Neural Networks - Backpropagation and beyond

September 13, 2016

```
Out[1]: <IPython.core.display.HTML object>
```

1 A little bit of history: Linear Perceptron

Mark 1 perceptron (Frank Rosenblatt, 1957):

- An image recognition apparatus;
- 400 photo cells
- Weights are potentiometers;
- Weights are changed by electric motors.

The New York Times, 1958: > [...] the embryo of an electronic computer that the Navy expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence.

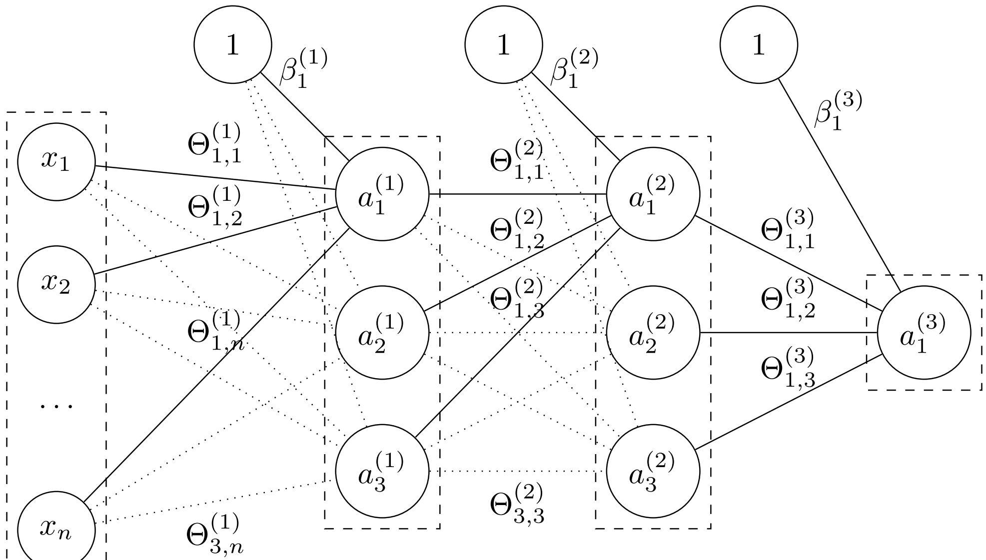
```
Out[2]: <IPython.lib.display.YouTubeVideo at 0x7f84f1e392e8>
```

1.1 Training the perceptron (no human guidance)

Training cycle (2000 "epochs"):

- holding an image in front of the digital camera (eg. triangle, circle, square,...);
- observing which of the two lamps lit up (binary classes);
- checking if the lamp is correct (arbitrarily chosen);
- sending "reward" or "penalty" signal.
- human operator only performs mechanical actions.

2 Multi-layer neural networks - Inference



$$
\begin{array}{llll}
 & z^{(1)} = \Theta^{(1)} a^{(0)} + \beta^{(1)} & z^{(2)} = \Theta^{(2)} a^{(1)} + \beta^{(2)} & z^{(3)} = \Theta^{(3)} a^{(2)} + \beta^{(3)} \\
a^{(0)} = x & g^{(1)}(x) = \tanh(x) & g^{(2)}(x) = \tanh(x) & g^{(3)}(x) = \tanh(x) \\
 & a^{(1)} = g^{(1)}(z^{(1)}) & a^{(2)} = g^{(2)}(z^{(2)}) & a^{(3)} = g^{(3)}(z^{(3)})
\end{array}
$$

- Given a n-layer neural network and its parameters $\Theta^1, \dots, \Theta^L$ oraz $\beta^1, \dots, \beta^L$, we calculate for $l \in \{1, \dots, L\}$:
$$a^l = g^l\left(\Theta^l a^{l-1} + \beta^l\right).$$
- Parameters Θ^l, weights on connection between neurons of layers a^{l-1} and a^l, have size $\dim(a^l) \times \dim(a^{l-1})$.
- Bias vectors β replace columns with "1" in feature matrix. The size of β^l is equal to the size of the corresponding layer $\dim(a^l)$.

