{\text{Layer 1}}))$$

Layer 2 (the inner $\mathbf{f}(W^{(2)}\,\mathbf{f}(W^{(1)}\mathbf{x}))$)

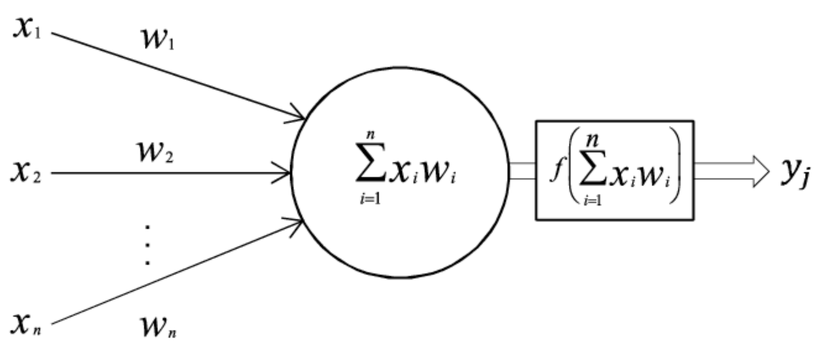
Output layer (the whole expression)

, or equivalently

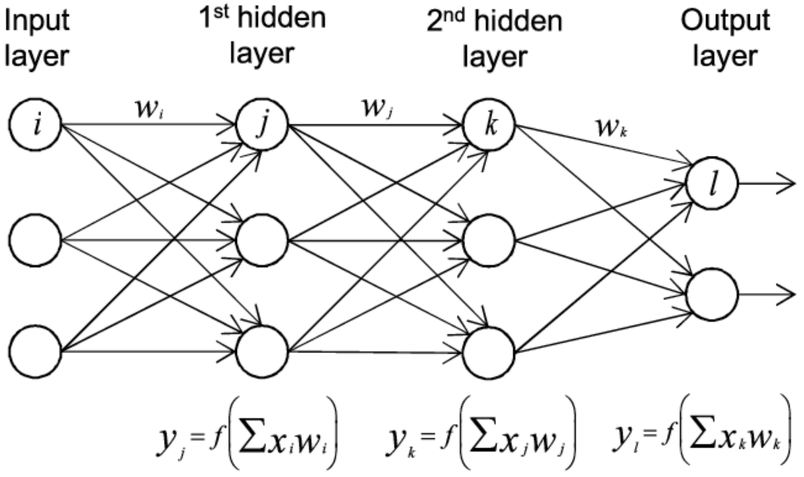
$$\begin{aligned} \mathbf{z}^{(1)} &= W^{(1)}\mathbf{x} \\ \mathbf{y}^{(1)} &= \mathbf{f}(\mathbf{z}^{(1)}) \\ \mathbf{z}^{(2)} &= W^{(2)}\mathbf{y}^{(1)} \\ \mathbf{y}^{(2)} &= \mathbf{f}(\mathbf{z}^{(2)}) \\ \mathbf{z}^{(3)} &= W^{(3)}\mathbf{y}^{(2)} \\ \mathbf{y}^{(3)} &= \mathbf{f}(\mathbf{z}^{(3)}) \end{aligned}$$

Alternating between **linear** transformation and **non-linear** activation functions

(a)



(b)



example of non-linear decision boundary

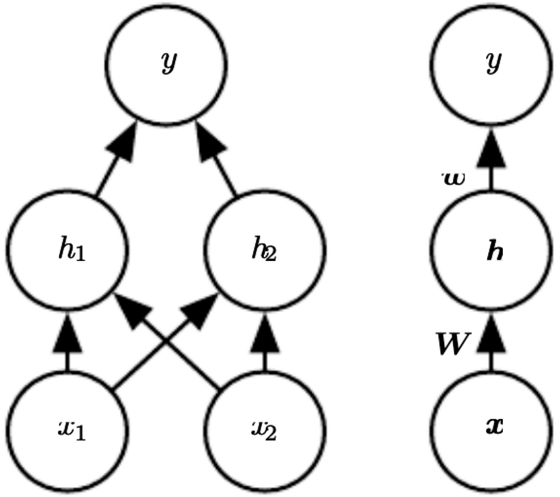
- Consider XOR classification function (i.e. “exclusive or”)
  - Outputs 1 only when exactly one of x_1 and x_2 is 1
  - Clearly not a linear decision boundary
- Can single layer NN handle this non-linear decision boundary problem?
- We will use simple two layer NN:

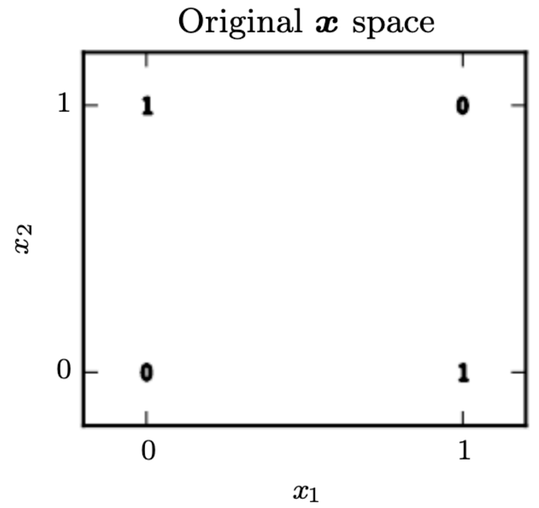
$$\mathbf{h} = \text{ReLU}(W\mathbf{x} + \mathbf{c}) = \max\{0, W\mathbf{x} + \mathbf{c}\}$$

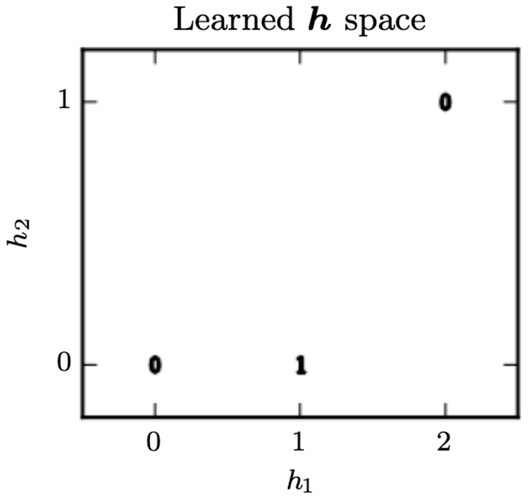
$$y = \mathbf{w}^T\mathbf{h}$$

- Solution:

$$W = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$$







https://www.deeplearningbook.org/contents/mlp.html

XOR example walkthrough

- We can verify that this two-layer NN implements the XOR function:
- $x_1 = 0$ and $x_2 = 0$: $\mathbf{h} = \text{ReLU}\left(\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}\begin{bmatrix}0\\0\end{bmatrix} + \begin{bmatrix}0\\-1\end{bmatrix}\right) = \text{ReLU}\left(\begin{bmatrix}0\\-1\end{bmatrix}\right) = \begin{bmatrix}0\\0\end{bmatrix}$,

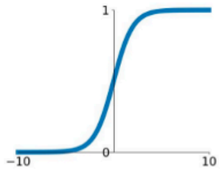
  $y = \begin{bmatrix}1 & -2\end{bmatrix}\begin{bmatrix}0\\0\end{bmatrix} = 0$
- $x_1 = 0$ and $x_2 = 1$: $\mathbf{h} = \text{ReLU}\left(\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} + \begin{bmatrix}0\\-1\end{bmatrix}\right) = \text{ReLU}\left(\begin{bmatrix}1\\0\end{bmatrix}\right) = \begin{bmatrix}1\\0\end{bmatrix}, y = \begin{bmatrix}1 & -2\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = 1$
- $x_1 = 1$ and $x_2 = 0$: $\mathbf{h} = \text{ReLU}\left(\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} + \begin{bmatrix}0\\-1\end{bmatrix}\right) = \text{ReLU}\left(\begin{bmatrix}1\\0\end{bmatrix}\right) = \begin{bmatrix}1\\0\end{bmatrix}, y = \begin{bmatrix}1 & -2\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = 1$
- $x_1 = 1$ and $x_2 = 1$: $\mathbf{h} = \text{ReLU}\left(\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}\begin{bmatrix}1\\1\end{bmatrix} + \begin{bmatrix}0\\-1\end{bmatrix}\right) = \text{ReLU}\left(\begin{bmatrix}2\\1\end{bmatrix}\right) = \begin{bmatrix}2\\1\end{bmatrix}, y = \begin{bmatrix}1 & -2\end{bmatrix}\begin{bmatrix}2\\1\end{bmatrix} = 0$

architecture and parameters of NN

- **Depth**: # of layers
- **Width**: # of neurons per layer
- **Activations**: sigmoid, ReLU, tanh, etc.

