



Automatic Differentiation

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Automatic Differentiation



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I think the first 40 years or so of automatic differentiation was largely people not using it because they didn't believe such an algorithm could possibly exist.

11:36 PM · Sep 17, 2019



9



26



159



13



Figure 1: When you got the idea



Figure 2: This is not autograd

Problem

Suppose we need to solve the following problem:

$$L(w) \rightarrow \min_{w \in \mathbb{R}^d}$$

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- You may use a lot of algorithms to approach this problem. Still, given the modern size of the problem, where d could be dozens of billions it is very challenging to solve this problem without information about the gradients using zero-order optimization algorithms.
- That is why it would be beneficial to be able to calculate the gradient vector $\nabla_w L = \left(\frac{\partial L}{\partial w_1}, \dots, \frac{\partial L}{\partial w_d} \right)^T$.

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- You may use a lot of algorithms to approach this problem. Still, given the modern size of the problem, where d could be dozens of billions it is very challenging to solve this problem without information about the gradients using zero-order optimization algorithms.
- That is why it would be beneficial to be able to calculate the gradient vector $\nabla_w L = \left(\frac{\partial L}{\partial w_1}, \dots, \frac{\partial L}{\partial w_d} \right)^T$.
- Typically, first-order methods perform much better in huge-scale optimization, while second-order methods require too much memory.

Example: multidimensional scaling

Suppose, we have a pairwise distance matrix for N d -dimensional objects $D \in \mathbb{R}^{N \times N}$. Given this matrix, we aim to recover the initial coordinates $W_i \in \mathbb{R}^d$, $i = 1, \dots, N$.

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$$L(W) = \sum_{i,j=1}^N (\|W_i - W_j\|_2^2 - D_{i,j})^2 \rightarrow \min_{W \in \mathbb{R}^{N \times d}}$$

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$$L(W) = \sum_{i,j=1}^N (\|W_i - W_j\|_2^2 - D_{i,j})^2 \rightarrow \min_{W \in \mathbb{R}^{N \times d}}$$

Link to a nice visualization ♣, where one can see, that gradient-free methods handle this problem much slower, especially in higher dimensions.

Question

Is it somehow connected with PCA?

Example: multidimensional scaling



Figure 3: Link to the animation

Example: Gradient Descent without gradient

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Suppose we need to solve the following problem:

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with the Gradient Descent (GD) algorithm:

$$w_{k+1} = w_k - \alpha_k \nabla_w L(w_k)$$

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One can consider 2-point gradient estimator^a G :

$$G = d \frac{L(w + \varepsilon v) - L(w - \varepsilon v)}{2\varepsilon} v,$$

where v is spherically symmetric.

^aI suggest a nice presentation about gradient-free methods

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Figure 4: "Illustration of two-point estimator of Gradient Descent"

Example: finite differences gradient descent

$$w_{k+1} = w_k - \alpha_k G$$

Example: finite differences gradient descent

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One can also consider the idea of finite differences:

$$G = \sum_{i=1}^d \frac{L(w + \varepsilon e_i) - L(w - \varepsilon e_i)}{2\varepsilon} e_i$$


Open In Colab 



Figure 5: "Illustration of finite differences estimator of Gradient Descent"

The curse of dimensionality for zero-order methods ¹

$$\min_{x \in \mathbb{R}^n} f(x)$$

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$$\text{Zero order GD: } x_{k+1} = x_k - \alpha_k G,$$

where G is a 2-point or multi-point estimator of the gradient.

¹Optimal rates for zero-order convex optimization: the power of two function evaluations

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	$f(x)$ - smooth	$f(x)$ - smooth and convex	$f(x)$ - smooth and strongly convex
GD	$\ \nabla f(x_k)\ ^2 \approx \mathcal{O}\left(\frac{1}{k}\right)$	$f(x_k) - f^* \approx \mathcal{O}\left(\frac{1}{k}\right)$	$\ x_k - x^*\ ^2 \approx \mathcal{O}\left(\left(1 - \frac{\mu}{L}\right)^k\right)$
Zero order GD	$\ \nabla f(x_k)\ ^2 \approx \mathcal{O}\left(\frac{n}{k}\right)$	$f(x_k) - f^* \approx \mathcal{O}\left(\frac{n}{k}\right)$	$\ x_k - x^*\ ^2 \approx \mathcal{O}\left(\left(1 - \frac{\mu}{nL}\right)^k\right)$

For 2-point estimators, you can't make the dependence better than on \sqrt{n} !

