Automatic Differentiation

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- Vector chain rule leads to matrix multiplication if we only take derivative of vector w.r.t. vector.
- We can still use chain rule notation when dealing with matrix derivatives, but we need to separately keep track what summation is meant with this.

Overview

Introduction

Forward Mode Automatic Differentiation

Reverse Mode Automatic Differentiation

Backpropagation in Neural Networks

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Automatic Differentiation

Will roughly be following the review article by Baydin et al. (2018).

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- Many ways to differentiate a function
- Can be very inefficient, if done carelessly

Example: Inefficient Symbolic Differentiation

$$L(\theta) = f(\boldsymbol{K}(\boldsymbol{D}(\theta)))\,,$$

$$f : \mathbb{R}^{N\times N} \to \mathbb{R}\,, \qquad \boldsymbol{K} : \mathbb{R}^{N\times N} \to \mathbb{R}^{N\times N}\,, \qquad \boldsymbol{D} : \mathbb{R}^{P} \to \mathbb{R}^{N\times N}\,.$$

$$\frac{\mathrm{d}L}{\mathrm{d}\boldsymbol{\theta}} = \underbrace{\frac{\partial L}{\partial \boldsymbol{K}}}_{1\times(N\times N)} \quad \underbrace{\frac{\partial \boldsymbol{K}}{\partial \boldsymbol{D}}}_{(N\times N)\times(N\times N)} \quad \underbrace{\frac{\partial \boldsymbol{D}}{\partial \boldsymbol{\theta}}}_{(N\times N)\times P}$$

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Scales with elements, so **at least** $N^2 + N^4 + N^2 P$.

2) Then we have two options:

- $\frac{\partial L}{\partial \boldsymbol{K}}\left(\frac{\partial \boldsymbol{K}}{\partial \boldsymbol{D}}\frac{\partial \boldsymbol{D}}{\partial \boldsymbol{\theta}}\right)$: $N^4 P + N^2 P$

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Problems:

- Cannot take advantage of structure (e.g. zero elements)
- Not clear which order to compute in to be efficient.

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Although unfortunately finding the optimal gradient in general (optimal jacobian accumulation problem) is NP-complete :(

Today: Answers / Topics

- Symbolic differentiation, and its problem
- Computational graphs (describing computation)
- Forward mode autodiff
- Reverse mode autodiff (backpropagation)
- Computational considerations

Computational Graphs

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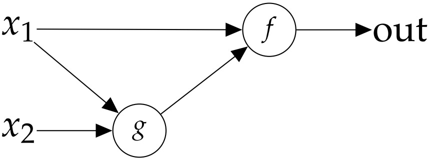

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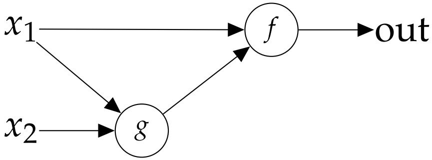

- To find the output, **traverse** the graph from the inputs.
- Gradient computation traverses the graph in various ways.

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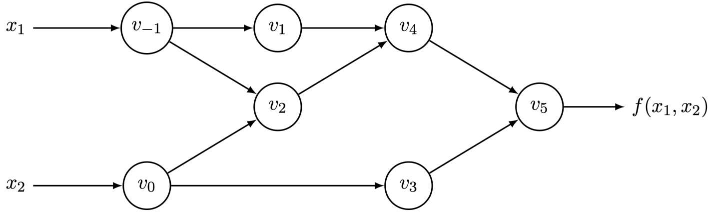
Repeat for all i to find all gradients.

Forward mode Autodiff: Example

Computational graph for $f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$



Forward Primal Trace

v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Forward Tangent (Derivative) Trace

$\dot{v}_{-1}$	$= \dot{x}_1$	$= 1$
$\dot{v}_0$	$= \dot{x}_2$	$= 0$
$\dot{v}_1$	$= \dot{v}_{-1}/v_{-1}$	$= 1/2$
$\dot{v}_2$	$= \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
$\dot{v}_3$	$= \dot{v}_0 \times \cos v_0$	$= 0 \times \cos 5$
$\dot{v}_4$	$= \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
$\dot{v}_5$	$= \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$
$\boldsymbol{\dot{y}}$	$\boldsymbol{= \dot{v}_5}$	$\mathbf{= 5.5}$

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The procedure above is efficient for vector inputs too!

