Introduction to Deep Learning for Scientists and Engineers

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Summary

- Part I
  - Problem definition (rely on supervised learning)
  - Compute graph and gradients
  - A little about deep learning libraries.
- Part II
  - Need for different architectures
  - Convolution networks
  - Recurrent networks
- Not covered
  - Diagram of neurons
  - History
  - Recent advances and business context
  - Tutorial on pytorch or keras
- Expectation and whats next

Extending derivatives to functions that accept vectors

For a function $f : \mathbb{R}^n \to \mathbb{R}$, or, equivalently, $y = f(\vec{x})$, the gradient is:

$$\nabla_x f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix} \tag{1}$$

For finding minima, use gradient descent (iterate):

$$\vec{x} = \vec{x} - \eta \nabla_x f \tag{2}$$

Extending this to $f : \mathbb{R}^n \to \mathbb{R}^n$, or $\vec{y} = f(\vec{x})$, we define the Jacobian as:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial y_1}{\partial x_{11}} & \frac{\partial y_1}{\partial x_{12}} & \dots & \frac{\partial y_1}{\partial x_{1n}} \\ \vdots & & & \\ \frac{\partial y_m}{\partial x_{11}} & \frac{\partial y_m}{\partial x_{12}} & \dots & \frac{\partial y_m}{\partial x_{1n}} \end{bmatrix} \tag{3}$$

Note: Gradient is defined for $y \in \mathbb{R}$.

- Can we define another function $L(\vec{y}) : \mathbb{R}^m \to \mathbb{R}$?
- What does this function mean?

Matrix multiplication as a function

$x \in \mathbb{R}^n$,$y \in \mathbb{R}^m$, $w \in \mathbb{R}^{m\times n}$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & \dots & w_{1n} \\ w_{21} & w_{22} & \dots & w_{2n} \\ \vdots & \vdots & & \vdots \\ w_{m1} & w_{m2} & \dots & w_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

$$\vec{y} = w\vec{x}$$

Derivatives

For $m = 2, n = 3$

$$y_1 = w_{11}x_1 + w_{12}x_2 + w_{13}x_3 \tag{4}$$

$$y_2 = w_{21}x_1 + w_{22}x_2 + w_{23}x_3 \tag{5}$$

$$\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \frac{\partial y_1}{\partial x_3} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \frac{\partial y_2}{\partial x_3} \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{bmatrix} \tag{6}$$

$$\frac{d\vec{y}}{d\vec{x}} = w \tag{7}$$

Element wise operations

$$\sigma(x) = \frac{1}{1 + e^{-x}} \tag{8}$$

$$\frac{d}{dx}\sigma(x) = \sigma(x)(1 - \sigma(x)) \tag{9}$$

$$\sigma(\begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{bmatrix}) = \begin{bmatrix} \sigma(z_1) \\ \sigma(z_2) \\ \vdots \\ \sigma(z_m) \end{bmatrix} \tag{10}$$

Derivatives in multiple dimensions

Partial derivatives of $f(x, y, z) = sin(x^2y) + e^z$

$$\frac{\partial f}{\partial x} = 2xycos(x^2y) \tag{11}$$

$$\frac{\partial f}{\partial y} = x^2cos(x^2y) \tag{12}$$

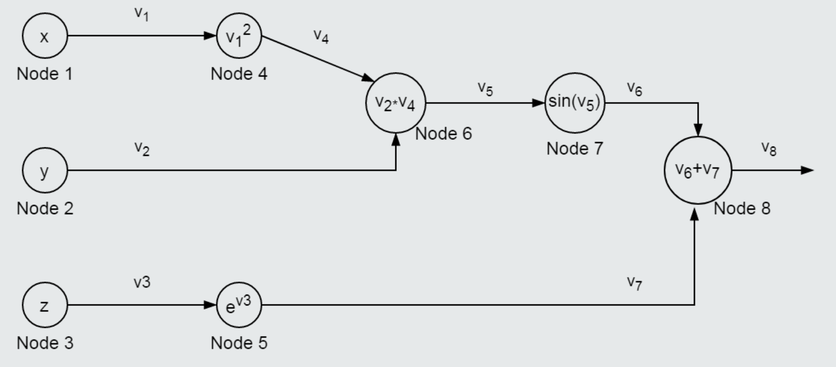
$$\frac{\partial f}{\partial z} = e^z \tag{13}$$