¹Optimal rates for zero-order convex optimization: the power of two function evaluations

Finite differences

The naive approach to getting approximate values of gradients is the **Finite differences** approach. For each coordinate, one can calculate the partial derivative approximation:

$$\frac{\partial L}{\partial w_k}(w) \approx \frac{L(w + \varepsilon e_k) - L(w)}{\varepsilon}, \quad e_k = (0, \dots, \frac{1}{k}, \dots, 0)$$

²Linnainmaa S. The representation of the cumulative rounding error of an algorithm as a Taylor expansion of the local rounding errors. Master's Thesis (in Finnish), Univ. Helsinki, 1970.

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If the time needed for one calculation of $L(w)$ is T , what is the time needed for calculating $\nabla_w L$ with this approach?

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If the time needed for one calculation of $L(w)$ is T , what is the time needed for calculating $\nabla_w L$ with this approach?

Answer $2dT$, which is extremely long for the huge scale optimization. Moreover, this exact scheme is unstable, which means that you will have to choose between accuracy and stability.

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Answer $2dT$, which is extremely long for the huge scale optimization. Moreover, this exact scheme is unstable, which means that you will have to choose between accuracy and stability.

Theorem

There is an algorithm to compute $\nabla_w L$ in $\mathcal{O}(T)$ operations. ²

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Forward mode automatic differentiation

To dive deep into the idea of automatic differentiation we will consider a simple function for calculating derivatives:

$$L(w_1, w_2) = w_2 \log w_1 + \sqrt{w_2 \log w_1}$$

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Let's draw a *computational graph* of this function:

$$L(w_1, w_2) = w_2 \log w_1 + \sqrt{w_2 \log w_1}$$

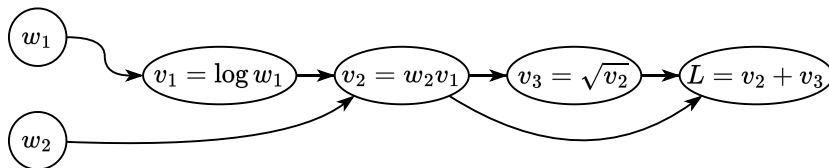


Figure 6: Illustration of computation graph of primitive arithmetic operations for the function $L(w_1, w_2)$

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Let's go from the beginning of the graph to the end and calculate the derivative $\frac{\partial L}{\partial w_1}$.

Forward mode automatic differentiation



Figure 7: Illustration of forward mode automatic differentiation

Function

$$w_1 = w_1, w_2 = w_2$$

Forward mode automatic differentiation



Figure 7: Illustration of forward mode automatic differentiation

Function

$$w_1 = w_1, w_2 = w_2$$

Derivative

$$\frac{\partial w_1}{\partial w_1} = 1, \frac{\partial w_2}{\partial w_1} = 0$$

Forward mode automatic differentiation

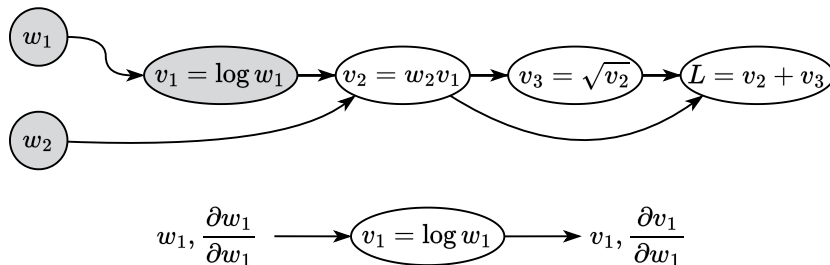


Figure 8: Illustration of forward mode automatic differentiation

Forward mode automatic differentiation



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Function

$$v_1 = \log w_1$$

Forward mode automatic differentiation



Figure 8: Illustration of forward mode automatic differentiation

Function

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Derivative

$$\frac{\partial v_1}{\partial w_1} = \frac{\partial v_1}{\partial w_1} \frac{\partial w_1}{\partial w_1} = \frac{1}{w_1} 1$$