- Function g^l is the so called **activation function**;
- For $i = 0$ we assume $a^0 =$ x (features or input layer) and $g^0(x) = x$ (identity);
- In the case of classifiers, for the last layer L often $g^L(x) = \mathrm{softmax}(x)$;
- Other activation functions are often sigmoids (eg. logistic function or hyperbolic tangens, tanh);
- In the case of regression networks, the last layer consists often of a single neuron.

2.1 Training multi-layer networks

- Parameters:
$$\Theta = (\Theta^1, \Theta^2, \Theta^3, \beta^1, \beta^2, \beta^3)$$
- Model:

$$h_\Theta(x) = \tanh(\Theta^3 \tanh(\Theta^2 \tanh(\Theta^1 x + \beta^1) + \beta^2) + \beta^3)$$

* Cost function (MSE):

$$J(\Theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\Theta(x^{(i)}) - y^{(i)})^2$$

* How do we calculate the gradients?

$$\nabla_{\Theta^l} J(\Theta) = ? \quad \nabla_{\beta^l} J(\Theta) = ? \quad l \in \{1, 2, 3\}$$

3 Backpropagation

- A hypothetical change Δz_j^l added to the j-th neuron in layer l propagates through the network and causes cost change:

$$\frac{\partial J(\Theta)}{\partial z_j^l}\Delta z_j^l$$

- If $\frac{\partial J(\Theta)}{\partial z_j^l}$ is large, Δz_j^l with an opposite sign can reduce the cost.
- If $\frac{\partial J(\Theta)}{\partial z_j^l}$ is close to zero, the cost cannot be much improved.
- We define the error δ_j^l of neuron j in layer l:

$$\delta_j^l \equiv \frac{\partial J(\Theta)}{\partial z_j^l} \qquad \delta^l \equiv \nabla_{z^l} J(\Theta) \text{ (vectorized)}$$

3.1 The four fundamental equations of Backpropagation (proofs anyone?)

$$\begin{aligned}
\delta^L &= \nabla_{a^L} J(\Theta) \odot (g^L)'(z^L) && (BP1)\\
\delta^l &= ((\Theta^{l+1})^T \delta^{l+1}) \odot (g^l)'(z^l) && (BP2)\\
\nabla_{\beta^l} J(\Theta) &= \delta^l && (BP3)\\
\nabla_{\Theta^l} J(\Theta) &= a^{l-1} \odot \delta^l && (BP4)
\end{aligned}$$

3.2 The Backpropagation Algorithm

For one training example (x,y):

1. **Input**: Set the activations of the input layers $a^0 = x$
2. **Forward step:** for $l = 1, \ldots, L$ calculate

$$z^l = \Theta^{(l)} a^{l-1} + \beta^l \text{ and } a^l = g^l(z^l)$$

3. **Output error δ^L:** calculate vector

$$\delta^L = \nabla_{a^L} J(\Theta) \odot (g^L)'(z^L)$$

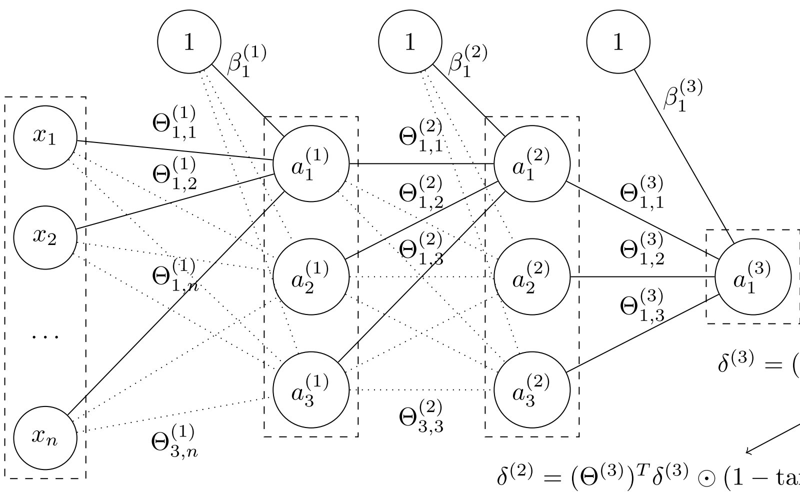
4. **Error backpropagation:** for $l = L-1, L-2, \ldots, 1$ calculate