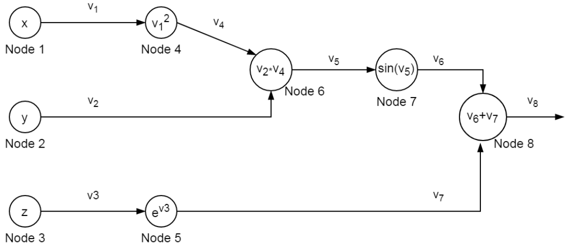
Computing the derivative

- Analytically (shown above)
- Numerically $f'(x) \approx \frac{f(x+\delta x)-f(x-\delta x)}{2\delta x}$
- Auto-diff. Deep learning libraries use reverse mode auto-diff.

Computation graph

Compute graph of $f(x, y, z) = sin(x^2y) + e^z$





$$\frac{\partial v_8}{\partial z} = \frac{\partial v_8}{\partial v_7}\frac{\partial v_7}{\partial v_3}\frac{\partial v_3}{\partial z} \tag{14}$$

$$= 1.e^{v_3}.1 \tag{15}$$

$$\frac{\partial v_8}{\partial z} = \frac{\partial f}{\partial z} = e^{v_3} = e^z \tag{16}$$

$$\frac{\partial v_8}{\partial y} = \frac{\partial v_8}{\partial v_6}\frac{\partial v_6}{\partial v_5}\frac{\partial v_5}{\partial v_2}\frac{\partial v_2}{\partial y} \tag{17}$$

$$= 1.cos(v_5).v_4.1 \tag{18}$$

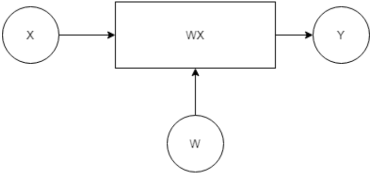
$$\frac{\partial f}{\partial y} = \frac{\partial v_8}{\partial y} = cos(v_5)v_4 \tag{19}$$

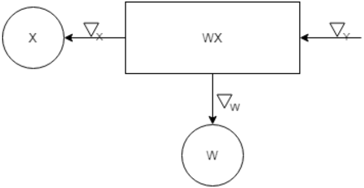
$$= cos(v_2 v_4)v_4 \tag{20}$$

$$= cos(v_1^2 y)v_1^2 \tag{21}$$

$$= cos(x^2 y)x^2 \tag{22}$$

Unit operations (and a little bit of python)






```python
class MultiplicationLayer1D:
    def __init__(self):
        self.cache = {}

    def forward(self, x, w):
        self.cache['x'] = x
        self.cache['w'] = w
        return w * x

    def backprop(self, incoming_grad):
        x_grad = self.cache['w']
        w_grad = self.cache['x']
        x_grad *= incoming_grad
        w_grad *= incoming_grad
        return x_grad, w_grad
```

```python
class AdditionLayer:
    def __init__(self):
        self.cache = {}

    def forward(self, x, w):
        self.cache['x'] = x
        self.cache['w'] = w
        return w + x

    def backprop(self, incoming_grad):
        x_grad = incoming_grad
        w_grad = incoming_grad
        return x_grad, w_grad
```

Fitting a function to data

Description (supervised learning)

Given a set of data $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, can we find a function $y = f(x)$ that "fits" this data?

Questions

- What is this function $f(x)$?
- What does "fit" mean?
- How do we know this works?
- What kinds of problems can we solve?