Forward mode automatic differentiation



Figure 9: Illustration of forward mode automatic differentiation

Forward mode automatic differentiation



Figure 9: Illustration of forward mode automatic differentiation

Function

$$v_2 = w_2 v_1$$

Forward mode automatic differentiation



Figure 9: Illustration of forward mode automatic differentiation

Function

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Derivative

$$\frac{\partial v_2}{\partial w_1} = \frac{\partial v_2}{\partial v_1} \frac{\partial v_1}{\partial w_1} + \frac{\partial v_2}{\partial w_2} \frac{\partial w_2}{\partial w_1} = w_2 \frac{\partial v_1}{\partial w_1} + v_1 \frac{\partial w_2}{\partial w_1}$$

Forward mode automatic differentiation



Figure 10: Illustration of forward mode automatic differentiation

Forward mode automatic differentiation



Figure 10: Illustration of forward mode automatic differentiation

Function

$$v_3 = \sqrt{v_2}$$

Forward mode automatic differentiation



Figure 10: Illustration of forward mode automatic differentiation

Function

$$v_3 = \sqrt{v_2}$$

Derivative

$$\frac{\partial v_3}{\partial w_1} = \frac{\partial v_3}{\partial v_2} \frac{\partial v_2}{\partial w_1} = \frac{1}{2\sqrt{v_2}} \frac{\partial v_2}{\partial w_1}$$

Forward mode automatic differentiation



Figure 11: Illustration of forward mode automatic differentiation

Forward mode automatic differentiation



Figure 11: Illustration of forward mode automatic differentiation

Function

$$L = v_2 + v_3$$

Forward mode automatic differentiation



Figure 11: Illustration of forward mode automatic differentiation

Function

$$L = v_2 + v_3$$

Derivative

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial v_2} \frac{\partial v_2}{\partial w_1} + \frac{\partial L}{\partial v_3} \frac{\partial v_3}{\partial w_1} = 1 \frac{\partial v_2}{\partial w_1} + 1 \frac{\partial v_3}{\partial w_1}$$

Make the similar computations for $\frac{\partial L}{\partial w_2}$

$$L(w_1, w_2) = w_2 \log w_1 + \sqrt{w_2 \log w_1}$$



Figure 12: Illustration of computation graph of primitive arithmetic operations for the function $L(w_1, w_2)$

Forward mode automatic differentiation example



Figure 13: Illustration of forward mode automatic differentiation

Function

$$w_1 = w_1, w_2 = w_2$$

Derivative

$$\frac{\partial w_1}{\partial w_2} = 0, \frac{\partial w_2}{\partial w_2} = 1$$

Forward mode automatic differentiation example



Figure 14: Illustration of forward mode automatic differentiation

Function

$$v_1 = \log w_1$$

Derivative

$$\frac{\partial v_1}{\partial w_2} = \frac{\partial v_1}{\partial w_1} \frac{\partial w_1}{\partial w_2} = \frac{1}{w_1} \cdot 0$$

Forward mode automatic differentiation example



Figure 15: Illustration of forward mode automatic differentiation

Function

$$v_2 = w_2 v_1$$

Derivative

$$\frac{\partial v_2}{\partial w_2} = \frac{\partial v_2}{\partial v_1} \frac{\partial v_1}{\partial w_2} + \frac{\partial v_2}{\partial w_2} \frac{\partial w_2}{\partial w_2} = w_2 \frac{\partial v_1}{\partial w_2} + v_1 \frac{\partial w_2}{\partial w_2}$$