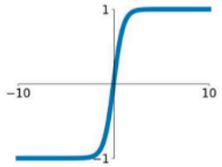
Sigmoid

$\sigma(x) = \frac{1}{1+e^{-x}}$



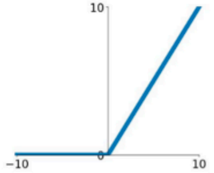
tanh

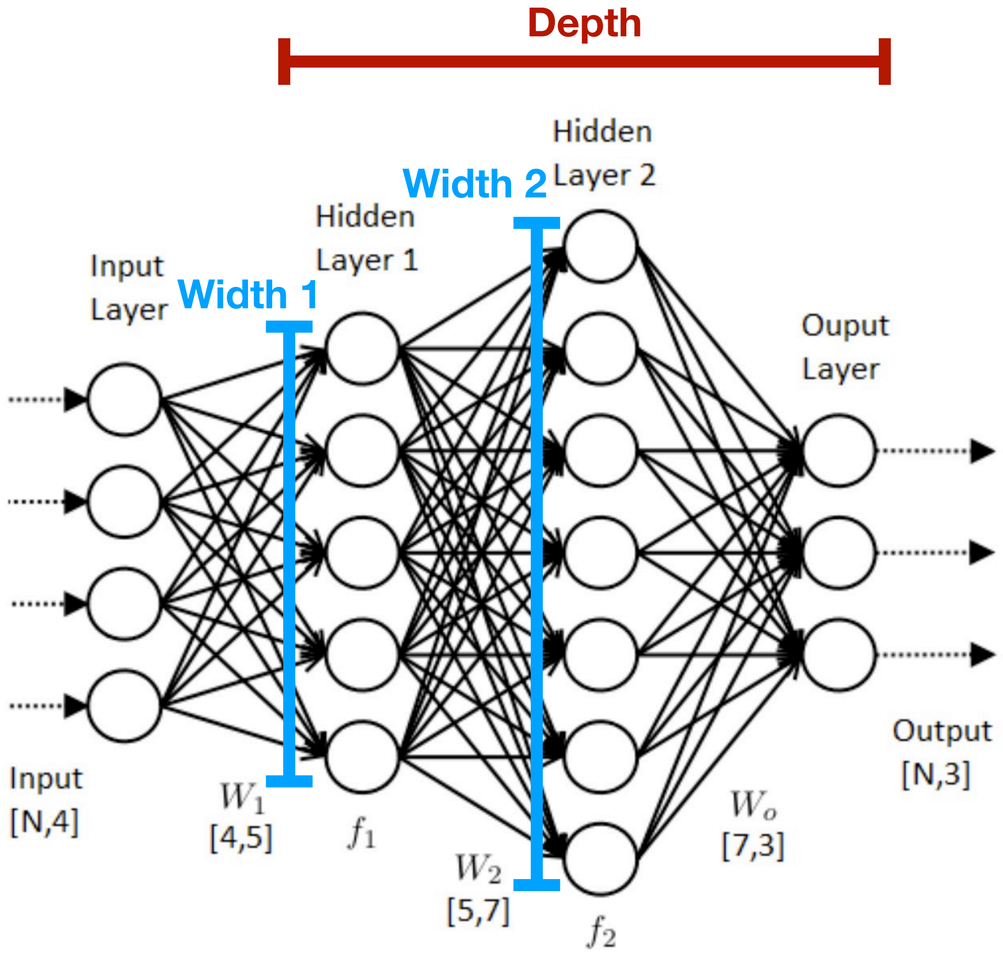
$\tanh(x)$



ReLU

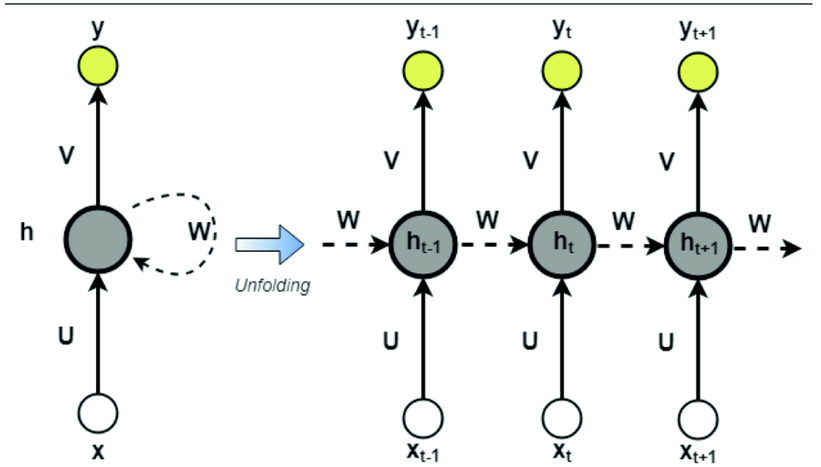
$\max(0, x)$

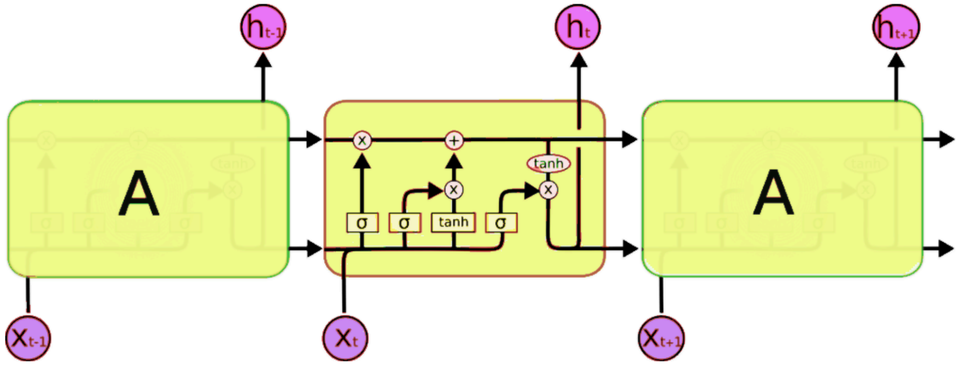




neural network architectures

- A plethora of neural network architectures have been proposed, for different applications
  - Multi-layer Perceptron (**MLP**): Cascading perceptrons
  - Recurrent Neural Networks (**RNN**): Sequential data modeling
  - Convolutional Neural Networks (**CNN**): Image recognition
  - Long Short Term Memory (**LSTM**): Memory cells with “forgetting” factors
  - Transformer (most recent), Gated Recurrent Units (**GRU**), Hopfield Networks, Boltzmann Machines, Generative Adversarial Networks (**GAN**), …