Forward mode: Computational complexity

Remember the key equation:

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- No memory overhead.
- **However**, cost scales linearly with the number of gradients!

Fun exercise

Prove the product rule using forward mode autodiff.

Board

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- Traverse the nodes of the graph, indexed by j, *backwards*, starting from the output.
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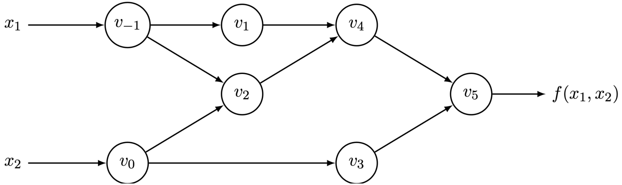
$$\frac{\partial \text{out}}{\partial v_j} = \sum_{k \in \text{outputs}(j)} \frac{\partial \text{out}}{\partial v_k} \frac{\partial v_k}{\partial v_j} \tag{3}$$

- We end up with $\partial \text{out}/\partial x_i$.

Repeat for all i to find all gradients.

Reverse mode Autodiff: Example

Computational graph for $f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$



Forward Primal Trace

$$
\begin{array}{lll}
v_{-1} & = x_1 & = 2 \\
v_0 & = x_2 & = 5 \\
\hline
v_1 & = \ln v_{-1} & = \ln 2 \\
v_2 & = v_{-1} \times v_0 & = 2 \times 5 \\
v_3 & = \sin v_0 & = \sin 5 \\
v_4 & = v_1 + v_2 & = 0.693 + 10 \\
v_5 & = v_4 - v_3 & = 10.693 + 0.959 \\
\hline
y & = v_5 & = 11.652
\end{array}
$$

Reverse Adjoint (Derivative) Trace

$$
\begin{array}{llll}
\boldsymbol{\bar{x}_1} & \boldsymbol{= \bar{v}_{-1}} & & \boldsymbol{= 5.5} \\
\boldsymbol{\bar{x}_2} & \boldsymbol{= \bar{v}_0} & & \boldsymbol{= 1.716} \\
\hline
\bar{v}_{-1} & = \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}} & = \bar{v}_{-1} + \bar{v}_1 / v_{-1} & = 5.5 \\
\bar{v}_0 & = \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0} & = \bar{v}_0 + \bar{v}_2 \times v_{-1} & = 1.716 \\
\bar{v}_{-1} & = \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}} & = \bar{v}_2 \times v_0 & = 5 \\
\bar{v}_0 & = \bar{v}_3 \frac{\partial v_3}{\partial v_0} & = \bar{v}_3 \times \cos v_0 & = -0.284 \\
\bar{v}_2 & = \bar{v}_4 \frac{\partial v_4}{\partial v_2} & = \bar{v}_4 \times 1 & = 1 \\
\bar{v}_1 & = \bar{v}_4 \frac{\partial v_4}{\partial v_1} & = \bar{v}_4 \times 1 & = 1 \\
\bar{v}_3 & = \bar{v}_5 \frac{\partial v_5}{\partial v_3} & = \bar{v}_5 \times (-1) & = -1 \\
\bar{v}_4 & = \bar{v}_5 \frac{\partial v_5}{\partial v_4} & = \bar{v}_5 \times 1 & = 1 \\
\hline
\bar{v}_5 & = \bar{y} & = 1 &
\end{array}
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The procedure above is efficient for vector inputs too!

Reverse mode: Computational complexity

Remember the key equation:

$$\frac{\partial \text{out}}{\partial v_j} = \sum_{k \in \text{outputs}(j)} \frac{\partial \text{out}}{\partial v_k} \frac{\partial v_k}{\partial v_j} \tag{4}$$

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Overview

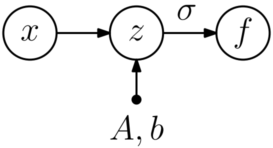
Introduction

Forward Mode Automatic Differentiation

Reverse Mode Automatic Differentiation

Backpropagation in Neural Networks

Gradients of a Single-Layer Neural Network



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- Find $\boldsymbol{A}, \boldsymbol{b}$, such that the squared loss

$$L(\boldsymbol{\theta}) = \tfrac{1}{2}\|\boldsymbol{e}\|^2 \in \mathbb{R}, \quad \boldsymbol{e} = \boldsymbol{y} - \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{z}) \in \mathbb{R}^M$$

is minimized

Putting Things Together

Partial derivatives:

$$
\begin{aligned}
\frac{\partial L}{\partial \boldsymbol{A}} &= \frac{\partial L}{\partial \boldsymbol{e}} \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{f}} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{A}} \\
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\end{aligned}
$$

$$\frac{\partial L}{\partial \boldsymbol{e}} = \underbrace{\boldsymbol{e}^\top}_{\in \mathbb{R}^{1\times M}} \qquad \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{f}} = \underbrace{-\boldsymbol{I}}_{\in \mathbb{R}^{M\times M}} \qquad \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} = \underbrace{\mathrm{diag}(1 - \tanh^2(\boldsymbol{z}))}_{\in \mathbb{R}^{M\times M}}$$

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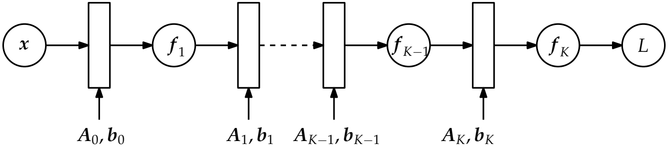
Gradients of a Multi-Layer Neural Network

$$L(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \boldsymbol{\theta}_3) = ||\mathbf{y} - \boldsymbol{f}_{\boldsymbol{\theta}_3}(\boldsymbol{f}_{\boldsymbol{\theta}_2}(\boldsymbol{f}_{\boldsymbol{\theta}_1}(\mathbf{x})))||^2 \tag{5}$$



- Inputs $\boldsymbol{x}$, observed outputs $\boldsymbol{y}$
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$$\boldsymbol{f}_0 = \boldsymbol{x}$$
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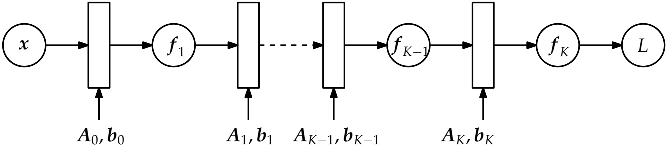

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- Find $\boldsymbol{A}_j, \boldsymbol{b}_j$ for $j = 0, \ldots, K-1$, such that the squared loss

$$L(\boldsymbol{\theta}) = \|\boldsymbol{y} - \boldsymbol{f}_{K,\boldsymbol{\theta}}(\boldsymbol{x})\|^2$$

is minimized, where $\boldsymbol{\theta} = \{\boldsymbol{A}_j, \boldsymbol{b}_j\}, \quad j = 0, \ldots, K-1$

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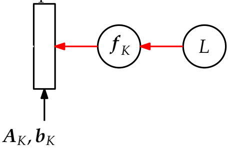

$$\frac{\partial L}{\partial \boldsymbol{\theta}_K} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{\theta}_K}$$

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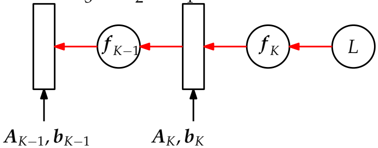
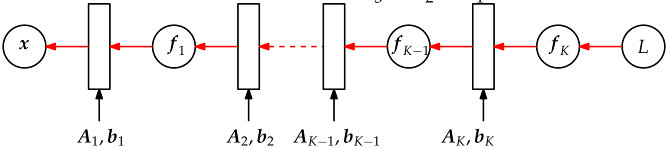


$$\frac{\partial L}{\partial \boldsymbol{\theta}_K} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{\theta}_K}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_{K-1}} = \frac{\partial L}{\partial \boldsymbol{f}_K} \boxed{\frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{f}_{K-1}} \frac{\partial \boldsymbol{f}_{K-1}}{\partial \boldsymbol{\theta}_{K-1}}}$$

Gradients of a Multi-Layer Neural Network

$$L(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \boldsymbol{\theta}_3) = ||\mathbf{y} - \boldsymbol{f}_{\boldsymbol{\theta}_3}(\boldsymbol{f}_{\boldsymbol{\theta}_2}(\boldsymbol{f}_{\boldsymbol{\theta}_1}(\mathbf{x})))||^2 \tag{6}$$