Forward mode automatic differentiation example



Figure 16: Illustration of forward mode automatic differentiation

Function

$$v_3 = \sqrt{v_2}$$

Derivative

$$\frac{\partial v_3}{\partial w_2} = \frac{\partial v_3}{\partial v_2} \frac{\partial v_2}{\partial w_2} = \frac{1}{2\sqrt{v_2}} \frac{\partial v_2}{\partial w_2}$$

Forward mode automatic differentiation example



Figure 17: Illustration of forward mode automatic differentiation

Function

$$L = v_2 + v_3$$

Derivative

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial v_2} \frac{\partial v_2}{\partial w_2} + \frac{\partial L}{\partial v_3} \frac{\partial v_3}{\partial w_2} = 1 \frac{\partial v_2}{\partial w_2} + 1 \frac{\partial v_3}{\partial w_2}$$

Forward mode automatic differentiation algorithm

Suppose, we have a computational graph $v_i, i \in [1; N]$.

Our goal is to calculate the derivative of the output of this graph with respect to some input variable w_k , i.e. $\frac{\partial v_N}{\partial w_k}$.

This idea implies propagation of the gradient with respect to the input variable from start to end, that is why we can introduce the notation:

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Figure 18: Illustration of forward chain rule to calculate the derivative of the function L with respect to w_k .

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- For $i = 1, \dots, N$:
 - Compute v_i as a function of its parents (inputs) x_1, \dots, x_{t_i} :

$$v_i = v_i(x_1, \dots, x_{t_i})$$

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- For $i = 1, \dots, N$:
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Note, that this approach does not require storing all intermediate computations, but one can see, that for calculating the derivative $\frac{\partial L}{\partial w_k}$ we need $\mathcal{O}(T)$ operations.

This means, that for the whole gradient, we need $d\mathcal{O}(T)$ operations, which is the same as for finite differences, but we do not have stability issues, or inaccuracies now (the formulas above are exact).

Figure 18: Illustration of forward chain rule to calculate the derivative of the function L with respect to w_k .

A close-up of Yoda's face from Star Wars, looking upwards with a slight smile. The background is dark with some blue and green light effects. The text "There is another" is overlaid at the bottom in white.

There is another

Backward mode automatic differentiation

We will consider the same function with a computational graph:

$$L(w_1, w_2) = w_2 \log w_1 + \sqrt{w_2 \log w_1}$$

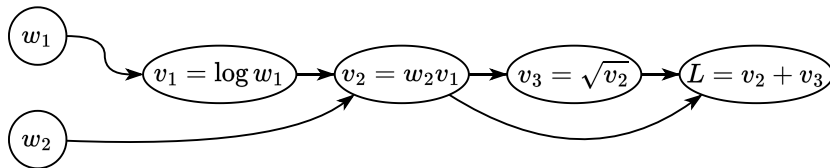


Figure 19: Illustration of computation graph of primitive arithmetic operations for the function $L(w_1, w_2)$

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Figure 19: Illustration of computation graph of primitive arithmetic operations for the function $L(w_1, w_2)$

Assume, that we have some values of the parameters w_1, w_2 and we have already performed a forward pass (i.e. single propagation through the computational graph from left to right). Suppose, also, that we somehow saved all intermediate values of v_i . Let's go from the end of the graph to the beginning and calculate the derivatives

$$\frac{\partial L}{\partial w_1}, \frac{\partial L}{\partial w_2}:$$

Backward mode automatic differentiation example



Figure 20: Illustration of backward mode automatic differentiation

Backward mode automatic differentiation example



Figure 20: Illustration of backward mode automatic differentiation

Derivatives

Backward mode automatic differentiation example



Figure 20: Illustration of backward mode automatic differentiation

Derivatives

$$\frac{\partial L}{\partial L} = 1$$

Backward mode automatic differentiation example



Figure 21: Illustration of backward mode automatic differentiation

Backward mode automatic differentiation example



Figure 21: Illustration of backward mode automatic differentiation

Derivatives

Backward mode automatic differentiation example



Figure 21: Illustration of backward mode automatic differentiation

Derivatives

$$\begin{aligned}\frac{\partial L}{\partial v_3} &= \frac{\partial L}{\partial L} \frac{\partial L}{\partial v_3} \\ &= \frac{\partial L}{\partial L} 1\end{aligned}$$

