

Automatic Differentiation

Benoît Legat

Full Width Mode Present Mode

≡ Table of Contents

Differentiation approaches

Chain rule

Forward Differentiation

Reverse differentiation

Comparison

Discontinuity

Neural network

Wine example 

Second-order

```
1 @htl("""  
2 <p align=center style="font-size: 40px;">Automatic Differentiation</p><p  
3 align=right><i>Benoît Legat</i></p>  
4 $(PlutoTeachingTools.ChooseDisplayStyle())  
5 $(PlutoUI.TableOfContents(depth=1))  
5 """)
```

Differentiation approaches

We can compute partial derivatives in different ways:

1. **Symbolically**, by fixing one of the variables and differentiating with respect to the others, either manually or using a computer.
2. **Numerically**, using the formula $f'(x) \approx (f(x + h) - f(x))/h$.
3. **Algorithmically**, either forward or reverse : this is what we will explore here.

Chain rule ↗

Consider $f(x) = f_3(f_2(f_1(x)))$. If we don't have the expression of f_1 but we can only evaluate $f_i(x)$ or $f'(x)$ for a given x ? The chain rule gives

$$f'(x) = f'_3(f_2(f_1(x))) \cdot f'_2(f_1(x)) \cdot f'_1(x).$$

Let's define $s_0 = x$ and $s_k = f_k(s_{k-1})$, we now have:

$$f'(x) = f'_3(s_2) \cdot f'_2(s_1) \cdot f'_1(s_0).$$

Two choices here:

Forward	Reverse
$t_0 = 1$	$r_3 = 1$
$t_k = f'_k(s_{k-1}) \cdot t_{k-1}$	$r_k = r_{k+1} \cdot f'_{k+1}(s_k)$

Forward Differentiation

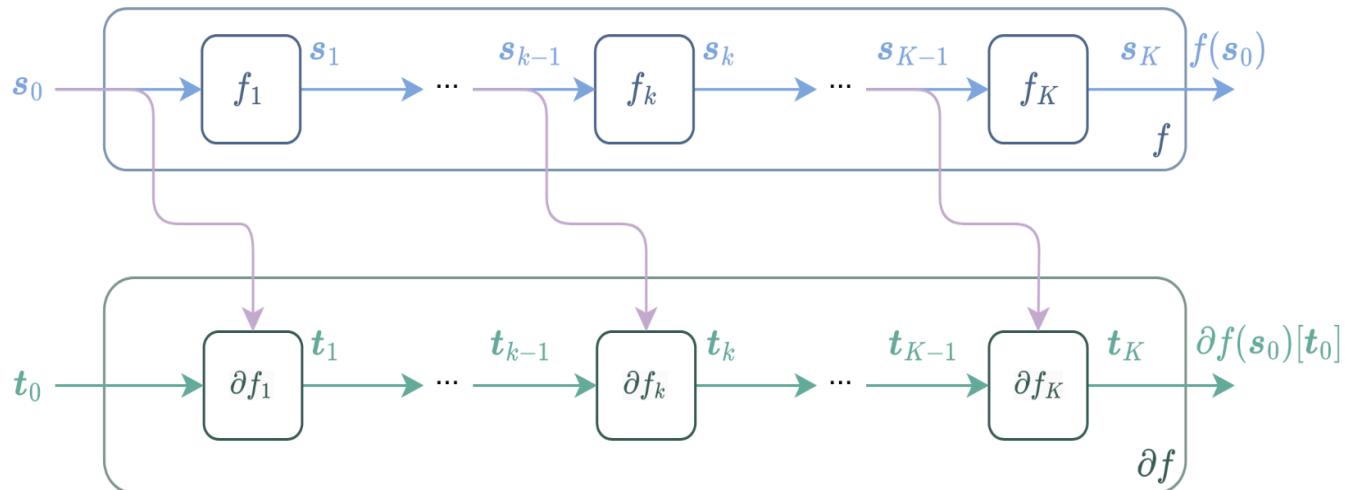


Figure 8.1

Implementation

```
1 struct Dual{T}
2     value::T # s_k
3     derivative::T # t_k
4 end
```

```
1 Base.:- (x::Dual{T}) where {T} = Dual(-x.value, -x.derivative)
```

```
1 Base.*(x::Dual{T}, y::Dual{T}) where {T} = Dual(x.value * y.value, x.value * y.derivative + x.derivative * y.value)
```

```
▶ Dual(-3, -10)
```

```
1 -Dual(1, 2) * Dual(3, 4)
```

```
f_1 (generic function with 1 method)
```

```
1 f_1(x, y) = x * y
```

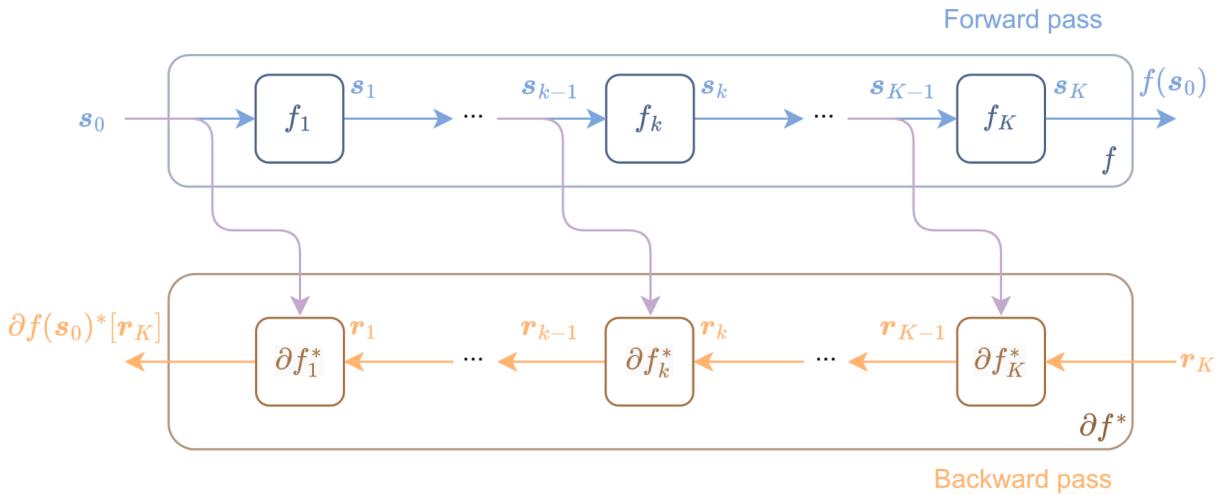
```
f_2 (generic function with 1 method)
```

```
1 f_2(s1) = -s1
```

