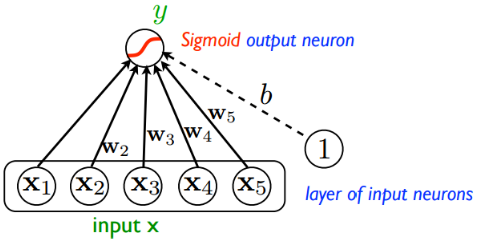
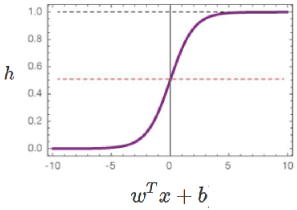
Basics of Training Neural Nets

Logistic Regression – Simplest Network



$$h(w^T x + b) = \frac{1}{1 + e^{-(w^T x + b)}}$$



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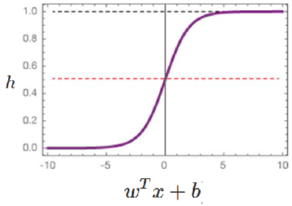

Can model class probabilities

$$P(y = 1 | w, b, x) = h(w^T x + b)$$

$$P(y = 0 | w, b, x) = 1 - h(w^T x + b)$$

Classification with Logistic Regression

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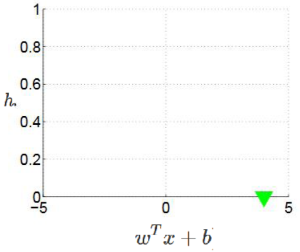
e.g.,

y=1 => Cat
y=0 => Dog



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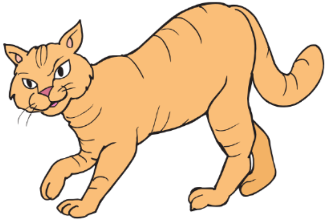

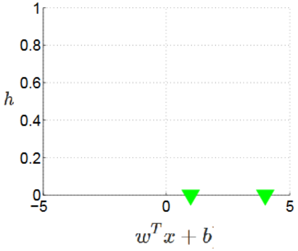

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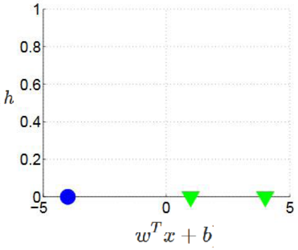

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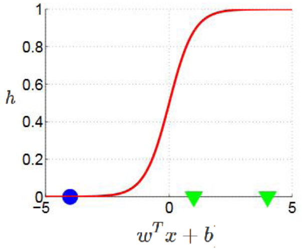

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The above two equations can be combined as:

$$P(y|w,b,x) = (h(w^T x + b))^y \; (1 - h(w^T x + b))^{1-y}$$

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The overall probability for M training examples:

$$P(Y|w,b,X) = \prod_{i=1}^{M} (h(w^T x_i + b))^{y_i} \ (1 - h(w^T x_i + b))^{1-y_i}$$

Classification with Logistic Regression

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$$\max_{w,b} \; P(Y|w,b,X)$$

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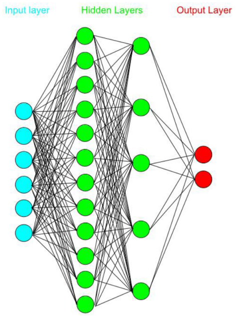
For a new example, x, we compute $h(w^T x + b)$ to get its probability for being a cat

Multiple Layers

To model more complex relations – we can go deep



Sometimes called Multilayer Perceptron (MLP)

How to Learn

Rumelhart, D.E., Hinton G.E, and Williams R.J. Learning representations by back-propagating errors. Nature 323 (Oct. 9, 1986), 533–536.

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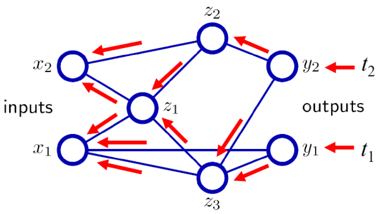
Intuitive explanation:

- Compute approximation error at the output
- Propagate error back by computing individual contributions of parameters to error



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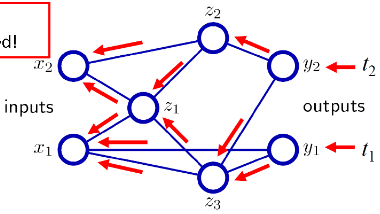
Very hand wavy
Confusion guaranteed!