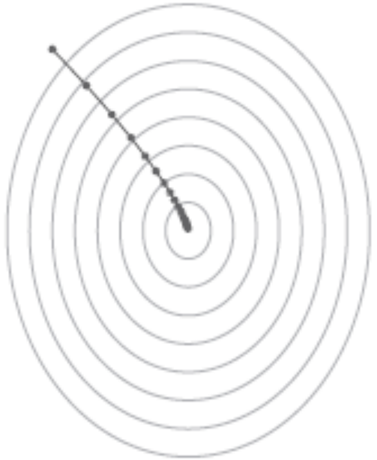
learning neural networks

- **(Batch) Gradient descent (GD)** can be computationally expensive for large datasets
  - E.g., if we have 1M images, *every update* requires computing and summing 10^6 gradients
    $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \alpha \sum_{i=1}^{n=10^6} \nabla F(x_i, y_i, \mathbf{w}^{(t)})$
  - If we add a normalizing constant of $1/n$, we can view this update as taking the expected gradient over all data samples:
    $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \alpha \frac{1}{n} \sum_{i=1}^{n} \nabla F(x_i, y_i, \mathbf{w}^{(t)}) = \mathbf{w}^{(t)} - \alpha \mathbb{E}[\nabla F(x_i, y_i, \mathbf{w}^{(t)})]$
- **Stochastic gradient descent (SGD)** massively reduces the computational complexity by only using 1 sample at each time step t, (x_t, y_t):