More about $f(x)$

Class of functions

Starting with a function $f(x; \theta_1, \theta_2, \ldots, \theta_n)$ where x is the input to the function and θs are its parameters, we need to find the set of θs that best "fits" the give data $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$

Class of linear functions

Consider $f(x) = ax + b$. If we can say, with some confidence, that our data is linearly related, we need to find $\theta_1 = a$, $\theta_2 = b$ that *fits* the given data. We can also write it as $f(x; a, b) = ax + b$. Preferred,

$$f(x; \theta_1, \theta_2) = \theta_1 x + \theta_2 \tag{23}$$

Fit

Mean squared Euclidean distance as one possible measure of fit

Let L_i be the squared Euclidean distance between the predicted value, $\hat{y}_i = f(x_i)$ and the actual, y_i. Then,

$$L_i = z_i^2 \tag{24}$$

$$z_i = y_i - f(x_i) \tag{25}$$

$$= y_i - \theta_1 x_i - \theta_2 \tag{26}$$

Minimizing L_i with respect to the parameters θ_1 and θ_2,

$$\frac{\partial L_i}{\partial \theta_1} = \frac{\partial z_i^2}{\partial z_i} \frac{\partial z_i}{\partial \theta_1} \tag{27}$$

$$\frac{\partial L_i}{\partial \theta_2} = \frac{\partial z_i^2}{\partial z_i} \frac{\partial z_i}{\partial \theta_2} \tag{28}$$

For n data points, mean loss is

$$L = \frac{1}{n}\sum_{i=1}^{i=n} L_i = \frac{1}{n}\sum_{i=1}^{i=n}(y_i - \theta_1 x_i - \theta_2)^2$$

In practice

- Choose a small (64 or 128) random subset of training data.
- Compute predicted values, then loss.
- Compute gradients of loss W.R.T. parameters then update parameters.

An **epoch** refers to a single iteration over all training data.

Two different spaces

- Space spanned by x and y. Optimization tries to find the surface (model) in this space that best fits the data.
- Space spanned by θs. We minimize the loss function in this space.

Using sigmoid

Definition

$$\sigma(x) = \frac{1}{1 + e^{-x}} \quad (29)$$

$$\frac{d}{dx}\sigma(x) = \sigma(x)(1 - \sigma(x)) \quad (30)$$

Assuming a non-linear function (sigmoidal + affine prior)

Let our function be $y = \sigma(\theta_1 x + \theta_2)$.

Making a non-linear function

New function and the squared error

$$z = \sigma(\hat{y}) \tag{31}$$

$$\hat{y} = \theta_1 x + \theta_2 \tag{32}$$

Error L_i for the ith data point

$$L_i = (\sigma(\theta_1 x_i + \theta_2) - y_i)^2 \tag{33}$$

Finding best θs

Minimizing L_i

$$L_i = \Delta_i^2 \tag{34}$$

$$\Delta_i = z_i - y_i \tag{35}$$

$$z_i = \sigma(\hat{y}_i) \tag{36}$$

$$\hat{y}_i = \theta_1 x_i + \theta_2 \tag{37}$$

$$\frac{\partial L_i}{\partial \theta_1} = \underbrace{\frac{\partial \Delta_i^2}{\partial \Delta_i} \frac{\partial \Delta_i}{\partial z_i} \frac{\partial z_i}{\partial \hat{y}_i}} \frac{\partial \hat{y}_i}{\partial \theta_1} \tag{38}$$

$$\frac{\partial L_i}{\partial \theta_2} = \underbrace{\frac{\partial \Delta_i^2}{\partial \Delta_i} \frac{\partial \Delta_i}{\partial z_i} \frac{\partial z_i}{\partial \hat{y}_i}} \frac{\partial \hat{y}_i}{\partial \theta_2} \tag{39}$$