Gradient Descent

$$\max_w f(w) \quad or \quad \min_w e(w)$$

Gradient descent $\min_w e(w)$

Algorithm: start with w_0, $t = 0$

1. Compute gradient $g_t = \frac{\partial e}{\partial w}\Big|_{w=w_t}$
2. Update $w_{t+1} = w_t - \eta g_t$
3. Set $t \leftarrow t + 1$

How to get gradients

1. Analytically Compute Gradients

$$\nabla e(w) = \frac{\partial e}{\partial w}$$

If you can do it, that's the best option!

Fast, Accurate, Exact!

BUT

Tedious to derive
Tedious to Implement
Error prone
Tedious to debug

How to get gradients

2. Numerically Compute Gradients

$$\frac{\partial e}{\partial w_i} = \frac{e(w_i + \epsilon \mid w \backslash w_i) - e(w_i - \epsilon \mid w \backslash w_i)}{2\epsilon}$$

Trivially Easy to Implement

BUT

Slow and Approximate

2N function calls if N parameters for every gradient descent step (Not Good)

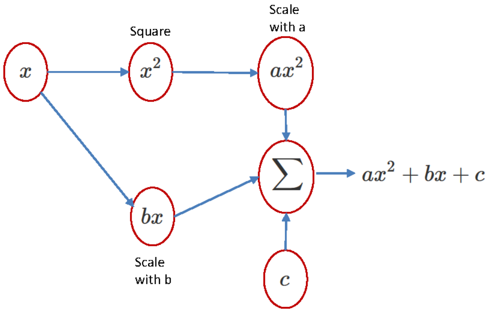
Exploiting Chain Rule

3. Automatic Differentiation (Exploit Chain Rule)

$$\frac{\partial}{\partial x} g(f(x)) = \frac{\partial g}{\partial f} \cdot \frac{\partial f}{\partial x}$$

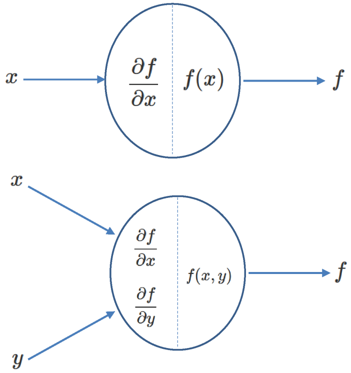
Computation Graph

$$f(x) = ax^2 + bx + c$$



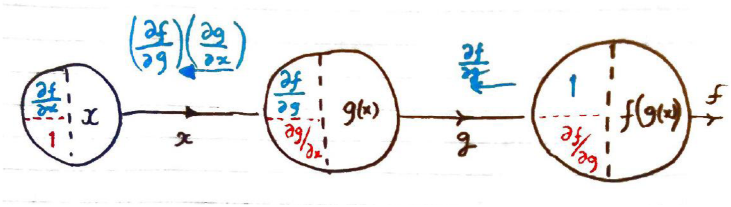
A function can be represented as a directed acyclic Computation Graph in terms of primitive functions. Once a function is represented as a computation graph, implementing chain rule becomes an exercise in memoization...

Memoization of Derivatives


x
$\frac{\partial f}{\partial x}$
$f(x)$
f
x
$\frac{\partial f}{\partial x}$
$\frac{\partial f}{\partial y}$
$f(x, y)$
f
y

While computing a node function in the graph store the derivative of the node output with respect of its input.

Memoization Example: Composition of Functions

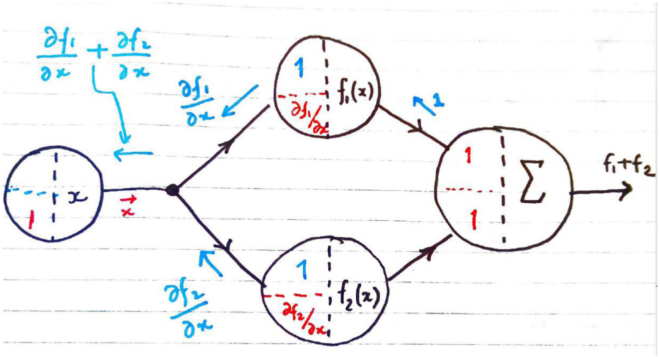


$\left(\frac{\partial f}{\partial g}\right)\left(\frac{\partial g}{\partial x}\right)$
$\frac{\partial f}{\partial g}$
$\frac{\partial f}{\partial x}$
1
x
x
$\frac{\partial f}{\partial g}$
$\partial g/\partial x$
$g(x)$
g
1
$\partial f/\partial g$
$f(g(x))$
f

Function Composition

- The terms in red represent the memoized derivatives stored during the forward pass. They are the derivatives of the respective node's output with respect to its input.
- The terms in blue flow and get collected during the backward pass. They represent the derivative of the main output function with respect to the output of the respective node.

