Deep Learning

Automatic Differentiation

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Automatic Differentiation (AD)

- Set of techniques to numerically evaluate the derivative of a function *specified by a computer program*.
- Analytic or symbolic differentiation evaluates the derivative of a function *specified by a math expression*.
- AD Also called *algorithmic differentiation* or *computational differentiation*.
- Backpropagation is a special case of AD.

Modern machine learning frameworks (TensorFlow, Theano, PyTorch) employ AD. The programmer only needs to implement the forward pass 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.*

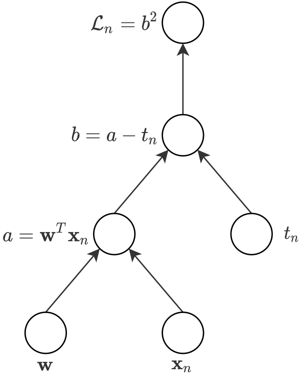
https://en.wikipedia.org/wiki/Automatic_differentiation

Linear Regression via Automatic Differentiation

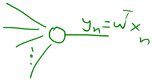
- Consider the squared loss function for linear regression.

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

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



Linear Regression via Automatic Differentiation



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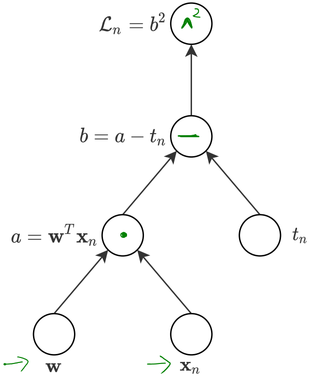
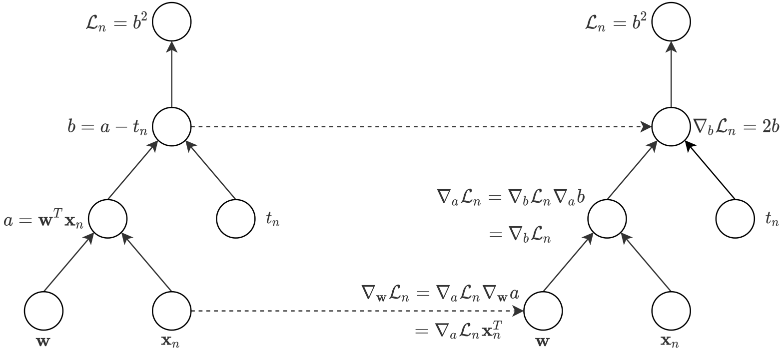


Linear Regression via Automatic Differentiation

- 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.



Linear Regression via Automatic Differentiation

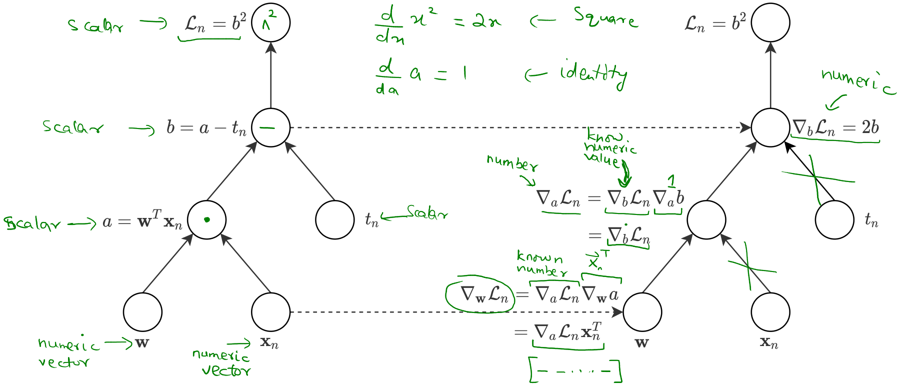
$L = (w^T x_n - t_n)^2$ $\boxed{\nabla_w L = 2(w^T x_n - t_n) x_n^T}$ No need anymore

- For training, we are interested in the gradient $\nabla_{\mathbf{w}} L_n$. $\left[\frac{\partial L}{\partial w_1} \; \frac{\partial L}{\partial w_2} \cdots \frac{\partial L}{\partial w_D}\right]$
- After the forward pass for a particular $\mathbf{w}$ and $\mathbf{x}_n$, gradients can be evaluated numerically.

$\frac{d}{d\vec{w}} \vec{w}^T \vec{x}_n = \vec{x}_n^T$ ← Dot-prod.

$\frac{d}{dx} x^2 = 2x$ ← Square

$\frac{d}{da} a = 1$ ← identity



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 $1, \cos, kx^{k-1}$*tc.*.
- If required, more sophisticated user-defined functions and their derivative implementations can be *registered* with Autograd.

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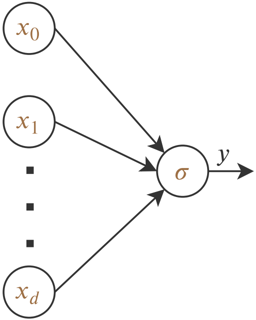
elementary functions $\begin{cases} \sigma(a) = \dfrac{1}{1+e^{-a}} \\ \sigma'(a) = \sigma(1-\sigma) \end{cases}$

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

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

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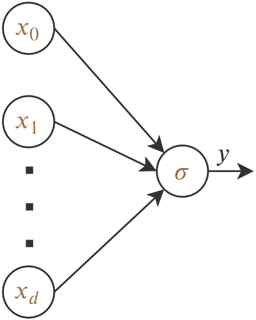

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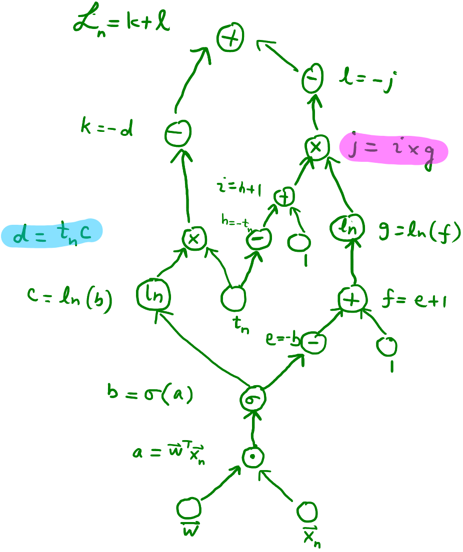
$\mathcal{L}_n(w) = -t_n \ln y_n - (1-t_n)\ln(1-y_n)$ where $y_n = \sigma(\vec{w}^T\vec{x}_n)$

Logistic Regression via Automatic Differentiation

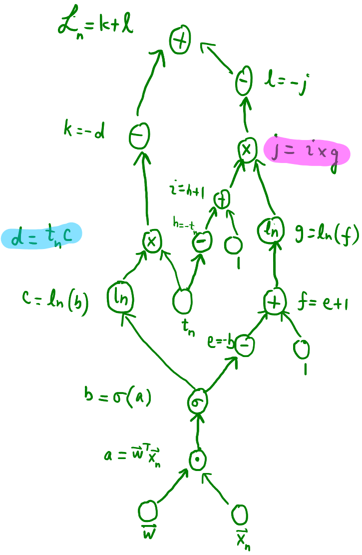
Step 1: Computational Graph for $\mathcal{L}_n$

$\mathcal{L}_n(w) = -t_n \ln y_n - (1-t_n)\ln(1-y_n)$ where $y_n = \sigma(\vec{w}^T\vec{x}_n)$



Logistic Regression via Automatic Differentiation

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



$\nabla_{\vec{w}} \mathcal{L}_n$?

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*.