$$\delta^l = ((\Theta^{l+1})^T \delta^{l+1}) \odot (g^l)'(z^l)$$

5. **Gradients:**

$$\nabla_{\Theta^l} J(\Theta) = a^{l-1} \odot \delta^l \text{ and } \nabla_{\beta^l} J(\Theta) = \delta^l$$

$$J(\Theta) = \frac{1}{2}(a^L - y)^2$$
$$\nabla_{a^L} J(\Theta) = a^L - y$$
$$\tanh'(x) = 1 - \tanh^2(x)$$



$$\delta^{(3)} = (a^{(3)} - y) \odot (1 - \tanh^2(z^{(3)}))$$

$$\delta^{(2)} = (\Theta^{(3)})^T \delta^{(3)} \odot (1 - \tanh^2(z^{(2)}))$$

$$\delta^{(1)} = (\Theta^{(2)})^T \delta^{(2)} \odot (1 - \tanh^2(z^{(1)}))$$

$$a^{(0)} = x \longrightarrow \begin{array}{l} z^{(1)} = \Theta^{(1)} a^{(0)} + \beta^{(1)} \\ g^{(1)}(x) = \tanh(x) \\ a^{(1)} = g^{(1)}(z^{(1)}) \end{array} \longrightarrow \begin{array}{l} z^{(2)} = \Theta^{(2)} a^{(1)} + \beta^{(2)} \\ g^{(2)}(x) = \tanh(x) \\ a^{(2)} = g^{(2)}(z^{(2)}) \end{array} \longrightarrow \begin{array}{l} z^{(3)} = \Theta^{(3)} a^{(2)} + \beta^{(3)} \\ g^{(3)}(x) = \tanh(x) \\ a^{(3)} = g^{(3)}(z^{(3)}) \end{array}$$

3.3 SGD with Backpropagation

One iteration: * For all parameters $\Theta = (\Theta^1, \ldots, \Theta^L)$ create zero-valued helper matrices $\Delta = (\Delta^1, \ldots, \Delta^L)$ of the same size (β omitted for simplicity). * For m examples in the batch, $i = 1, \ldots, m$: * Perform backpropagation for example $(x^{(i)}, y^{(i)})$ and store the gradients $\nabla_\Theta J^{(i)}(\Theta)$ * $\Delta := \Delta + \frac{1}{m} \nabla_\Theta J^{(i)}(\Theta)$ * Update the weights: $\Theta := \Theta - \alpha\Delta$

3.4 What about more complicated networks?

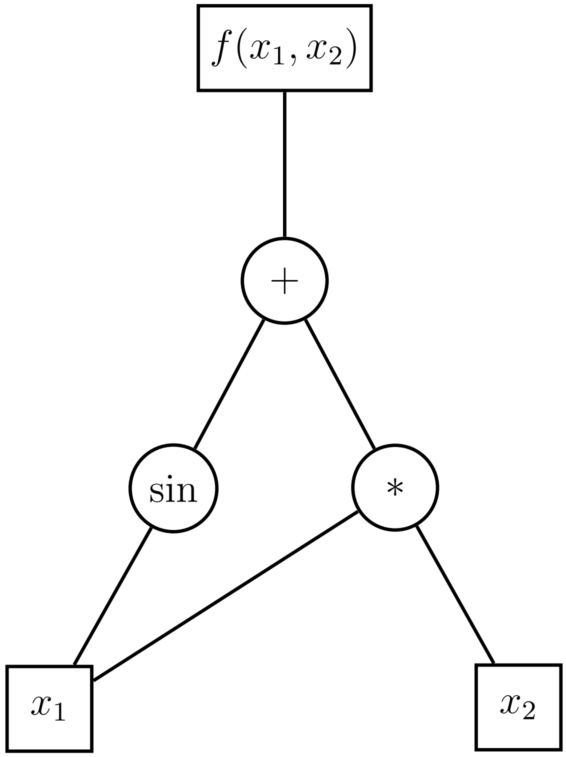
- Backprogagation is usually formulated in the language of (Feedforward) Neural Networks (layers, weights, biases, activations, weighted inputs, …)
- Today's NNs contain more complicated operation, e.g. concatenation of bidirectional RNN states, …
- But: what's the derivation of the "concatenation" operation and where does that fit into the BP equations?