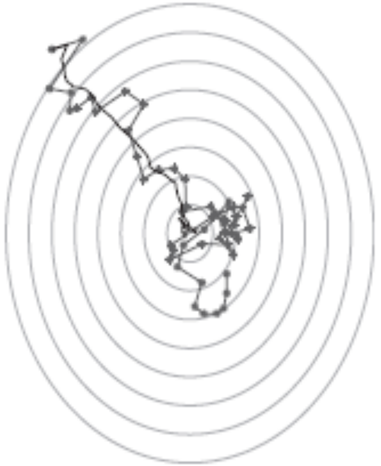
  $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \alpha \mathbb{E}[\nabla F(x_i, y_i, \mathbf{w}^{(t)})] \rightarrow \mathbf{w}^{(t)} - \alpha \nabla F(x_t, y_t, \mathbf{w}^{(t)})$

  - Note that the *variance of the steps* is much higher but the *cost is much lower*
  - Sometimes called **amortized learning** because it amortizes (spreads out) the computational cost across many iterations
  - **Mini-batch gradient descent** is actually used in practice, where often 64, 128 or 256 samples are used in each batch (bridging between SGD and GD)

Gradient descent



Stochastic Gradient Descent



SGD for a sigmoidal neuron

- Letting y_i be the label of datapoint i, $\mathbf{w} = (w_1, w_2, \dots)$ be the vector of weights, and $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots)$ be the datapoint vector, define the error $E(\mathbf{x}_i)$ of the output of a specific input:

$$E(\mathbf{x}_i) = \frac{1}{2}\left(y_i - f(sum)\right)^2 = \frac{1}{2}\left(y_i - f(\mathbf{w}^T\mathbf{x}_i)\right)^2$$

- For SGD, we only need the partial derivative for one specific input

$$\frac{\partial E(\mathbf{x}_i)}{\partial w_j} = \frac{\partial E(\mathbf{x}_i)}{\partial f(sum)} \cdot \frac{\partial f(sum)}{\partial sum} \cdot \frac{\partial sum}{\partial w_j} = -\underbrace{(y_i - f(sum)) \cdot f(sum)(1 - f(sum))}_{\text{Denote as } \delta_0 \text{ since same for every } w_j} \cdot x_{ij}$$

  - Remember that $\frac{\partial f(x)}{\partial x} = f(x)(1 - f(x))$ when f is a sigmoid

SGD for a sigmoidal neuron

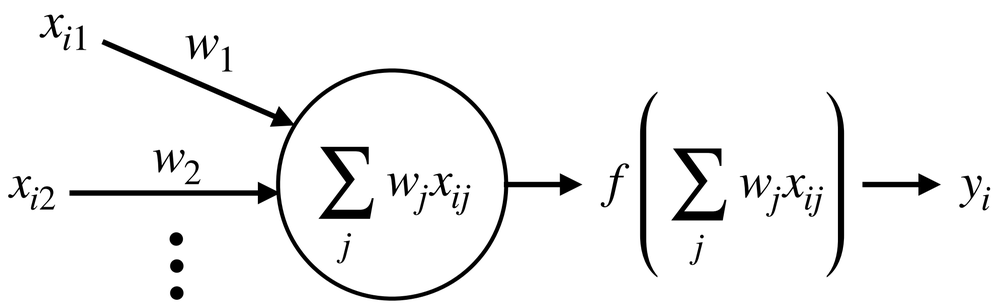
- From previous slide:

$$\frac{\partial E(\mathbf{x}_i)}{\partial w_j} = \frac{\partial E(\mathbf{x}_i)}{\partial f(sum)} \cdot \frac{\partial f(sum)}{\partial sum} \cdot \frac{\partial sum}{\partial w_j} = -\underbrace{(y_i - f(sum)) \cdot f(sum)(1 - f(sum))}_{\text{Denote as } \delta_0 \text{ since same for every } w_j} \cdot x_{ij}$$

- Thus, our SGD update rule becomes:

$$w_j^{(t+1)} = w_j^{(t)} + \alpha \cdot \delta_0 \cdot x_{ij}$$

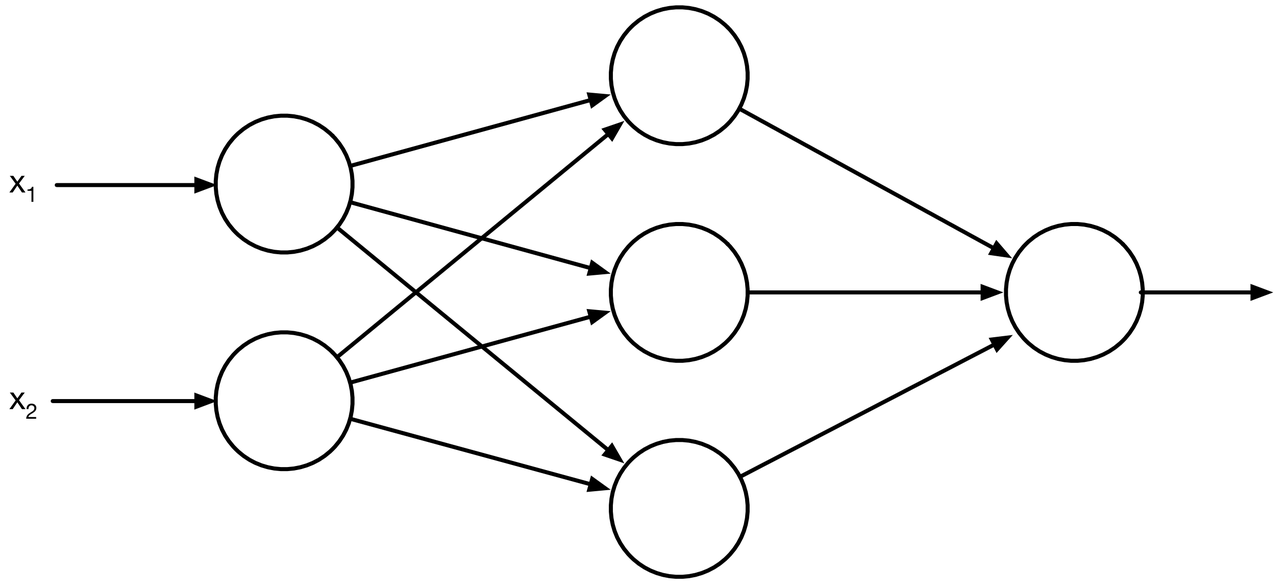
$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \alpha \cdot \delta_0 \cdot \mathbf{x}_i$$



  - Importantly, δ_0 is reused for every w_j, so we only have to compute it once for each t

learning complex separators

- Let’s build up to more complex models by cascading neurons
- Learning the weights of the edges to the output neuron is easy — same as learning for a single neuron
- But what about the weights on the inputs to the hidden layer?



updating the deltas

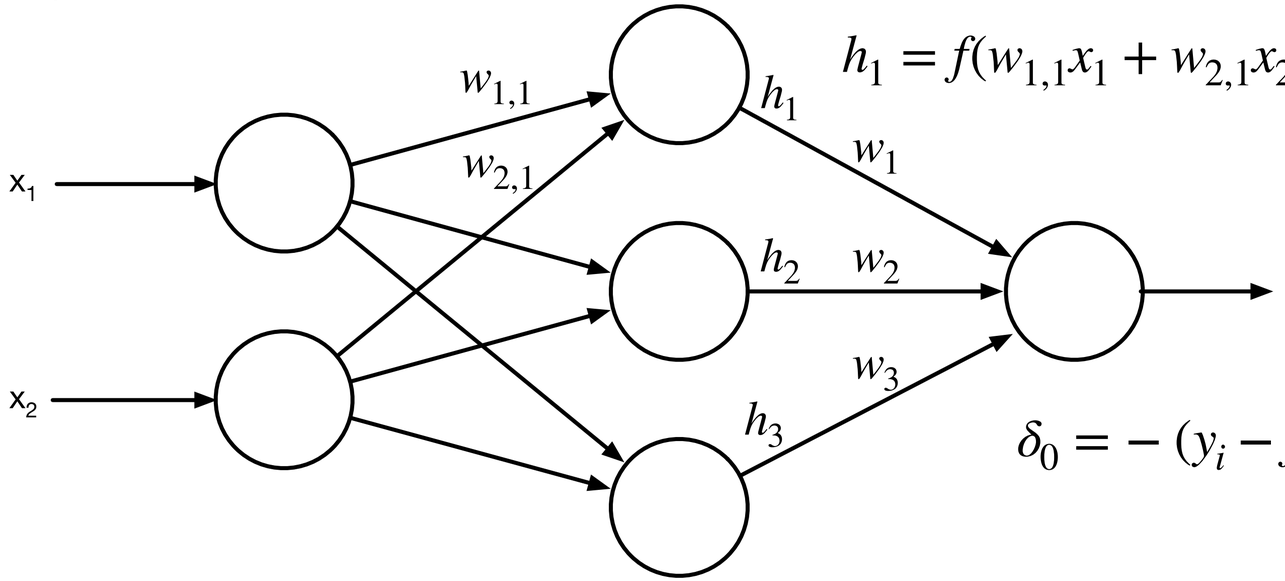
- Consider the network below. The output of this hidden layer is a vector $\mathbf{h}$. We can write the error of the network as:

$$E(\mathbf{w}) = \frac{1}{2}(y_i - f(w_1 h_1 + w_2 h_2 + w_3 h_3))^2 = \frac{1}{2}(y_i - f(w_1 f(w_{1,1} x_1 + w_{2,1} x_2) + w_2 h_2 + w_3 h_3))^2$$