► Dual(-3, -10)

1 (f_2 ° f_1)(Dual(1, 2), Dual(3, 4))

Reverse differentiation



Two different takes on the multivariate chain rule

The chain rule gives us

$$\frac{\partial f_3}{\partial x}(f_1(x), f_2(x)) = \partial_1 f_3(s_1, s_2) \cdot \frac{\partial s_1}{\partial x} + \partial_2 f_3(s_1, s_2) \cdot \frac{\partial s_2}{\partial x}$$

To compute this expression, we need the values of $s_1(x)$ and $s_2(x)$ as well as the derivatives $\partial s_1/\partial x$ and $\partial s_2/\partial x$.

Common to forward and reverse: Given s_1, s_2 , computes **local** derivatives $\partial_1 f_3(s_1, s_2)$ and $\partial_2 f_3(s_1, s_2)$, shortened $\partial_1 f_3, \partial_2 f_3$ for conciseness.

Forward

$$\begin{aligned} t_3 &= \partial_1 f_3 \cdot t_1 + \partial_2 f_3 \cdot t_2 \\ &= [\partial_1 f_3 \quad \partial_2 f_3] \cdot \begin{bmatrix} t_1 \\ t_2 \end{bmatrix} \\ &= \partial f_3 \cdot \begin{bmatrix} t_1 \\ t_2 \end{bmatrix} \end{aligned}$$

Reverse

$$\begin{aligned} [r_1 \quad r_2] &+= r_1 \cdot \partial f_3 \\ &+= r_1 \cdot [\partial_1 f_3 \quad \partial_2 f_3] \\ &+= [r_1 \cdot \partial_1 f_3 \quad r_1 \cdot \partial_2 f_3] \end{aligned}$$

Reverse*

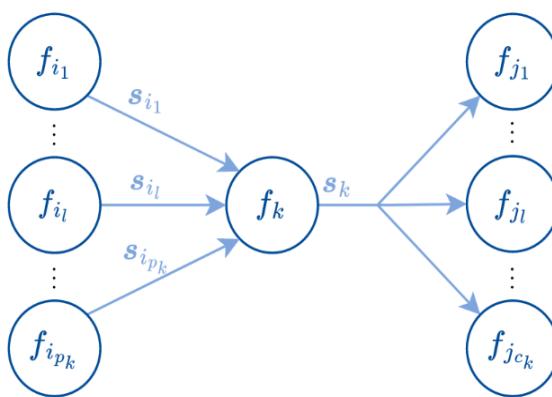
$$\begin{aligned} \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} &+= \partial f_3^* \cdot r_1 \\ &+= \begin{bmatrix} \partial_1 f_3 \\ \partial_2 f_3 \end{bmatrix} \cdot r_1 \\ &+= \begin{bmatrix} \partial_1 f_3 \cdot r_1 \\ \partial_2 f_3 \cdot r_1 \end{bmatrix} \end{aligned}$$

When using automatic differentiation, don't forget that we must always evaluate the derivatives. For the following example we choose to evaluate it in $x = 3$

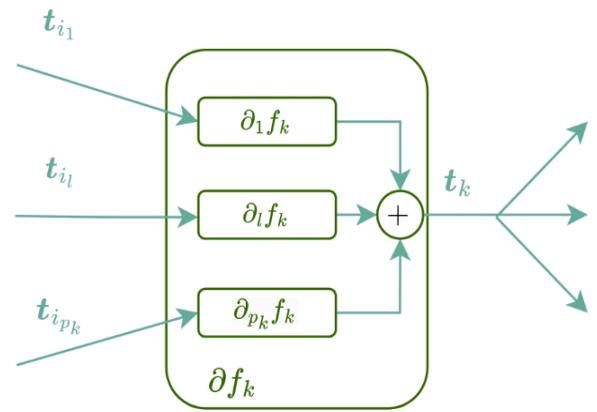
- ▶ Apply the automatic differentiation to $s_3 = f_3(s_1, s_2) = s_1 + s_2$, with $s_1 = f_1(x) = x$ and $s_2 = f_2(x) = x^2$