4 Reverse-mode Autodiff

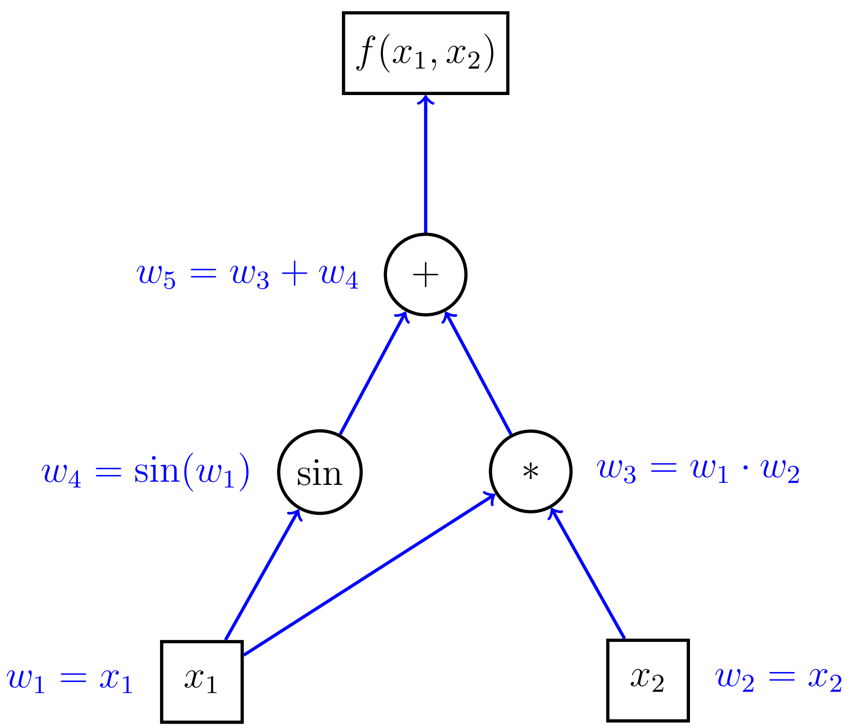
4.1 Let's calculate gradients for anything … automatically!

$$f(x_1, x_2) = \sin(x_1) + x_1 x_2$$

4.2 An example computation graph



4.3 Forward propagations of values



4.4 The idea of reverse-mode auto-differentiation:

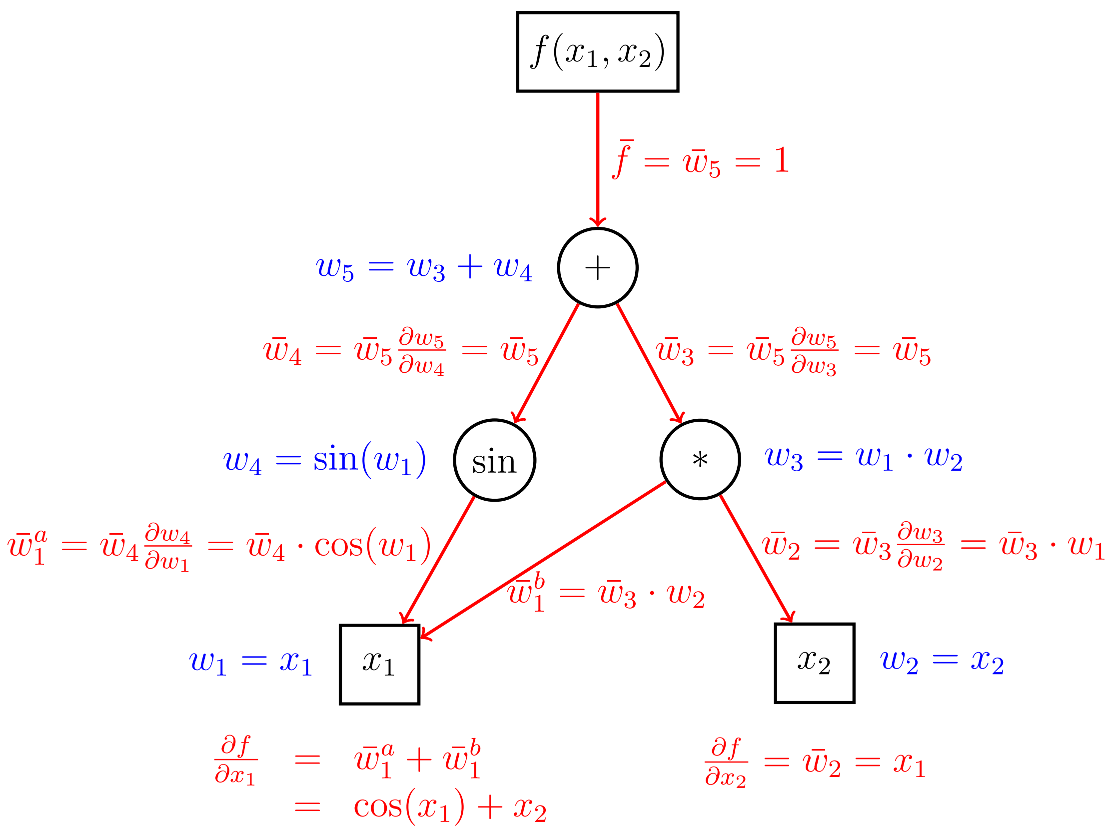
- Repeatedly substitute the derivative of the outer functions in the chain rule;
- Sub-expression follow the structure of the computation graph.