Backward mode automatic differentiation example



Figure 22: Illustration of backward mode automatic differentiation

Backward mode automatic differentiation example



Figure 22: Illustration of backward mode automatic differentiation

Derivatives

Backward mode automatic differentiation example



Figure 22: Illustration of backward mode automatic differentiation

Derivatives

$$\begin{aligned}\frac{\partial L}{\partial v_2} &= \frac{\partial L}{\partial v_3} \frac{\partial v_3}{\partial v_2} + \frac{\partial L}{\partial L} \frac{\partial L}{\partial v_2} \\ &= \frac{\partial L}{\partial v_3} \frac{1}{2\sqrt{v_2}} + \frac{\partial L}{\partial L} 1\end{aligned}$$

Backward mode automatic differentiation example



Figure 23: Illustration of backward mode automatic differentiation

Backward mode automatic differentiation example



Figure 23: Illustration of backward mode automatic differentiation

Derivatives

Backward mode automatic differentiation example



Figure 23: Illustration of backward mode automatic differentiation

Derivatives

$$\begin{aligned}\frac{\partial L}{\partial v_1} &= \frac{\partial L}{\partial v_2} \frac{\partial v_2}{\partial v_1} \\ &= \frac{\partial L}{\partial v_2} w_2\end{aligned}$$

Backward mode automatic differentiation example



Figure 24: Illustration of backward mode automatic differentiation

Backward mode automatic differentiation example



Figure 24: Illustration of backward mode automatic differentiation

Derivatives

Backward mode automatic differentiation example



Figure 24: Illustration of backward mode automatic differentiation

Derivatives

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial v_1} \frac{\partial v_1}{\partial w_1} = \frac{\partial L}{\partial v_1} \frac{1}{w_1}$$

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial v_2} \frac{\partial v_2}{\partial w_2} = \frac{\partial L}{\partial v_1} v_1$$

Backward (reverse) mode automatic differentiation

i Question

Note, that for the same price of computations as it was in the forward mode we have the full vector of gradient $\nabla_w L$. Is it a free lunch? What is the cost of acceleration?

Backward (reverse) mode automatic differentiation

Question

Note, that for the same price of computations as it was in the forward mode we have the full vector of gradient $\nabla_w L$. Is it a free lunch? What is the cost of acceleration?

Answer Note, that for using the reverse mode AD you need to store all intermediate computations from the forward pass. This problem could be somehow mitigated with the gradient checkpointing approach, which involves necessary recomputations of some intermediate values. This could significantly reduce the memory footprint of the large machine-learning model.

Reverse mode automatic differentiation algorithm

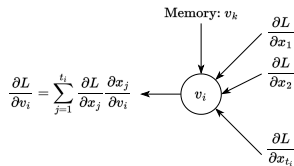
Suppose, we have a computational graph $v_i, i \in [1; N]$.

Our goal is to calculate the derivative of the output of this graph with respect to all inputs variable w ,

i.e. $\nabla_w v_N = \left(\frac{\partial v_N}{\partial w_1}, \dots, \frac{\partial v_N}{\partial w_d} \right)^T$. This idea implies

propagation of the gradient of the function with respect to the intermediate variables from the end to the origin, that is why we can introduce the notation:

$$\overline{v_i} = \frac{\partial L}{\partial v_i} = \frac{\partial v_N}{\partial v_i}$$



- **FORWARD PASS**

For $i = 1, \dots, N$:

Figure 25: Illustration of reverse chain rule to calculate the derivative of the function L with respect to the node v_i .