Forward tangents ↗

Forward pass

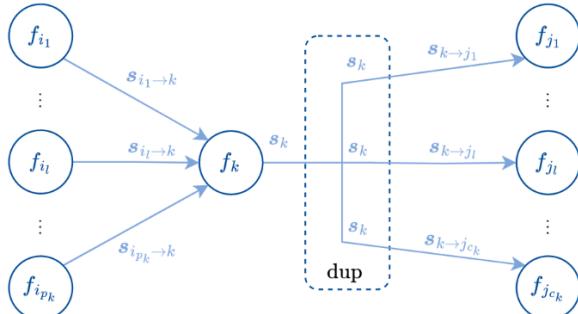


Forward mode

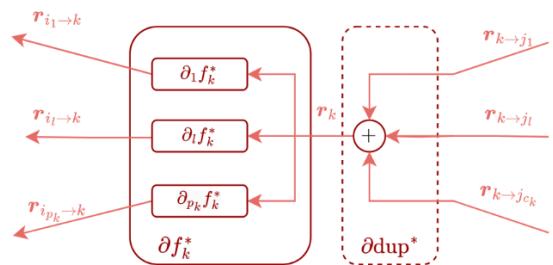


Reverse tangents ↗

Forward pass

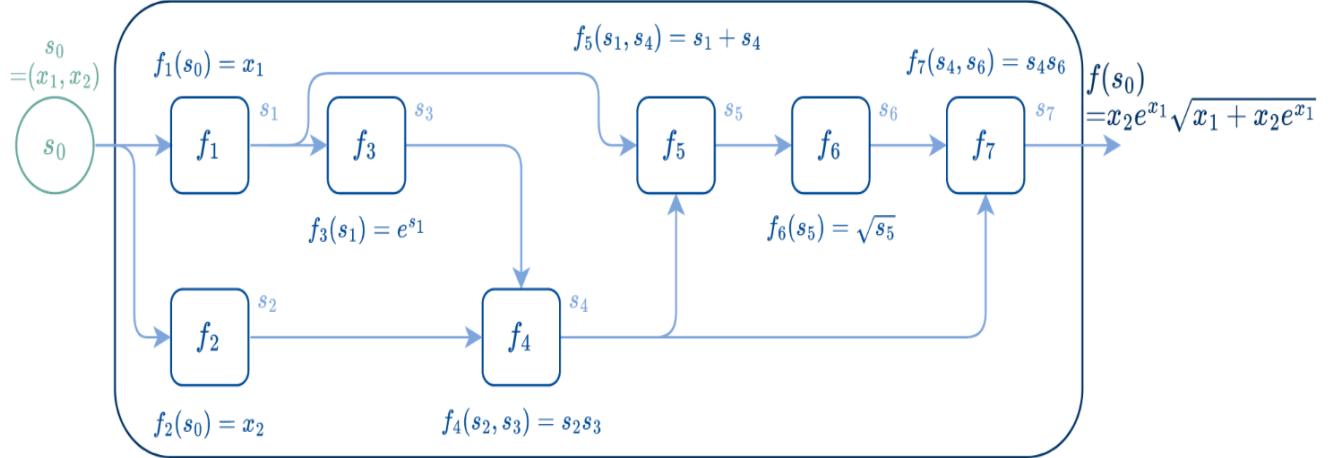


Reverse mode



- ▶ Why is ∂dup^* a sum ?

Expression graph ↴



► Can this directed graph have cycles ?

► What happens if f_4 is handled before f_5 in the backward pass ?

► How to prevent this from happening ?

Comparison ↵

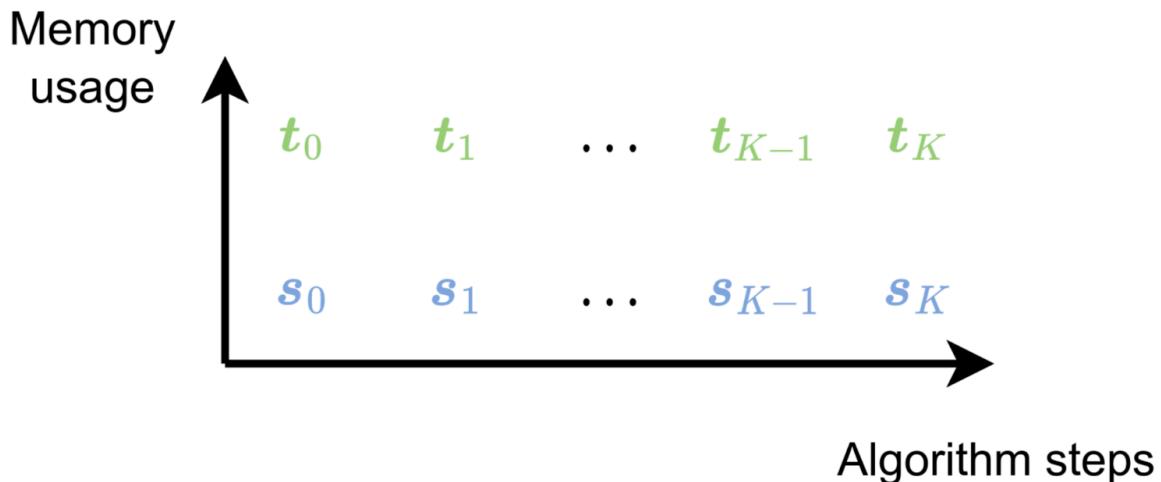
- Forward mode of $f(\mathbf{x})$ with dual numbers $\text{Dual.}(\mathbf{x}, \mathbf{v})$ computes Jacobian-Vector Product (JVP) $\mathbf{J}_f(\mathbf{x}) \cdot \mathbf{v}$
- Reverse mode of $f(\mathbf{x})$ computes Vector-Jacobian Product (VJP) $\mathbf{v}^\top \mathbf{J}_f(\mathbf{x})$ or in other words $\mathbf{J}_v(\mathbf{x})^\top \mathbf{v}$

► How can we compute the full Jacobian ?

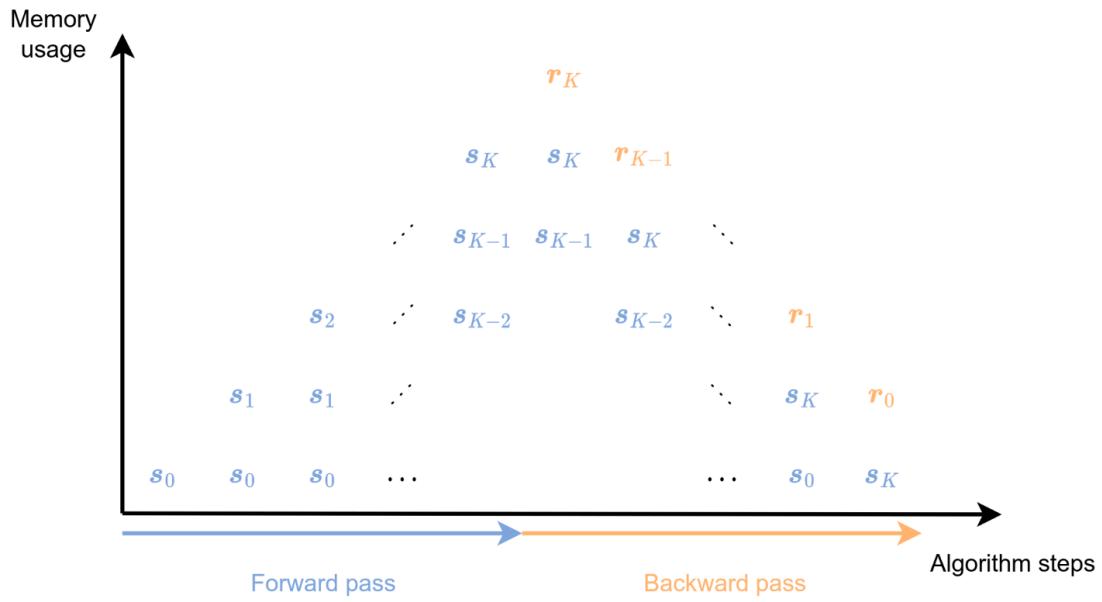
► When is each mode faster than the other one to compute the full Jacobian ?

