ECE 20875
Python for Data Science
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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
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:

\[
\text{sum} = \begin{bmatrix} b & w_1 & w_2 \end{bmatrix} \begin{bmatrix} 1.0 \\ x \\ y \end{bmatrix}
\]

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

• 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

\[
o = f(\text{sum}) = \frac{1}{1 + e^{-\text{sum}}}
\]
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

\[
\text{Sigmoid} \quad \sigma(x) = \frac{1}{1 + e^{-x}}
\]

\[
\text{tanh} \quad \tanh(x)
\]

\[
\text{ReLU} \quad \max(0, x)
\]

\[
\text{Leaky ReLU} \quad \max(0.1x, x)
\]
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!
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)

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

$$z_j = \sum_{i=1}^{n} w_{ij}x_i = w_j^T x$$

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

$$z_1 = w_1^T x$$
$$z_2 = w_2^T x$$
$$\vdots$$
$$z_n = w_n^T x$$

which can be written as $z = Wx$

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

$$y_1 = f(z_1)$$
$$y_2 = f(z_2)$$
$$\vdots$$
$$y_n = f(z_n)$$

which can be written as $y = f(z)$

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

$$DNN(x) = f(W(3)f(W(2)f(W(1)x)))$$

or equivalently

$$z^{(1)} = W^{(1)}x$$
$$y^{(1)} = f(z^{(1)})$$
$$z^{(2)} = W^{(2)}y^{(1)}$$
$$y^{(2)} = f(z^{(2)})$$
$$z^{(3)} = W^{(3)}y^{(2)}$$
$$y^{(3)} = f(z^{(3)})$$

Alternating between linear transformation and non-linear activation functions
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:

$$h = \text{ReLU}(Wx + c) = \max\{0, Wx + c\}$$

$$y = w^T h$$

• Solution:

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

https://www.deeplearningbook.org/contents/mlp.html
XOR example walkthrough

• We can verify that this two-layer NN implements the XOR function:

\[
\begin{align*}
  \text{• } x_1 &= 0 \text{ and } x_2 = 0: \\ h &= \text{ReLU} \left( \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 0 \end{bmatrix} + \begin{bmatrix} 0 \end{bmatrix} \right) = \text{ReLU} \left( \begin{bmatrix} 0 \end{bmatrix} \right) = \begin{bmatrix} 0 \end{bmatrix}, \\
  y &= \begin{bmatrix} 1 & -2 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} = 0
\end{align*}
\]

\[
\begin{align*}
  \text{• } x_1 &= 0 \text{ and } x_2 = 1: \\ h &= \text{ReLU} \left( \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \end{bmatrix} + \begin{bmatrix} 0 \end{bmatrix} \right) = \text{ReLU} \left( \begin{bmatrix} 1 \end{bmatrix} \right) = \begin{bmatrix} 1 \end{bmatrix}, \\
  y &= \begin{bmatrix} 1 & -2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 1
\end{align*}
\]

\[
\begin{align*}
  \text{• } x_1 &= 1 \text{ and } x_2 = 0: \\ h &= \text{ReLU} \left( \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \end{bmatrix} + \begin{bmatrix} 0 \end{bmatrix} \right) = \text{ReLU} \left( \begin{bmatrix} 1 \end{bmatrix} \right) = \begin{bmatrix} 1 \end{bmatrix}, \\
  y &= \begin{bmatrix} 1 & -2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 1
\end{align*}
\]

\[
\begin{align*}
  \text{• } x_1 &= 1 \text{ and } x_2 = 1: \\ h &= \text{ReLU} \left( \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \end{bmatrix} + \begin{bmatrix} 0 \end{bmatrix} \right) = \text{ReLU} \left( \begin{bmatrix} 2 \end{bmatrix} \right) = \begin{bmatrix} 2 \end{bmatrix}, \\
  y &= \begin{bmatrix} 1 & -2 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = 0
\end{align*}
\]
architecture and parameters of NN

- **Depth**: # of layers
- **Width**: # of neurons per layer
- **Activations**: sigmoid, ReLU, tanh, etc.
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), …
(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
  
  $$w^{(t+1)} = w^{(t)} - \alpha \sum_{i=1}^{10^6} \nabla F(x_i, y_i, w^{(t)})$$

- If we add a normalizing constant of $1/n$, we can view this update as taking the expected gradient over all data samples:
  
  $$w^{(t+1)} = w^{(t)} - \alpha \frac{1}{n} \sum_{i=1}^{n} \nabla F(x_i, y_i, w^{(t)}) = w^{(t)} - \alpha \mathbb{E}[\nabla F(x_i, y_i, w^{(t)})]$$

Stochastic gradient descent (SGD) massively reduces the computational complexity by only using 1 sample at each time step $t$, $(x_t, y_t)$:

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

- 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)
SGD for a sigmoidal neuron

- Letting $y_i$ be the label of datapoint $i$, $\mathbf{w} = (w_1, w_2, \ldots)$ be the vector of weights, and $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots)$ 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

$$\frac{\partial E(\mathbf{x}_i)}{\partial w_j} = \frac{\partial E(\mathbf{x}_i)}{\partial f(sum)} \cdot \frac{\partial f(sum)}{\partial \text{sum}} \cdot \frac{\partial \text{sum}}{\partial w_j} = - (y_i - f(sum)) \cdot f(sum)(1 - f(sum)) \cdot x_{ij}$$

Denote as $\delta_0$ since same for every $w_j$

- 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:

\[
\frac{\partial E(x_i)}{\partial w_j} = \frac{\partial E(x_i)}{\partial f(sum)} \cdot \frac{\partial f(sum)}{\partial \text{sum}} \cdot \frac{\partial \text{sum}}{\partial w_j} = - (y_i - f(sum)) \cdot f(sum)(1 - f(sum)) \cdot x_{ij}
\]

Denote as \(\delta_0\) since same for every \(w_j\)

• Thus, our SGD update rule becomes:

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

\[
w^{(t+1)} = w^{(t)} + \alpha \cdot \delta_0 \cdot x_i
\]

• Importantly, \(\delta_0\) 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?
• 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:

\[
\frac{\partial E}{\partial w_{1,1}} = \frac{\partial E}{\partial h_1} \cdot \frac{\partial h_1}{\partial \text{sum}_{h_1}} \cdot \frac{\partial \text{sum}_{h_1}}{\partial w_{1,1}} = - \delta_0 w_1 \cdot f(\text{sum}_{h_1}) \cdot x_1 = - \delta_{h_1} \cdot x_1
\]

\( \delta_0 = -(y_i - f(\mathbf{w}^T \mathbf{h})) \cdot f(\mathbf{w}^T \mathbf{h})(1 - f(\mathbf{w}^T \mathbf{h})) \)
The 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:

```python
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/](https://pytorch.org/))
  • tensorflow ([https://www.tensorflow.org/](https://www.tensorflow.org/))

• Both have Python interfaces
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 data points
  - Each input data point’s dimension is $n$, output dimension is $o$
  - MLP 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

```python
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)
```

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