- The change in output error with respect to $w_{1,1}$ is:

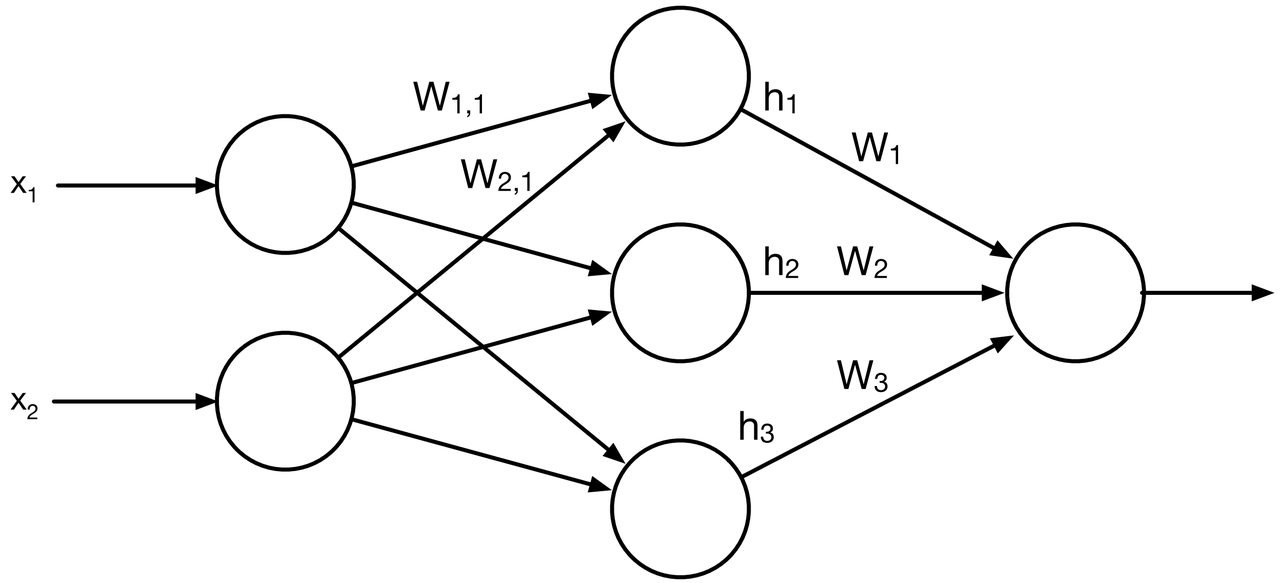
$$\frac{\partial E}{\partial w_{1,1}} = \frac{\partial E}{\partial h_1} \cdot \frac{\partial h_1}{\partial sum_{h_1}} \cdot \frac{\partial\, sum_{h_1}}{\partial w_{1,1}} = -\delta_0 w_1 \cdot f'(sum_{h_1}) \cdot x_1 = -\delta_{h_1} \cdot x_1$$

this term has the same form as what we derived for a single neuron previously



essence of backpropagation

- Computing the gradient for each neuron gives us the delta ($\delta_0, \delta_{h_1}, \ldots$) for the “upstream” neurons, so we can keep pushing error back
- This gives us the essence of **backpropagation** for training neural networks
  - **Forward pass**: Compute outputs of each neuron
  - **Backward pass**: Push errors (deltas, $\delta_0, \delta_{h_1}, \ldots$) weighted by edges to compute how the weights change.
  - Update: Apply stochastic gradient descent to each weight. Repeat.



implementing neural networks

- sklearn now has a built in MLP module:

```
from sklearn.neural_network import MLPClassifier

mlp = MLPClassifier(hidden_layer_sizes=(13,13,13),max_iter=500)
```