► When is the speed of numerical differentiation comparable to autodiff ?

Memory usage of forward mode ↵

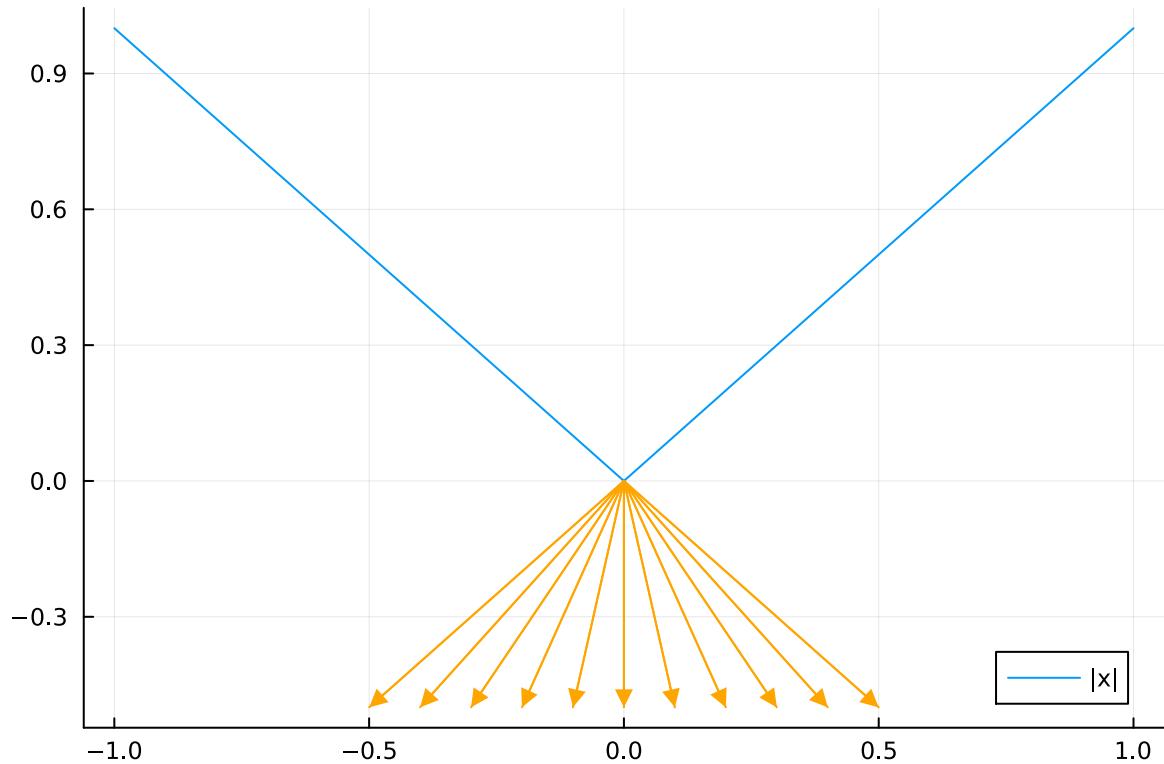


Memory usage of reverse mode \Leftrightarrow



Discontinuity ↴

► Is the function $|x|$ is differentiable at $x = 0$?.



► What about returning a convex combination of the derivative from the left and right ?

Forward mode ↴

```
abs (generic function with 1 method)
```

```
1 abs(x) = ifelse(x < 0, -x, x)
```

```
abs_bis (generic function with 1 method)
```

```
1 abs_bis(x) = ifelse(x > 0, x, -x)
```

```
1 Base.isless(x::Dual, y::Real) = isless(x.value, y)
```

```
1 Base.isless(x::Real, y::Dual) = isless(x, y.value)
```

```
► Dual(0, 1)
```

```
1 abs(Dual(0, 1))
```

```
► Dual(0, -1)
```

```
1 abs_bis(Dual(0, 1))
```

Neural network

Two equivalent approaches, b_k is a **column** vector, S_i, X, W_i, Y are matrices.

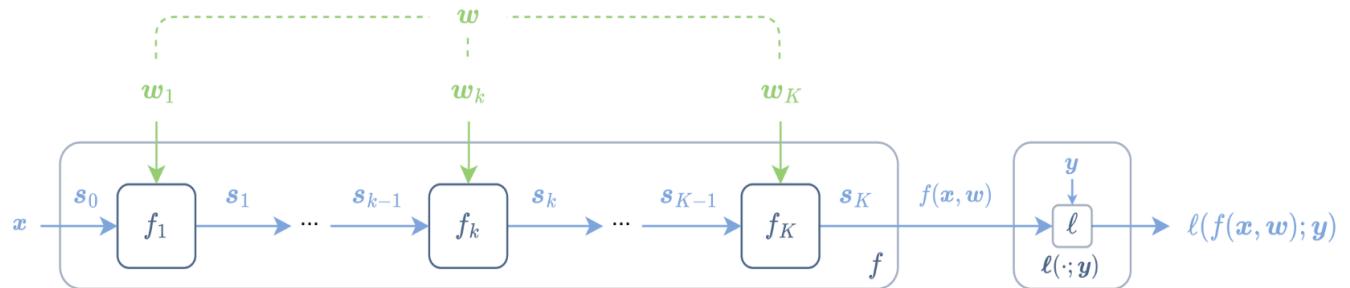
Right-to-left

$$\begin{aligned} S_0 &= X \\ S_{2k-1} &= W_k S_{2k-2} + b_k \mathbf{1}^\top \\ S_{2k} &= \sigma(S_{2k-1}) \\ S_{2H+1} &= W_{k+1} S_{2H} \\ S_{2H+2} &= \ell(S_{2H+1}; Y) \end{aligned}$$

