"How to Train Your Neural Network"

Alexander G. Ororbia II

Introduction to Machine Learning

CSCI-335

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Background

A Recipe for Machine Learning

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^{N}$$

2. Choose each of these:

- Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

- Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with SGD:

(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Background

A Recipe for

Gradients

Backpropagation can compute this gradient!

And it's a **special case of a more general algorithm** called reverse-mode automatic differentiation that can compute the gradient of any differentiable function efficiently!

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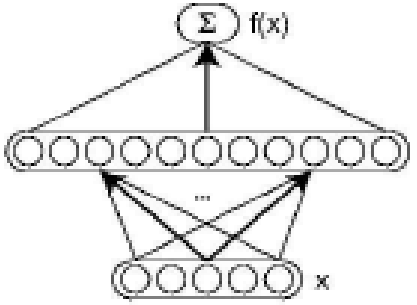
White Board Time!

(Backprop & Computational Graphs)



Approaches to Differentiation

1. Finite Difference Method
   - Pro: Great for testing implementations of backpropagation
   - Con: Slow for high dimensional inputs / outputs
   - Required: Ability to call the function f(**x**) on any input **x**
2. Symbolic Differentiation
   - Note: The method you learned in high-school
   - Note: Used by Mathematica / Wolfram Alpha / Maple
   - Pro: Yields easily interpretable derivatives
   - Con: Leads to exponential computation time if not carefully implemented
   - Required: Mathematical expression that defines f(**x**)
3. Automatic Differentiation - Reverse Mode
   - Note: Called *Backpropagation* when applied to Neural Nets
   - Pro: Computes partial derivatives of one output $f(\mathbf{x})_i$ with respect to all inputs x_j in time proportional to computation of f(**x**)
   - Con: Slow for high dimensional outputs (e.g. vector-valued functions)
   - Required: Algorithm for computing f(**x**)
4. Automatic Differentiation - Forward Mode
   - Note: Easy to implement. Uses dual numbers.
   - Pro: Computes partial derivatives of all outputs $f(\mathbf{x})_i$ with respect to one input x_j in time proportional to computation of f(**x**)
   - Con: Slow for high dimensional inputs (e.g. vector-valued **x**)
   - Required: Algorithm for computing f(**x**)

Given $f : \mathbb{R}^A \rightarrow \mathbb{R}^B, f(\mathbf{x})$

Compute $\frac{\partial f(\mathbf{x})_i}{\partial x_j} \forall i, j$

The Finite Difference Method

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

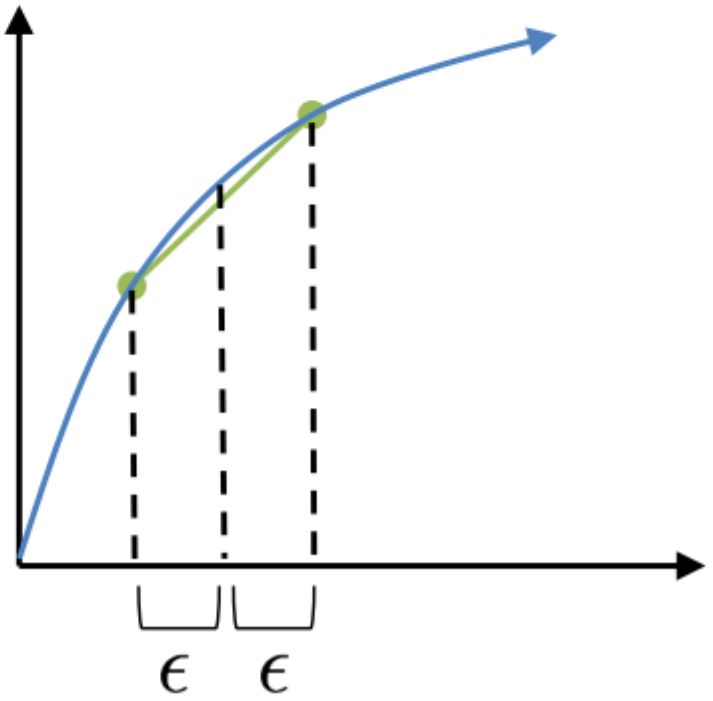
The *centered* finite difference approximation is:

$$\frac{\partial}{\partial \theta_i} J(\boldsymbol{\theta}) \approx \frac{(J(\boldsymbol{\theta} + \epsilon \cdot \boldsymbol{d}_i) - J(\boldsymbol{\theta} - \epsilon \cdot \boldsymbol{d}_i))}{2\epsilon}$$

