CS-568 Deep Learning

Automatic Differentiation

Nazar Khan
Department of Computer Science
University of the Punjab

Automatic Differentiation (AD)

- Set of techniques to numerically evaluate the derivative of a function that is *specified by a computer program*.
- Analytic or symbolic differentiation evaluates the derivative of a function *specified by a math expression*.
- Also called *algorithmic differentiation* or *computational differentiation*.
- Backpropagation is a special case of AD.
- Modern machine learning frameworks (TensorFlow, PyTorch) employ AD.
- Programmer implements the forward-pass only, up to the loss function.
- Derivatives are handled *automatically!*

Automatic Differentiation

AD exploits the fact that every computer program, no matter how complicated, executes a ***sequence*** *of* ***elementary arithmetic operations*** *(addition, subtraction, multiplication, division, etc.) and* ***elementary functions*** *(*exp, log, sin, cos, *etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.*

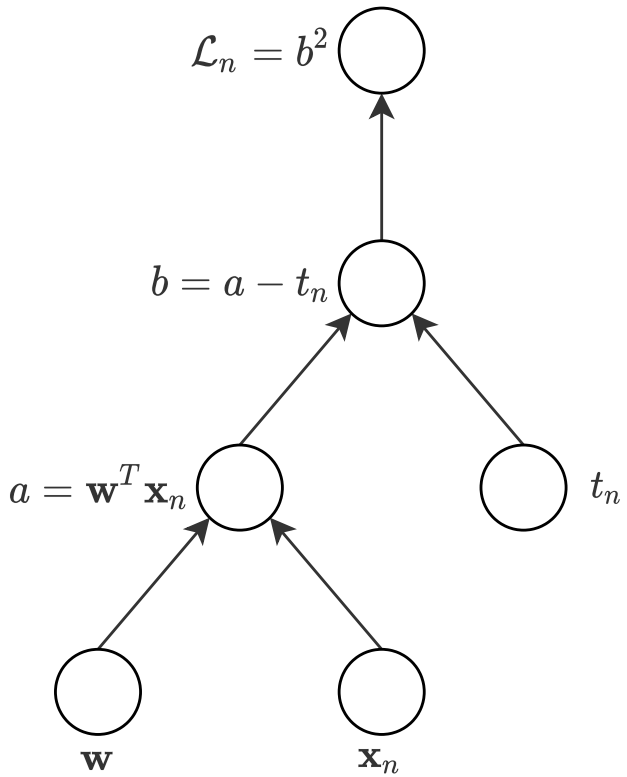
https://en.wikipedia.org/wiki/Automatic_differentiation

Linear Regression via Automatic Differentiation

- Consider the squared loss function for linear regression.

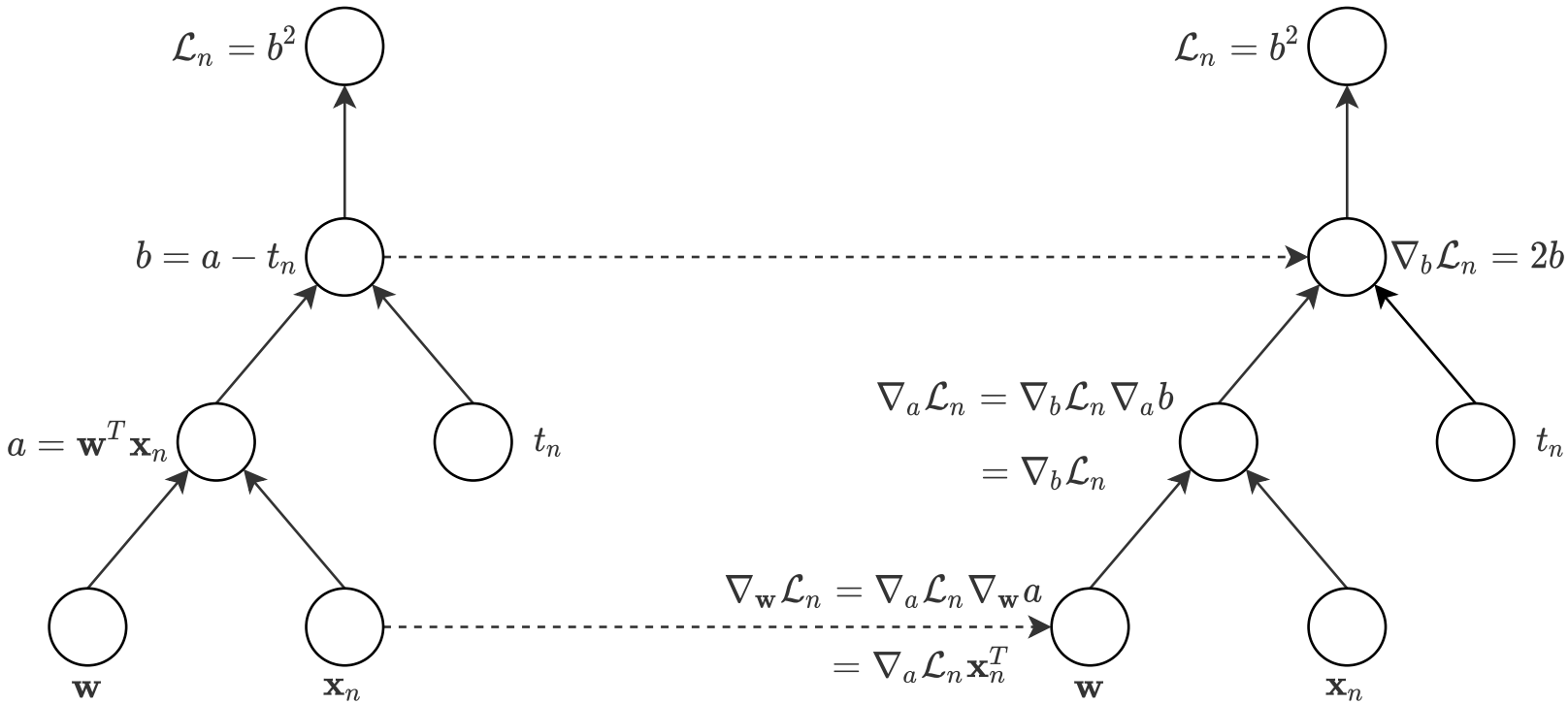
$$\mathcal{L}_n(\mathbf{w}) = \left(\mathbf{w}^T \mathbf{x}_n - t_n\right)^2$$