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For $i = 1, \dots, N$:

- Compute and store the values of v_i as a function of its parents (inputs)

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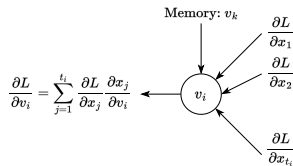
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For $i = 1, \dots, N$:

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For $i = N, \dots, 1$:

- Compute the derivative $\overline{v_i}$ using the backward chain rule and information from all of its children (outputs) (x_1, \dots, x_{t_i}) :

$$\overline{v_i} = \frac{\partial L}{\partial v_i} = \sum_{j=1}^{t_i} \frac{\partial L}{\partial x_j} \frac{\partial x_j}{\partial v_i}$$

Figure 25: Illustration of reverse chain rule to calculate the derivative of the function L with respect to the node v_i .

Choose your fighter



i Question

Which of the AD modes would you choose (forward/ reverse) for the following computational graph of primitive arithmetic operations? Suppose, you are needed to compute the jacobian

$$J = \left\{ \frac{\partial L_i}{\partial w_j} \right\}_{i,j}$$

Figure 26: Which mode would you choose for calculating gradients there?

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Answer Note, that the reverse mode computational time is proportional to the number of outputs here, while the forward mode works proportionally to the number of inputs there. This is why it would be a good idea to consider the forward mode AD.

Figure 26: Which mode would you choose for calculating gradients there?

Choose your fighter



Figure 27: ♣ This graph nicely illustrates the idea of choice between the modes. The $n = 100$ dimension is fixed and the graph presents the time needed for Jacobian calculation w.r.t. x for $f(x) = Ax$

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Figure 28: Which mode would you choose for calculating gradients there?

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Answer It is generally impossible to say it without some knowledge about the specific structure of the graph G . Note, that there are also plenty of advanced approaches to mix forward and reverse mode AD, based on the specific G structure.

Figure 28: Which mode would you choose for calculating gradients there?

Feedforward Architecture

FORWARD

- $v_0 = x$ typically we have a batch of data x here as an input.



BACKWARD

Figure 29: Feedforward neural network architecture

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- $v_0 = x$ typically we have a batch of data x here as an input.
- For $k = 1, \dots, t-1, t$:
 - $v_k = \sigma(v_{k-1} w_k)$. Note, that practically speaking the data has dimension $x \in \mathbb{R}^{b \times d}$, where b is the batch size (for the single data point $b = 1$). While the weight matrix w_k of a k layer has a shape $n_{k-1} \times n_k$, where n_k is the dimension of an inner representation of the data.

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- $L = L(v_t)$ - calculate the loss function.

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- For $k = t, t-1, \dots, 1$:
 - $\frac{\partial L}{\partial v_k} = \frac{\partial L}{\partial v_{k+1}} \frac{\partial v_{k+1}}{\partial v_k}$
 $b \times n_k \quad b \times n_{k+1} \quad n_{k+1} \times n_k$



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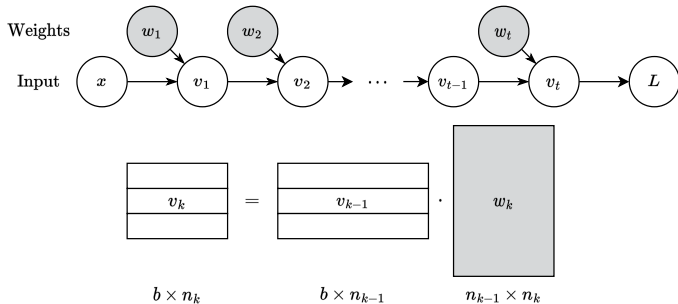


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 - $\frac{\partial L}{\partial w_k} = \frac{\partial L}{\partial v_{k+1}} \cdot \frac{\partial v_{k+1}}{\partial w_k}$
 $b \times n_{k-1} \cdot n_k \quad b \times n_{k+1} \quad n_{k+1} \times n_{k-1} \cdot n_k$

Hessian vector product without the Hessian

When you need some information about the curvature of the function you usually need to work with the hessian. However, when the dimension of the problem is large it is challenging. For a scalar-valued function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, the Hessian at a point $x \in \mathbb{R}^n$ is written as $\nabla^2 f(x)$. A Hessian-vector product function is then able to evaluate

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for any vector $v \in \mathbb{R}^n$. We have to use the identity

$$\nabla^2 f(x)v = \nabla[x \mapsto \nabla f(x) \cdot v] = \nabla g(x),$$

where $g(x) = \nabla f(x)^T \cdot v$ is a new vector-valued function that dots the gradient of f at x with the vector v .