Left-to-right

$$\begin{aligned} S_0 &= X \\ S_{2k-1} &= S_{2k-2} W_k + \mathbf{1} b_k^\top \\ S_{2k} &= \sigma(S_{2k-1}) \\ S_{2H+1} &= S_{2H} W_{k+1} \\ S_{2H+2} &= \ell(S_{2H+1}; Y) \end{aligned}$$

Evaluation



Matrix multiplication (Vectorized way)

Useful: $\text{vec}(AXB) = (B^\top \otimes A)\text{vec}(X)$

$$\begin{aligned} F(X) &= AX \\ G(\text{vec}(X)) &\triangleq \text{vec}(F(X)) = (I \otimes A)\text{vec}(X) \\ J_G &= (I \otimes A) \\ J_G^\top \text{vec}(R) &= (I \otimes A^\top)\text{vec}(R) \\ \partial F^*[R] &= \text{mat}(J_G^\top \text{vec}(R)) = A^\top R \end{aligned}$$

► How should we store the Jacobian in the forward pass to save it for the backward pass ?

Matrix multiplication (Scalar product way)

The adjoint of a linear map A for a given scalar product $\langle \cdot, \cdot \rangle$ is the linear map A^* such that

$$\forall x, y, \quad \langle A(x), y \rangle = \langle x, A^*(y) \rangle.$$

For the scalar product

$$\langle X, Y \rangle = \sum_{i,j} X_{ij} Y_{ij} = \langle \text{vec}(X), \text{vec}(Y) \rangle = \text{tr}(XY^\top), \quad A^* = A^\top$$

Now, given a forward tangent T and a reverse tangent R

$$\langle AT, R \rangle = \langle T, A^\top R \rangle$$

so the backward pass computes $A^\top R$.

► How to prove that $A^* = A^\top$?

Broadcasting (Vectorized way)

Consider applying a scalar function f (e.g. **tanh**) to each entry of a matrix X .)

$$\begin{aligned} (F(X))_{ij} &= f(X_{ij}) = f \cdot (X) \\ G(\text{vec}(X)) &\triangleq \text{vec}(F(X)) = \text{vec}(f \cdot (X)) \\ J_G &= \text{Diag}(\text{vec}(f' \cdot (X))) \\ J_G \text{vec}(T) &= \text{Diag}(\text{vec}(f' \cdot (X))) \text{vec}(T) \\ \partial F[T] &= \text{mat}(J_G \text{vec}(T)) = f' \cdot (X) \odot T \\ J_G^\top \text{vec}(R) &= \text{Diag}(\text{vec}(f' \cdot (X))) \text{vec}(R) \\ \partial F^*[R] &= \text{mat}(J_G^\top \text{vec}(R)) = f' \cdot (X) \odot R \end{aligned}$$

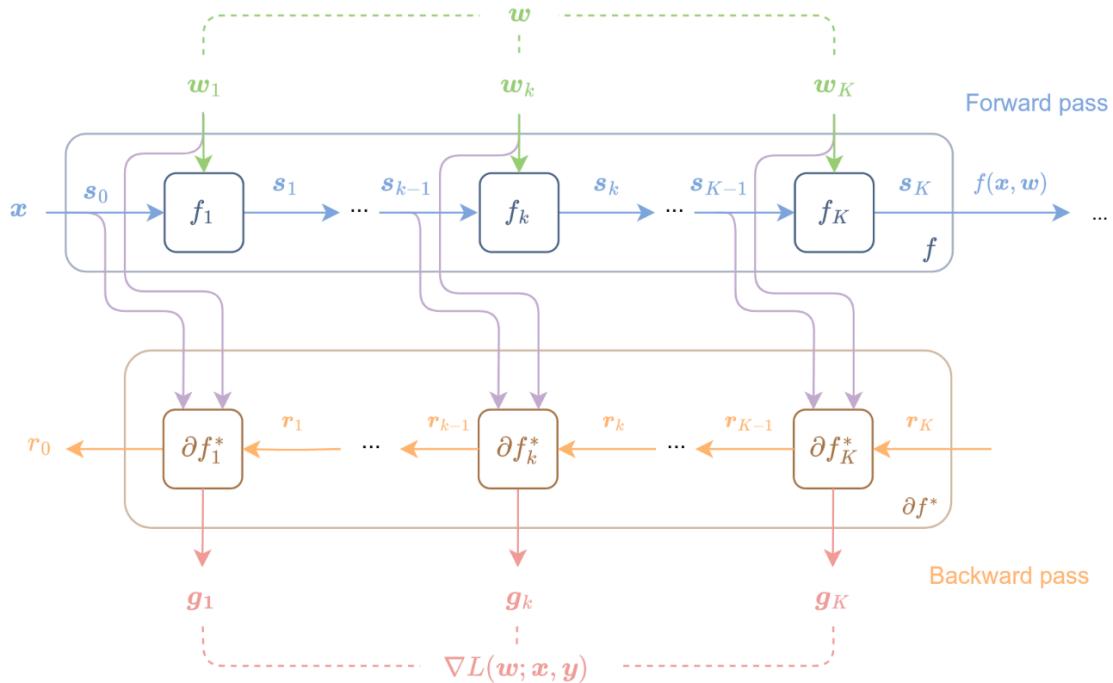
Broadcasting (Scalar product way)

$$\langle f' \cdot (X) \odot T, R \rangle = \langle T, f' \cdot (X) \odot R \rangle.$$

► Let $A(X) = B \odot X$, what is the adjoint A^* ?