- Can be represented as a **computational graph** consisting of *elementary operations*.



Linear Regression via Automatic Differentiation

- For training, we are interested in the gradient $\nabla_{\mathbf{w}} \mathcal{L}_n$.
- After the forward pass for a particular $\mathbf{w}$ and $\mathbf{x}_n$, gradients can be evaluated numerically.



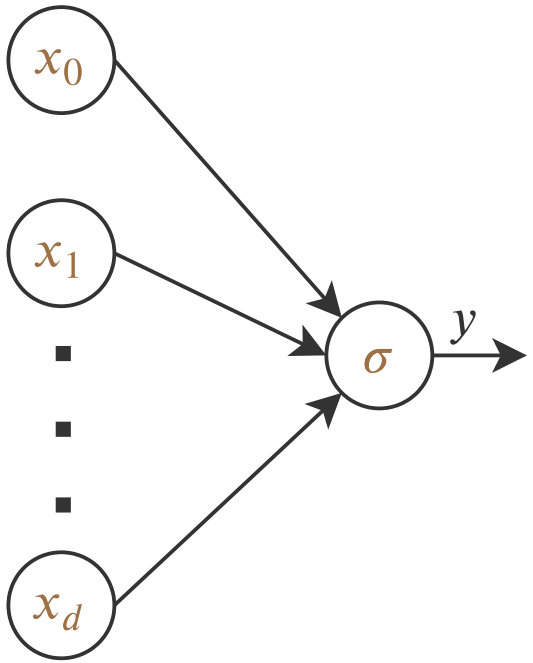
AD in Python

- A Python package called *Autograd* implements *reverse mode* automatic differentiation.
- Elementary operations such as $+, \sin, x^k$ *etc.* are *overloaded* by also computing their derivates $1, \cos, kx$ *etc.*.
- If required, more sophisticated user-defined functions and their derivative implementations can be *registered* with Autograd.

Logistic Regression via Automatic Differentiation

Binary classifier with no hidden layer

Just a perceptron with logistic sigmoid activation function. Models probability of class 1 instead of decision.



$$y = p(\mathcal{C}_1|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x})$$
$$1 - y = p(\mathcal{C}_2|\mathbf{x}) = 1 - p(\mathcal{C}_1|\mathbf{x})$$

Binary cross-entropy loss

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N} t_n \ln y_n + (1 - t_n) \ln (1 - y_n)$$

Logistic Regression via Automatic Differentiation

Step 1: Computational Graph for $\mathcal{L}_n$

Logistic Regression via Automatic Differentiation

Step 2: AutoDiff till $\nabla_{\mathbf{w}} \mathcal{L}_n$

Summary

- Modern machine learning frameworks such as TensorFlow and PyTorch do not require a programmer to write code for derivatives.
- Programmer implements the forward-pass up to the loss function only.
- Derivatives and backpropagation are handled automatically via automatic differentiation.
- It is a set of techniques to numerically evaluate the derivative of any function that is *specified by a computer program*.