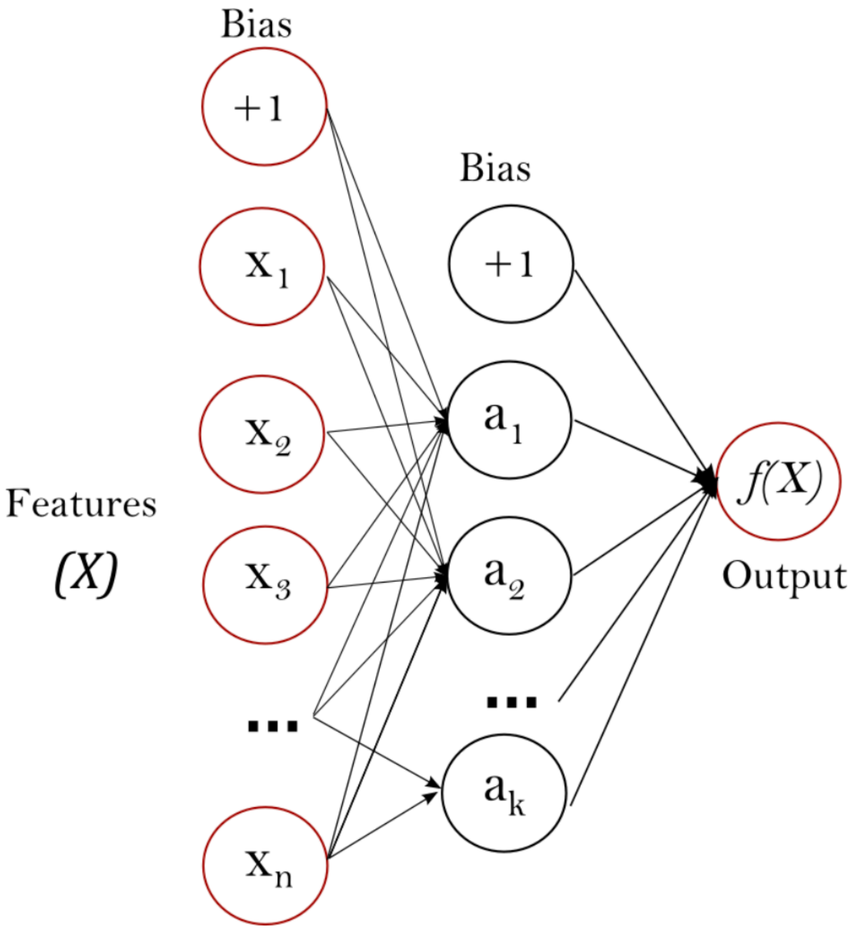
- For more complex neural networks, we typically leverage other machine learning libraries/platforms:
  - pytorch (https://pytorch.org/)
  - tensorflow (https://www.tensorflow.org/)
  - Both have Python interfaces

TensorFlow

PyTorch

Multi-layer Perceptron (MLP)

- Generally speaking, learns a function $f(\cdot) : \mathbb{R}^n \rightarrow \mathbb{R}^o$ by training on a dataset of input datapoints
  - Each input datapoint's dimension is n, output dimension is o
  - ML**P** is a misnomer, because it uses anything *except* a perceptron activation
- Architecture of an MLP:
  - Input layer, where each of the n input features is represented as a neuron
  - l hidden layers, where each layer performs a linear transformation followed by a non-linear activation
  - Output which has one non-linear activation for each of the o output dimensions



- Single hidden layer ($l = 1$)
- Single output ($o = 1$)

MLP in Python

- sklearn has a built in MLP (multi-layer perception) module

```
from sklearn.neural_network import MLPClassifier

mlp = MLPClassifier(hidden_layer_sizes=(13,13,13), max_iter=500)

mlp.fit(train_X, train_y)

print(mlp.coefs_[i])  # weight matrix corresponding to layer i (i=0,…,3)

print(mlp.intercept_[i])  # bias vector for neurons in layer i+1 (i=0,…,2)

results = mlp.predict(test_X)
```

- Check out https://scikit-learn.org/stable/modules/generated/sklearn.neural_network.MLPClassifier.html

deep learning training

- With deep learning, we have non-linear (and non-convex) error functions
- Therefore SGD is not guaranteed to converge to the global optimum solution
- A lot of research is devoted to …
  - Speeding up backpropagation, with methods like the Adam optimizer, or by distributing training across many nodes
  - Finding conditions for global solutions in neural networks