► What should be saved for the backward pass ?

Putting everything together ↗



Product of Jacobians ↗

Suppose that we need to differentiate a composition of functions: $(f_n \circ f_{n-1} \circ \dots \circ f_2 \circ f_1)(w)$. For each function, we can compute a jacobian given the value of its input. So, during a forward pass, we can compute all jacobians. We now just need to take the product of these jacobians:

$$J_n J_{n-1} \cdots J_2 J_1$$

While the product of matrices is associative, its computational complexity depends on the order of the multiplications! Let $d_i \times d_{i-1}$ be the dimension of J_i .

► What is the complexity of forward mode

► What is the complexity of reverse mode

► What about the complexity of meeting in the middle between k and $k + 1$?

► Which mode should be used depending on the d_i ?

► What about neural networks ?

Wine example



```
wine = dataset Wine:  
    metadata  => Dict{String, Any} with 4 entries  
    features  => 13x178 Matrix{Float64}  
    targets   => 1x178 Matrix{Int64}  
    dataframe => nothing  
1 wine = MLDatasets.Wine(; as_df = false)
```

```
normalise (generic function with 1 method)
```

```
1 function normalise(x)  
2     μ = Statistics.mean(x, dims=2)  
3     σ = Statistics.std(x, dims=2, mean=μ)  
4     return (x .- μ) ./ σ  
5 end
```

```
X = 13x178 Matrix{Float32}:
```

1.51434	0.245597	0.196325	1.68679	...	0.331822	0.208643	1.39116
-0.560668	-0.498009	0.0211715	-0.345835		1.73984	0.227053	1.57871
0.2314	-0.825667	1.10621	0.486554		-0.38826	0.0126963	1.36137
-1.1663	-2.48384	-0.267982	-0.806975		0.151234	0.151234	1.49872
1.90852	0.018094	0.0881098	0.9283		1.41841	1.41841	-0.261969
0.806722	0.567048	0.806722	2.48444	...	-1.12665	-1.03078	-0.391646
1.03191	0.731565	1.21211	1.4624		-1.3408	-1.35081	-1.27072
-0.657708	-0.818411	-0.497005	-0.979113		0.547563	1.35108	1.59213
1.22144	-0.543189	2.12996	1.02925		-0.420888	-0.228701	-0.420888
0.251009	-0.292496	0.268263	1.18273		2.21798	1.82976	1.78663
0.361158	0.404908	0.317409	-0.426341	...	-1.60759	-1.56384	-1.52009
1.84272	1.11032	0.786369	1.18074		-1.48127	-1.39676	-1.42493
1.01016	0.962526	1.39122	2.32801		0.279786	0.295664	-0.593486

```
1 X = Float32.(normalise(wine.features))
```

```
y =
```

```
1x178 Matrix{Float32}:
```

```
-1.0 -1.0 -1.0 -1.0 -1.0 -1.0 ... 1.0 1.0 1.0 1.0 1.0 1.0 1.0
```

```
1 y = Float32.(wine.targets .- 2)
```

Neural network



h = 16

```

W =
► [16×13 Matrix{Float32}:
 0.505036 0.487785 0.00554371 0.297242 ... 0.555753 0.587209 0.66508 , 1×16 ]
 1 W = [rand(Float32, h, size(x, 1)), rand(Float32, size(y, 1), h)]

```

35.68883f0

```
1 sum((W[2] * tanh.(W[1] * X) - y).^2) / size(y, 2)
```

Forward mode ↗

forward_pass (generic function with 1 method)

```

1 function forward_pass(W, X, y)
2   W1, W2 = W
3   y_1 = tanh.(W1 * X)
4   local_der_tanh = 1 .- y_1.^2
5   local_der_mse = 2 * (W2 * y_1 - y) / size(y, 2)
6   return local_der_tanh, local_der_mse
7 end

```

forward_diff (generic function with 1 method)

```

1 function forward_diff(W, X, y, j, k)
2   W1, W2 = W
3   T_1 = onehot(j, axes(W1, 1)) * onehot(k, axes(W1, 2))'
4   J_1, J_2 = forward_pass(W, X, y)
5   only((W2 * (J_1 .* (T_1 * X))) * J_2') # only: 1x1 matrix -> scalar
6 end

```

forward_diff (generic function with 2 methods)

```

1 function forward_diff(W, X, y)
2   [forward_diff(W, X, y, i, j) for i in axes(W[1], 1), j in axes(W[1], 2)]
3 end

```

```
16×13 Matrix{Float32}:
0.0492459 -0.0151014 0.204655 ... 0.126389 0.164975 0.147873
0.644999 -0.183911 0.0655422 0.0740547 0.0675947 0.51252
0.156035 -0.532178 -0.2059 1.11036 1.69756 0.897393
0.46117 0.126852 0.221034 0.0335679 0.217164 0.786164
0.144001 -0.338128 0.0209725 0.474271 0.620907 0.251471
0.186354 0.277661 0.181377 ... 0.0542061 0.0704498 0.139791
0.0264179 0.0244104 0.017131 -0.0109521 -0.00464136 0.0245121
⋮ ⋮ ⋮
0.755716 0.373341 0.813124 ... -0.402573 -0.365702 0.895789
0.506101 -0.685985 0.0714243 0.904638 0.997983 0.651869
0.21363 -0.244871 0.175721 0.19688 0.270057 0.512348
0.0111615 -0.00103121 0.0026915 0.0101704 0.027334 0.0134008
-0.15025 -0.315693 -0.0169707 0.380187 0.485116 0.227788
0.375061 0.441373 0.316326 ... -0.324608 -0.0673226 0.271744
```

```
1 if h < 200 # Forward Diff start being too slow for 'h > 200'
2   @time forward_diff(W, X, y)
3 end
```