Memoization Example: Addition of functions

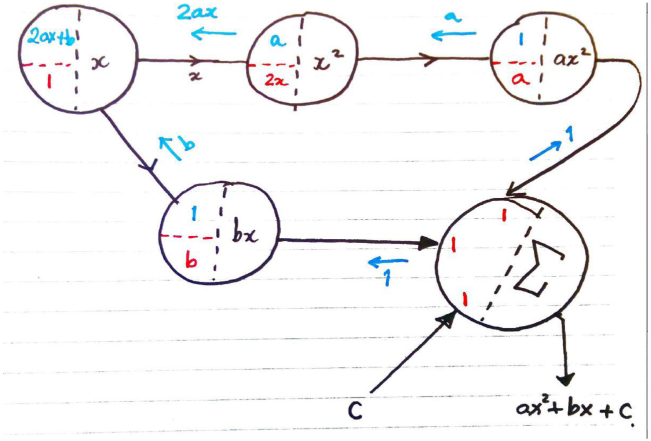


$\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial x}$
$\frac{\partial f_1}{\partial x}$
$\frac{\partial f_2}{\partial x}$
x
1
$\vec{x}$
1
$f_1(x)$
$\partial f_1/\partial x$
1
$f_2(x)$
$\partial f_2/\partial x$
1
Σ
1
1
f_1+f_2

Function Summation

- The red and blue terms represent the same quantities as in the previous slide. In this example, when two paths merge during backward pass, the sum of the two quantities flow backwards.

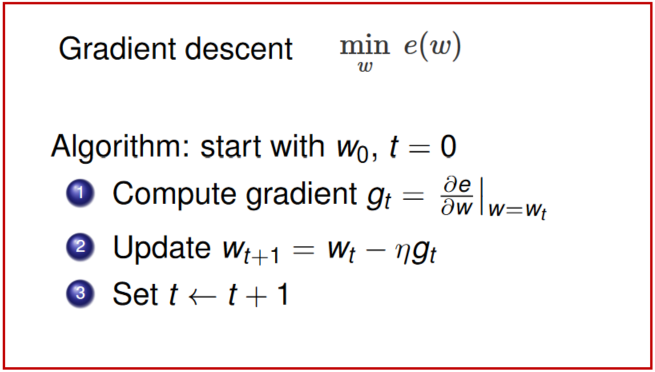
Memoization Example: Quadratic



Chain Rule on our Quadratic Example

Now we know how to compute gradients – so run Gradient Descent

$$\max_{w} f(w) \quad or \quad \min_{w} e(w)$$



Gradient descent $\min_{w} e(w)$

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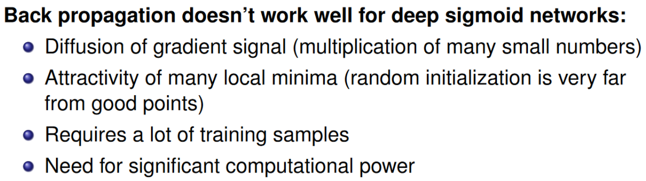
Problems with Back Propagation



Back propagation doesn't work well for deep sigmoid networks:

- Diffusion of gradient signal (multiplication of many small numbers)
- Attractivity of many local minima (random initialization is very far from good points)
- Requires a lot of training samples
- Need for significant computational power

Tricks to handle problems

To obtain more flexibility/non-linearity we use additional function prototypes:

- Sigmoid
- Rectified linear unit (ReLU)
- Pooling
- Dropout
- Convolutions

Tricks to handle problems

Rectified Linear Unit (ReLU)

- Drop information if smaller than zero
- **Fixes the problem of vanishing gradients to some degree**

Dropout

- Drop information at random
- Kind of a regularization