Finding best θs

Updates to θ_1 and θ_2

$$\frac{\partial L_i}{\partial \theta_1} = \underbrace{\frac{\partial \Delta_i^2}{\partial \Delta_i} \frac{\partial \Delta_i}{\partial z_i} \frac{\partial z_i}{\partial \hat{y}_i}} \frac{\partial \hat{y}_i}{\partial \theta_1} \tag{40}$$

$$\frac{\partial L_i}{\partial \theta_2} = \underbrace{\frac{\partial \Delta_i^2}{\partial \Delta_i} \frac{\partial \Delta_i}{\partial z_i} \frac{\partial z_i}{\partial \hat{y}_i}} \frac{\partial \hat{y}_i}{\partial \theta_2} \tag{41}$$

$$\theta_{1_{p+1}} = \theta_{1_p} - \eta \frac{\partial L_i}{\partial \theta_1} \tag{42}$$

$$\theta_{2_{p+1}} = \theta_{2_p} - \eta \frac{\partial L_i}{\partial \theta_2} \tag{43}$$

Finding best θs

Updates to θ_1 and θ_2

$$\theta_{1_{p+1}} = \theta_{1_p} - \eta \frac{\partial L_i}{\partial \theta_1} \tag{44}$$

$$\theta_{2_{p+1}} = \theta_{2_p} - \eta \frac{\partial L_i}{\partial \theta_2} \tag{45}$$

Vectorized format

$$\vec{\theta_{p+1}} = \vec{\theta_p} - \eta \nabla_{\vec{\theta}} L \tag{46}$$

Using vectors

$x \in \mathbb{R}^n$,$y \in \mathbb{R}^m$, $w \in \mathbb{R}^{m\times n}$

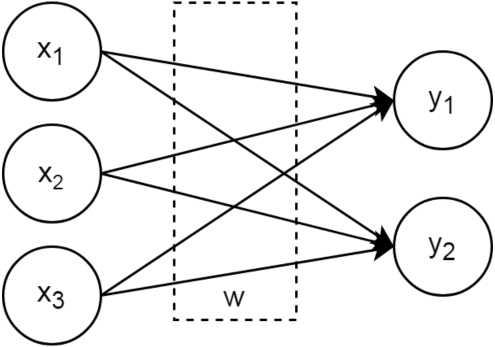
$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & \dots & w_{1n} \\ w_{21} & w_{22} & \dots & w_{2n} \\ \vdots & \vdots & & \vdots \\ w_{m1} & w_{m2} & \dots & w_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

For $m = 2, n = 3$

$$y_1 = w_{11}x_1 + w_{12}x_2 + w_{13}x_3 + b_1 \tag{47}$$

$$y_2 = w_{21}x_1 + w_{22}x_2 + w_{23}x_3 + b_2 \tag{48}$$

Mandatory network diagram



More layers

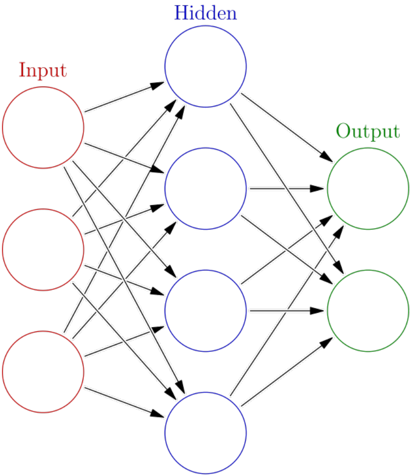
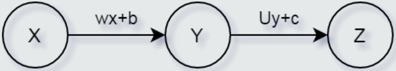


Image from https://en.wikipedia.org/wiki/Artificial_neural_network

Multiple layers

Layers (composition) of $ax + b$ style functions



$$
\begin{aligned}
y &= \mathbb{W}x + b \\
z &= \mathbb{U}y + c = \mathbb{U}(\mathbb{W}x + b) + c \\
&= (\mathbb{U}\mathbb{W})x + (\mathbb{U}b + c) = \mathbb{V}x + d
\end{aligned}
$$

Introducing non-linearity with element-wise sigmoid

$$
\begin{aligned}
y &= \sigma(\mathbb{W}x + b) \\
z &= \sigma(\mathbb{U}y + c)
\end{aligned}
$$