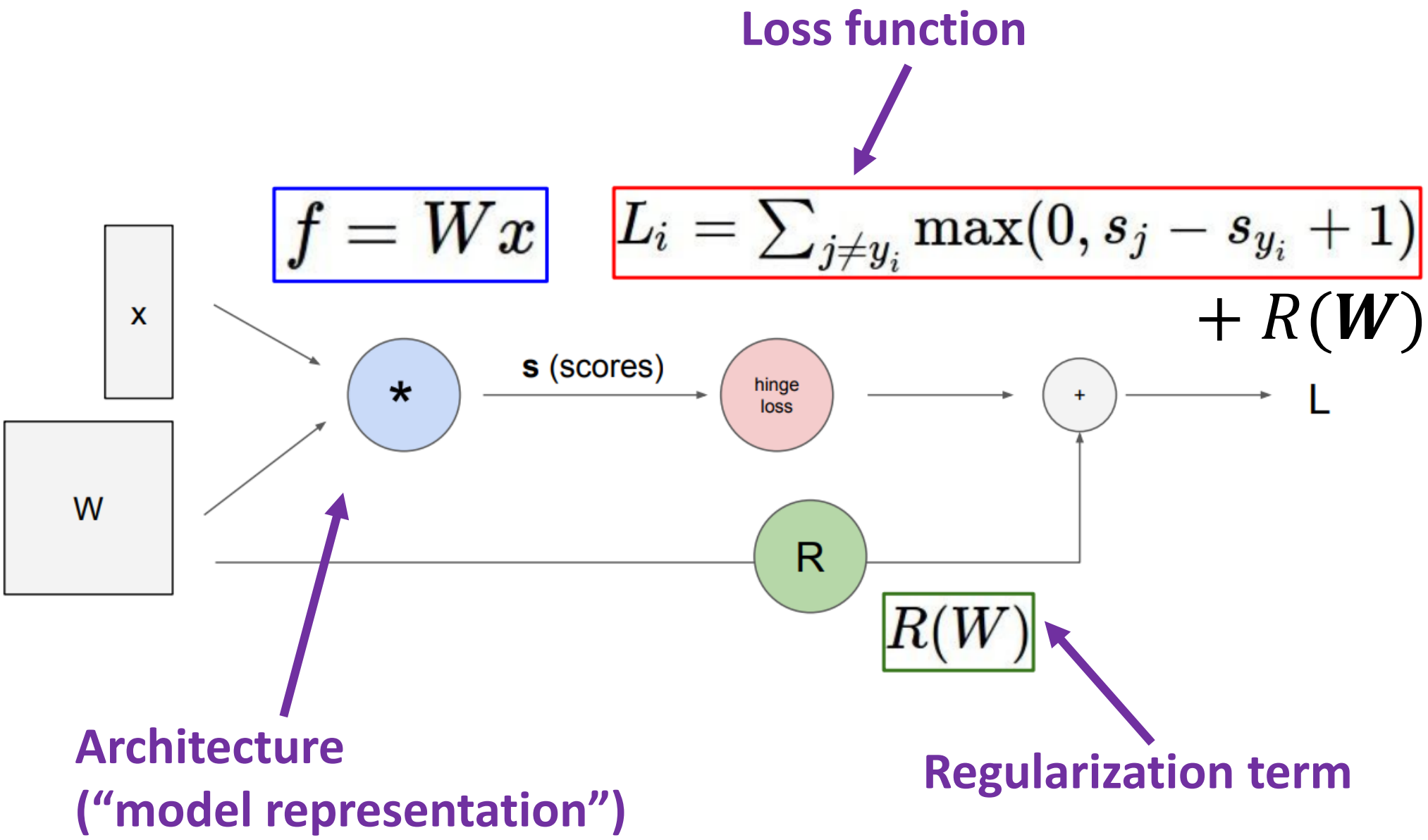
where $\boldsymbol{d}_i$ is a 1-hot vector consisting of all zeros except for the ith entry of $\boldsymbol{d}_i$, which has value 1.