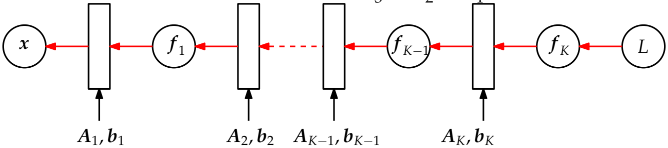
$$\frac{\partial L}{\partial \boldsymbol{\theta}_K} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{\theta}_K}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_{K-1}} = \frac{\partial L}{\partial \boldsymbol{f}_K} \boxed{\frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{f}_{K-1}} \frac{\partial \boldsymbol{f}_{K-1}}{\partial \boldsymbol{\theta}_{K-1}}}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_{K-2}} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{f}_{K-1}} \boxed{\frac{\partial \boldsymbol{f}_{K-1}}{\partial \boldsymbol{f}_{K-2}} \frac{\partial \boldsymbol{f}_{K-2}}{\partial \boldsymbol{\theta}_{K-2}}}$$

Gradients of a Multi-Layer Neural Network

$$L(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \boldsymbol{\theta}_3) = ||\mathbf{y} - \boldsymbol{f}_{\boldsymbol{\theta}_3}(\boldsymbol{f}_{\boldsymbol{\theta}_2}(\boldsymbol{f}_{\boldsymbol{\theta}_1}(\mathbf{x})))||^2 \tag{6}$$



$$\frac{\partial L}{\partial \boldsymbol{\theta}_K} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{\theta}_K}$$

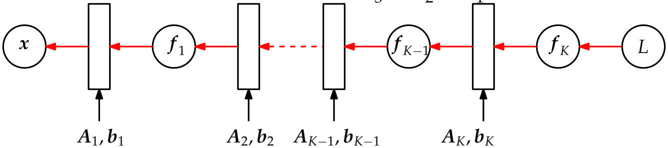
$$\frac{\partial L}{\partial \boldsymbol{\theta}_{K-1}} = \frac{\partial L}{\partial \boldsymbol{f}_K} \boxed{\frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{f}_{K-1}} \frac{\partial \boldsymbol{f}_{K-1}}{\partial \boldsymbol{\theta}_{K-1}}}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_{K-2}} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{f}_{K-1}} \boxed{\frac{\partial \boldsymbol{f}_{K-1}}{\partial \boldsymbol{f}_{K-2}} \frac{\partial \boldsymbol{f}_{K-2}}{\partial \boldsymbol{\theta}_{K-2}}}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_i} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{f}_{K-1}} \cdots \boxed{\frac{\partial \boldsymbol{f}_{i+1}}{\partial \boldsymbol{f}_i} \frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{\theta}_i}}$$

Gradients of a Multi-Layer Neural Network

$$L(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \boldsymbol{\theta}_3) = ||\mathbf{y} - \boldsymbol{f}_{\boldsymbol{\theta}_3}(\boldsymbol{f}_{\boldsymbol{\theta}_2}(\boldsymbol{f}_{\boldsymbol{\theta}_1}(\mathbf{x})))||^2 \tag{6}$$



$$\frac{\partial L}{\partial \boldsymbol{\theta}_K} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{\theta}_K}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_{K-1}} = \frac{\partial L}{\partial \boldsymbol{f}_K} \boxed{\frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{f}_{K-1}} \frac{\partial \boldsymbol{f}_{K-1}}{\partial \boldsymbol{\theta}_{K-1}}}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_{K-2}} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{f}_{K-1}} \boxed{\frac{\partial \boldsymbol{f}_{K-1}}{\partial \boldsymbol{f}_{K-2}} \frac{\partial \boldsymbol{f}_{K-2}}{\partial \boldsymbol{\theta}_{K-2}}}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_i} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{f}_{K-1}} \cdots \boxed{\frac{\partial \boldsymbol{f}_{i+1}}{\partial \boldsymbol{f}_i} \frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{\theta}_i}}$$

▶▶ Intermediate derivatives are stored during the forward pass

Summary: Differentiation

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- Flavours of automatic differentiation
- Computational cost analysis of automatic differentiation
- Application: Backpropagation in NNs

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If you have a spare 1.5 hours, and want to see how **minimal** an implementation of this can be, I **highly** recommend Conal Elliott's talk on *The Simple Essence of Automatic Differentiation*: https://www.youtube.com/watch?v=ne99laPUxN4

References I

Atilim Gunes Baydin, Barak A. Pearlmutter, Alexey Andreyevich Radul, and Jeffrey Mark Siskind. Automatic differentiation in machine learning: a survey. **Journal of Machine Learning Research**, 18(153):1–43, 2018. URL `http://jmlr.org/papers/v18/17-468.html`.