Multi-layer, feed forward, non-polynomial

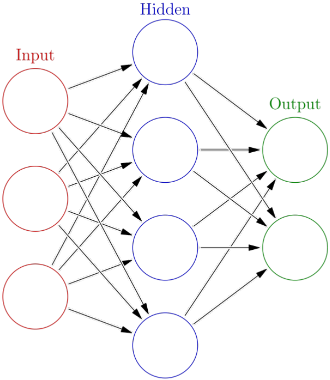
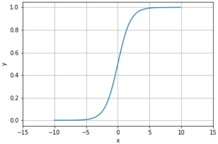


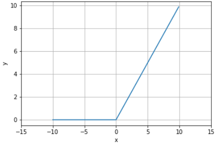
Image from https://en.wikipedia.org/wiki/Artificial_neural_network

Activation functions

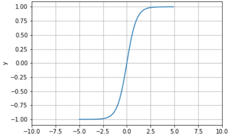
$$f(x) = \frac{1}{1 + e^{-x}}$$



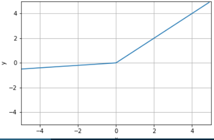
$$f(x) = max(x, 0)$$



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



$$f(x) = \begin{cases} x, & \text{if } x \geq 0 \\ 0.1x, & \text{otherwise} \end{cases}$$



What can these functions (neural networks) do?

A standard multilayer feed-forward network with a locally bounded piecewise continuous activation function can approximate any continuous function to any degree of accuracy if and only if the network's activation function is not a polynomial.

-Leshno et al.,1993

In particular, we show that arbitrary decision regions can be arbitrarily well approximated by continuous feed forward neural networks with only a single internal, hidden layer and any continuous sigmoidal nonlinearity.

-Cybenko, 1989

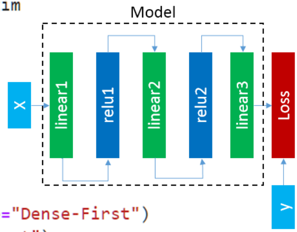
Python code

```python
# Build the network
import core.np.Activations as act
import core.np.Loss as loss
from core.np.utils import to_one_hot
import core.np.Optimization as autodiff_optim
import core.np.regularization as reg
from core import info, debug, log_at_info
import time
import matplotlib.pyplot as plt

x_node = node.VarNode('x')
y_target_node = node.VarNode('yt')

linear1 = node.DenseLayer(x_node, 100, name="Dense-First")
relu1 = act.RelUNode(linear1, name="RelU-First")
linear2 = node.DenseLayer(relu1, 200, name="Dense-Second")
relu2 = act.RelUNode(linear2, name="RelU-Second")
linear3 = node.DenseLayer(relu2, 10, name="Dense-Third")

loss_node = loss.LogitsCrossEntropy(linear3, y_target_node, name="XEnt")
```



Steps

- Settle on a class of function with parameters to be optimized.
- Define a secondary function - the loss function.
- Split data into training set, validation set and test set. Use randomization. For the following discussion, we ignore validation set.
- Initialize model weights (W's or θs), typically using small random numbers.
- Iterate over the data in batches
  - compute the predicted value
  - compute the loss
  - compute gradients
  - update parameters
- Keep track of loss and stop when loss stops decreasing.
- Compute loss for test set.

Why now?

- Activation functions
- Initialization approaches
- New optimization algorithms*
- Architectures for better propagation of gradients
- Availability of massive amounts of data - generation + storage
- Advances in processor speeds and GPUs
- New ways of working and collaborating

Learning, libraries etc.

Why use libraries

- Define compute graph easily
- calculates gradient
- Move between CPU and GPU
- Model libraries, trained models, utilities

Libraries

- Torch and Theano
- Tensorflow
- Keras
- Pytorch

Next

Part II

- Autoencoders and PCA
- Convolution neural networks
- Recurrent neural networks
- Transfer learning
- GANs (possibly!)

References

Automatic differentiation in machine learning: A survey

Atilim Gunes Baydin, Barak A. Pearlmutter & Alexey Andreyevich Radul
arxiv http://arxiv.org/abs/1502.05767