0.014277 seconds (6.24 k allocations: 12.209 MiB)

Reverse mode ↴

► How to deduce the backward pass for reverse mode from the forward mode ?

reverse_diff (generic function with 1 method)

```
1 function reverse_diff(W, X, y)
2   J_1, J_2 = forward_pass(W, X, y)
3   (J_1 .* (W[2]' * J_2)) * X'
4 end
```

```
16×13 Matrix{Float32}:
0.0492459 -0.0151014 0.204655 ... 0.126389 0.164975 0.147873
0.644998 -0.183911 0.0655422 ... 0.0740547 0.0675947 0.51252
0.156035 -0.532178 -0.2059 ... 1.11036 1.69756 0.897393
0.46117 0.126851 0.221034 ... 0.0335679 0.217164 0.786164
0.144001 -0.338128 0.0209725 ... 0.474271 0.620907 0.251471
0.186354 0.277661 0.181377 ... 0.0542061 0.0704498 0.139791
0.0264179 0.0244104 0.017131 ... -0.0109521 -0.00464136 0.0245121
⋮ ⋮ ⋮
0.755716 0.37334 0.813124 ... -0.402573 -0.365702 0.895789
0.506101 -0.685985 0.0714242 ... 0.904638 0.997983 0.651869
0.21363 -0.244871 0.175721 ... 0.19688 0.270057 0.512348
0.0111615 -0.00103121 0.00269151 ... 0.0101704 0.027334 0.0134008
-0.15025 -0.315693 -0.0169707 ... 0.380187 0.485116 0.227788
0.375061 0.441373 0.316326 ... -0.324608 -0.0673226 0.271744
```

```
1 @time reverse_diff(w, x, y)
```

0.000066 seconds (25 allocations: 60.039 KiB)

GPU acceleration

```
1 if CUDA.functional()
2     X_gpu = CUDA.CuArray(x)
3     y_gpu = CUDA.CuArray(y)
4     W_gpu = CUDA.CuArray.(w)
5     @time reverse_diff(W_gpu, X_gpu, y_gpu)
6 end
```

► Why is the GPU version slower than the CPU version ?

Second-order ↴

Consider a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, we want to compute the Hessian $\nabla^2 f(x)$, defined by

$$(\nabla^2 f(x))_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

Application: Given the optimization problem:

$$\begin{aligned} \min_x f(x) \\ g_i(x) = 0 \quad \forall i \in \{1, \dots, m\} \end{aligned}$$

The Hessian of the Lagrangian $\mathcal{L}(x, \lambda) = f(x) - \lambda_1 g_1(x) - \dots - \lambda_m g_m(x)$ is obtained as

$$\nabla_x^2 \mathcal{L}(x, \lambda) = \nabla^2 f(x) - \sum_{i=1}^m \lambda_i \nabla^2 g_i(x)$$

Second-order AD ↴

► How can the Hessian of f be computed given an AD for Jacobian and gradient.

► Does the AD need to be the same for the gradient and the Jacobian ?

Notation ↴

- Let $f_k : \mathbb{R}^{d_{k-1}} \rightarrow \mathbb{R}^{d_k}$. $\partial f_k \triangleq \partial f_k(s_{k-1}) \in \mathbb{R}^{d_k \times d_{k-1}}$, $\partial^2 f_k \triangleq \partial^2 f_k(s_{k-1}) \in \mathbb{R}^{d_k \times d_{k-1} \times d_{k-1}}$ is a 3D array/tensor.
- Given $v \in \mathbb{R}^{d_{k-1}}$, by the product $(\partial^2 f_k \cdot v) \in \mathbb{R}^{d_k \times d_{k-1}}$, we denote the contraction of the the 3rd (or 2nd since the tensor is symmetric over its last 2 dimensions) dimension:

$$(\partial^2 f_k \cdot v)_{ij} = \sum_{l=1}^{d_{k-1}} (\partial^2 f_k)_{ijl} \cdot v_l$$

- Given $\mathbf{u} \in \mathbb{R}^{d_k}$, by the product $(\mathbf{u} \cdot \partial^2 f_k) \in \mathbb{R}^{d_{k-1} \times d_{k-1}}$, we denote the contraction of the the 1st dimension.

$$(\mathbf{u} \cdot \partial^2 f_k)_{ij} = \sum_{l=1}^{d_k} u_l \cdot (\partial^2 f_k)_{lij}$$

- Both $\partial^2 f_k \cdot \mathbf{v}$ and $\mathbf{u} \cdot \partial^2 f_k$ are matrices so then we're back to matrix notations.

Chain rule \Leftrightarrow

$$\begin{aligned} \frac{\partial^2(f_2 \circ f_1)}{\partial x_i \partial x_j} &= \frac{\partial}{\partial x_j} \left(\frac{\partial(f_2 \circ f_1)}{\partial x_i} \right) \\ &= \frac{\partial}{\partial x_j} \left(\partial f_2 \cdot \frac{\partial f_1}{\partial x_i} \right) \\ &= \left(\partial^2 f_2 \cdot \frac{\partial f_1}{\partial x_j} \right) \cdot \frac{\partial f_1}{\partial x_i} + \partial f_2 \cdot \frac{\partial^2 f_1}{\partial x_i \partial x_j} \end{aligned}$$

In terms of the matrices $J_k = \partial f_k$ and $H_{kj} = \frac{\partial}{\partial x_j} J_k = \partial^2 f_k \cdot \frac{\partial s_{k-1}}{\partial x_j}$, it becomes

$$\frac{\partial^2(f_2 \circ f_1)}{\partial x_i \partial x_j} = H_{2j} \cdot \frac{\partial f_1}{\partial x_i} + J_2 \cdot \frac{\partial^2 f_1}{\partial x_i \partial x_j}$$

Forward on forward \Leftrightarrow

Given $\text{Dual}(s_1, t_1)$ with $s_1 = \text{Dual}(f_1(x), \frac{\partial f_1}{\partial x_j})$ and $t_1 = \text{Dual}(\frac{\partial f_1}{\partial x_i}, \frac{\partial^2 f_1}{\partial x_i \partial x_j})$