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```
import jax.numpy as jnp

def hvp(f, x, v):
    return grad(lambda x: jnp.vdot(grad(f)(x), v))(x)
```

Neural network training dynamics via Hessian spectra and hvp³



Figure 30: Large negative eigenvalues disappeared after training for ResNet-32

³An Investigation into Neural Net Optimization via Hessian Eigenvalue Density

Hutchinson Trace Estimation ⁴

This example illustrates the estimation of the Hessian trace of a neural network using Hutchinson's method, which is an algorithm to obtain such an estimate from matrix-vector products:

Let $X \in \mathbb{R}^{d \times d}$ and $v \in \mathbb{R}^d$ be a random vector such that $\mathbb{E}[vv^T] = I$. Then,

$$\text{Tr}(X) = \mathbb{E}[v^T X v] = \frac{1}{V} \sum_{i=1}^V v_i^T X v_i$$



Figure 31: Source

Activation checkpointing

The animated visualization of the above approaches 

An example of using a gradient checkpointing 

⁵ZeRO: Memory Optimizations Toward Training Trillion Parameter Models

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Real world example from **GPT-2**⁵:

- Activations in naive mode can occupy much more memory: for a sequence length of 1K and a batched size of 32, 60 GB is needed to store all intermediate activations.

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Real world example from **GPT-2**⁵:

- Activations in naive mode can occupy much more memory: for a sequence length of 1K and a batched size of 32, 60 GB is needed to store all intermediate activations.
- Checkpointing activations can reduce consumption by up to 8 GB by recomputing them (33% computational overhead)

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Figure 32: Different approaches for taking derivatives

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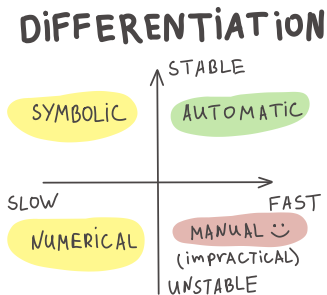


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What automatic differentiation (AD) is NOT:

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- AD (reverse mode) is time-efficient and numerically stable

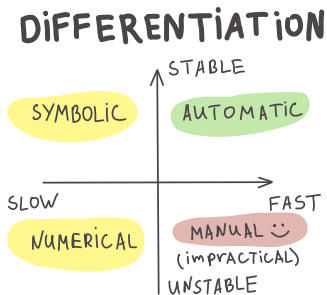


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- AD is not just the chain rule
- AD is not just backpropagation
- AD (reverse mode) is time-efficient and numerically stable
- AD (reverse mode) is memory inefficient (you need to store all intermediate computations from the forward pass).



Figure 32: Different approaches for taking derivatives

Further reading

- I recommend reading the official Jax Autodiff Cookbook. Open In Colab ♣

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Summary

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Определения

1. Формула для приближенного вычисления производной функции $f(x) : \mathbb{R}^n \rightarrow \mathbb{R}$ по k -ой координате с помощью метода конечных разностей.
2. Пусть $f = f(x_1(t), \dots, x_n(t))$. Формула для вычисления $\frac{\partial f}{\partial t}$ через $\frac{\partial x_i}{\partial t}$ (Forward chain rule).
3. Пусть L - функция, возвращающая скаляр, а v_k - функция, возвращающая вектор $x \in \mathbb{R}^t$. Формула для вычисления $\frac{\partial L}{\partial v_k}$ через $\frac{\partial L}{\partial x_i}$ (Backward chain rule).
4. Идея Хатчинсона для оценки следа матрицы с помощью matvec операций.

Теоремы

1. Автоматическое дифференцирование.
Вычислительный граф. Forward/ Backward mode
(в этом вопросе нет доказательств, но необходимо подробно описать алгоритмы).