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial w_1}\frac{\partial w_1}{\partial x} = \left(\frac{\partial f}{\partial w_2}\frac{\partial w_2}{\partial w_1}\right)\frac{\partial w_1}{\partial x} = \left(\left(\frac{\partial f}{\partial w_3}\frac{\partial w_3}{\partial w_2}\right)\frac{\partial w_2}{\partial w_1}\right)\frac{\partial w_1}{\partial x} = \dots$$

- We calculate the ***adjoint***:

$$\bar{w} = \frac{\partial f}{\partial w}$$

4.5 Back propagation of adjoints



4.6 2-layer Neural Network

```
auto x = input(shape={whatevs, 784});
auto y = input(shape={whatevs, 10});
```

```
auto w1 = param(shape={784, 100});
auto b1 = param(shape={1, 100});
auto l1 = tanh(dot(x, w1) + b1);

auto w2 = param(shape={100, 10});
auto b2 = param(shape={1, 10});
auto l2 = softmax(dot(l1, w2) + b2, axis=1);

auto graph = -mean(sum(y * log(l2), axis=1), axis=0);

x = Tensor({500, 784}, 1);
y = Tensor({500, 10}, 1);

graph.forward();
graph.backward();

auto dw = w.grad();
auto db = b.grad();
```

4.7 Unary node for Tanh operation in Marian

```
struct TanhNodeOp : public UnaryNodeOp {
  template <typename ...Args>
  TanhNodeOp(Args ...args)
  : UnaryNodeOp(args...) { }

  void forward() {
    Element(_1 = Tanh(_2),
            val_, a_->val());
  }

  void backward() {
    Element(_1 += _2 * (1 - Tanh(_3) * Tanh(_3)),
            a_->grad(), adj_, a_->val());
  }
};
```

4.8 Binary node for Division operation in Marian

```
struct DivNodeOp : public BroadcastingNodeOp {
  template <typename ...Args>
  DivNodeOp(Args ...args) : BroadcastingNodeOp(args...) { }

  void forward() {
    Element(_1 = _2 / _3,
            val_, a_->val(), b_->val());
  }

  void backward() {
    Element(_1 += _2 * 1.0f / _3,
            a_->grad(), adj_, b_->val());
    Element(_1 -= _2 * _3 / (_4 * _4),
            b_->grad(), adj_, a_->val(), b_->val());
```

```
  }
};
```

4.9 Complex Softmax node defined by other operators

```
template <typename ...Args>
inline Expr softmax(Expr a, Args ...args) {
  Expr e = exp(a);
  return e / sum(e, args...);
}
```