Notes:

- Suffers from issues of floating point precision, in practice
- Typically only appropriate to use on small examples with an appropriately chosen epsilon

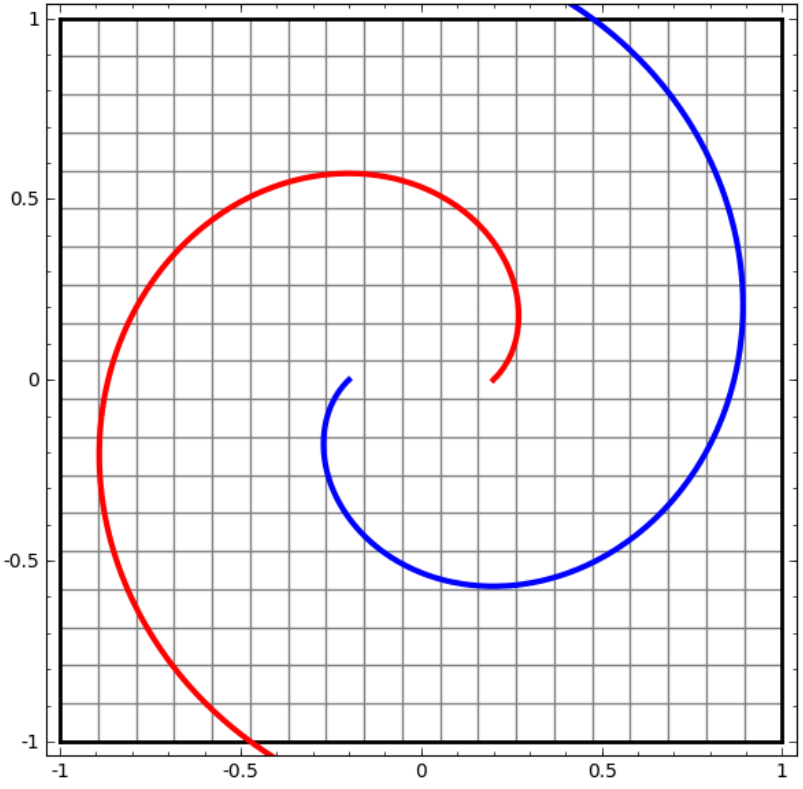


Computational Graph (Example)



Reverse Mode Differentiation

- Application of the chain-rule from calculus
- Can view ANNs at level of processing elements (PEs)— "neuronal graph"
  - Follow dot-arrow diagram to get partial derivative scalars
  - Limited flexibility, but simple to understand
- Can view this at lowest level— computation graph
  - Follow graph of operators & get partial derivatives using sub-rules (sum rule, product rule, etc.)
  - Highly flexible
  - Tools that do this:
    - ***Theano***: http://deeplearning.net/software/theano/
    - ***TensorFlow2***: https://www.tensorflow.org/
    - ***PyTorch***: https://pytorch.org/



'Deep calculus"!

The Vanishing Gradient Problem

- Solving credit assignment problem with back-propagation (backprop) too difficult
  - Difficult to know how much importance to accord to remote inputs (Bengio et al., 1994)
  - Information passed through chain of multiplications back through network
    - Any value slightly less than 1 in Hadamard product, derivative signal quickly shrinks to useless values (near zero)
  - Learning long-term dependencies in temporal sequences becomes near impossible
- Complementary problem: Exploding gradients
  - Any value greater than 1 in Hadamard product, derivative signal increases dramatically (numerical overflow)

QUESTIONS?