- Compute $s_2 = f_2(s_1) = (f_2(f_1(x)), J_2 \cdot \frac{\partial f_1}{\partial x_j}) = ((f_2 \circ f_1)(x), \partial(f_2 \circ f_1)/\partial x_j)$
- Compute $J_{f_2}(s_1)$ which gives $\text{Dual}(J_2, H_{2j})$
- Compute

$$\begin{aligned} J_{f_2}(s_1) \cdot t_1 &= \text{Dual}(J_2, H_{2j}) \cdot \text{Dual}(\frac{\partial f_1}{\partial x_i}, \frac{\partial^2 f_1}{\partial x_i \partial x_j}) \\ &= \text{Dual}(J_2 \cdot \frac{\partial f_1}{\partial x_i}, J_2 \cdot \frac{\partial^2 f_1}{\partial x_i \partial x_j} + H_{2j} \cdot \frac{\partial f_1}{\partial x_i}) \\ &= \text{Dual}(\frac{\partial(f_2 \circ f_1)}{\partial x_i}, \frac{\partial^2(f_2 \circ f_1)}{\partial x_i \partial x_j}) \end{aligned}$$

- What is the closed form expression for t_k in terms of the matrices J_k and H_{kj} ?

Forward on reverse ↲

Forward pass: Given $s_1 = \text{Dual}(f_1(x), \frac{\partial f_1}{\partial x_j})$

1. Compute $s_2 = f_2(s_1) \rightarrow$ same as forward on forward
2. Compute $J_{f_2}(s_1) \rightarrow$ same as forward on forward

Reverse pass: Given $r_2 = \text{Dual}((r_2)_1, (r_2)_2)$, compute

$$\begin{aligned} r_2 \cdot J_2 &= \text{Dual}((r_2)_1, (r_2)_2) \cdot \text{Dual}(J_2, H_{2j}) \cdot \\ &= \text{Dual}((r_2)_1 \cdot J_2, (r_2)_2 \cdot J_2 + (r_2)_1 \cdot H_{2j}) \end{aligned}$$

- Which value of r_k is solution for this recurrence equation ?

- What is the closed form expression for r_k in terms of the matrices J_k and H_{kj} ?

Reverse on forward ↲

Forward pass: Given $s_1 = \text{Dual}(f_1(x), \frac{\partial f_1}{\partial x_i})$

1. Forward mode computes

$$s_2 = f_2(s_1) = (f_2(f_1(x)), J_2 \cdot \frac{\partial f_1}{\partial x_i}) = ((f_2 \circ f_1)(x), \partial(f_2 \circ f_1)/\partial x_i)$$

2. The reverse mode computes the local Jacobian of this operation : $\partial s_2 / \partial s_1$. The local Jacobian of $(s_1)_1 \mapsto f_2((s_1)_1)$ is J_2 . The local Jacobian of $s_1 \mapsto \partial f_2((s_1)_1)(s_1)_2$ is $(\partial^2 f_2((s_1)_1) \cdot (s_1)_2, \partial f_2((s_1)_1)) = (\partial^2 f_2(f_1(x)) \cdot \frac{\partial f_1}{\partial x_i}, \partial f_2(f_1(x))) = (H_{2i}, J_2)$

Reverse pass:

$$\begin{aligned} (r_1)_1 &= (r_2)_1 \cdot J_2 + (r_2)_2 \cdot H_{2i} \\ (r_1)_2 &= (r_2)_2 \cdot J_2 \end{aligned}$$

- Which value of r_k is solution for this recurrence equation ?

Reverse on reverse ↳

Forward pass (2nd):

1. Forward pass computes $s_2 = f_2(s_1) \rightarrow$ Jacobian $\partial s_2 / \partial s_1 = J_2$
2. Local Jacobian $J_2 = \partial f_2(s_1) \rightarrow$ The Jacobian is the 3D array $\partial J_2 / \partial s_1 = \partial^2 f_2$
3. Backward pass computes $r_1 = r_2 \cdot \partial f_2(s_1) \rightarrow$ Jacobian of $(s_1, r_2) \mapsto r_2 \cdot \partial f_2(s_1)$ is $(r_2 \cdot \partial^2 f_2(s_1), \partial f_2(s_1)) = (r_2 \cdot \partial^2 f_2, J_2)$. Note that here $r_2 \in \mathbb{R}^{d_k}$ is multiplying the first dimension of the tensor $\partial^2 f_2(s_1) \in \mathbb{R}^{d_k \times d_{k-1} \times d_{k-1}}$ so the result is a symmetric matrix of dimension $\mathbb{R}^{d_{k-1} \times d_{k-1}}$

Reverse pass (2nd): The result is r_0 , let \dot{r}_k be the second-order reverse tangent for r_k and \dot{s}_k be the second-order reverse tangent of s_k . We have

$$\begin{aligned}\dot{r}_2 &= J_2 \cdot \dot{r}_1 \\ \dot{s}_1 &= (r_2 \cdot \partial^2 f_2(s_1)) \cdot \dot{r}_1 + \dot{s}_2 \cdot J_2\end{aligned}$$

► Which value of \dot{s}_k, \dot{r}_k is solution for this recurrence equation ?

► What is the difference with reverse on forward and forward on reverse ?

Acknowledgements and further readings ↳

- Dual is inspired from [ForwardDiff](#)
- Node is inspired from [micrograd](#)
- [Here](#) is a good intro to AD
- Figures are from the [The Elements of Differentiable Programming book](#)

The End

Utils ↵

```
1 using Plots, PlutoUI, PlutoUI.ExperimentalLayout, HypertextLiteral; @htl, @htl_str  
PlutoTeachingTools, DataFrames, MLDatasets, Statistics, CUDA, OneHotArrays
```

```
img (generic function with 3 methods)
```

```
qa (generic function with 2 methods)
```