Automatic Differentiation

Benoît Legat

☐ Full Width Mode ☐ Present Mode

Table of Contents


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

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:

$$\begin{array}{ll} \text{Forward} & \text{Reverse} \\ t_0 = 1 & r_3 = 1 \\ t_k = f_k'(s_{k-1}) \cdot t_{k-1} & r_k = r_{k+1} \cdot f_{k+1}'(s_k) \end{array}$$

Forward Differentiation

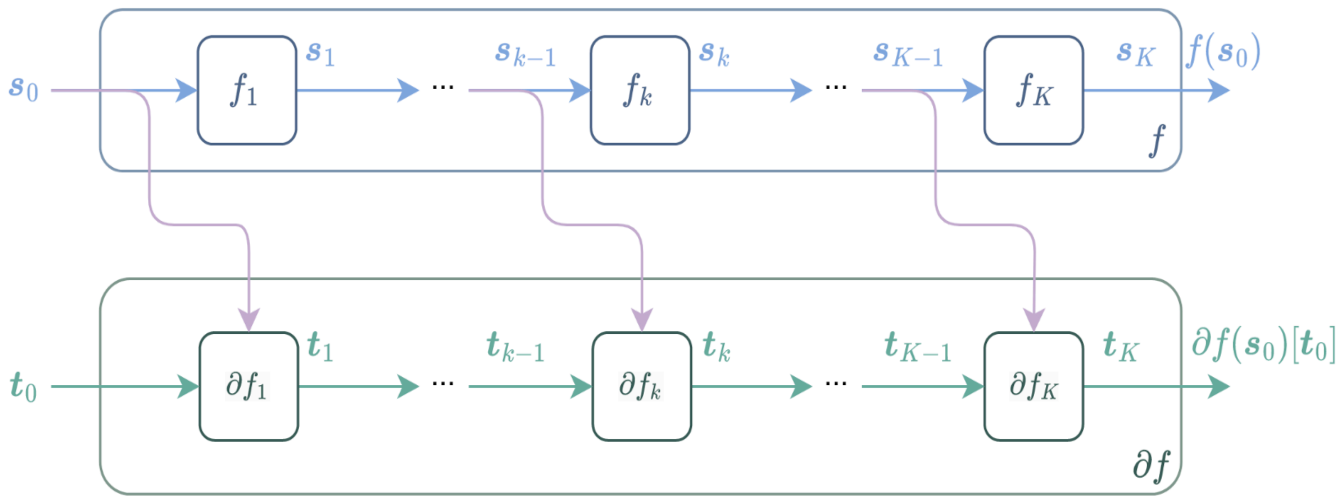


Figure 8.1

Implementation

```julia
struct Dual{T}
    value::T # s_k
    derivative::T # t_k
end
```

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

```julia
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)
```

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

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

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

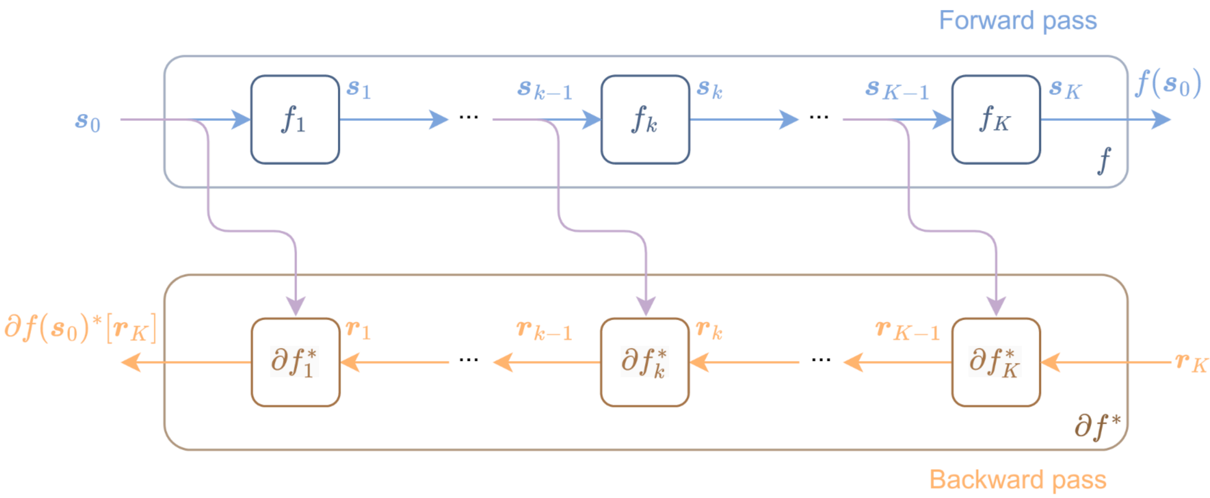
```
f_2 (generic function with 1 method)
```

```julia
f_2(s1) = -s1
```

Dual(-3, -10)

```
(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

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

Reverse

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

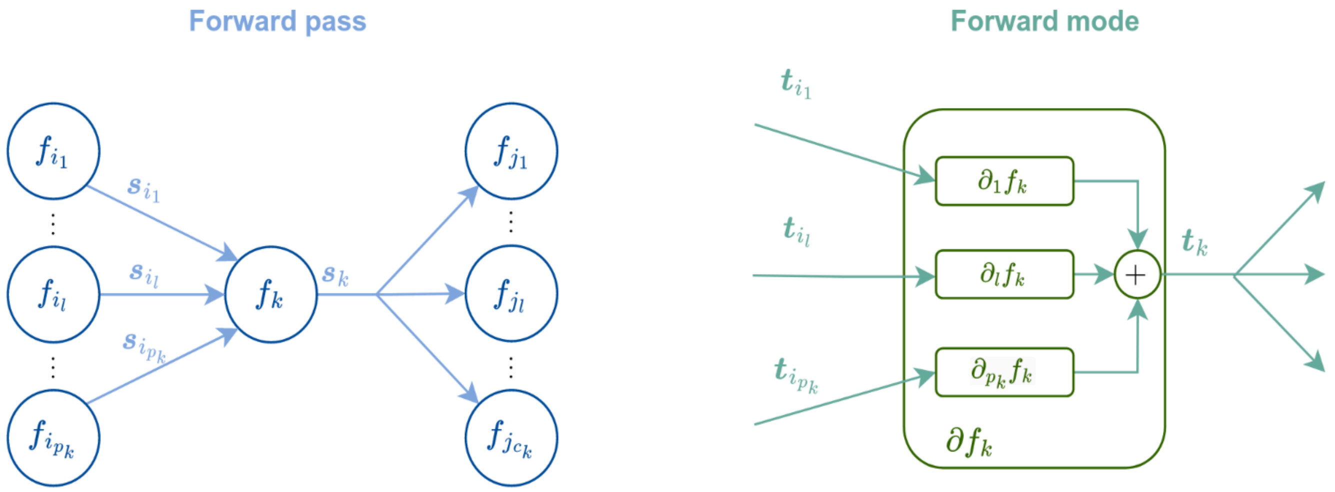
Reverse*

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

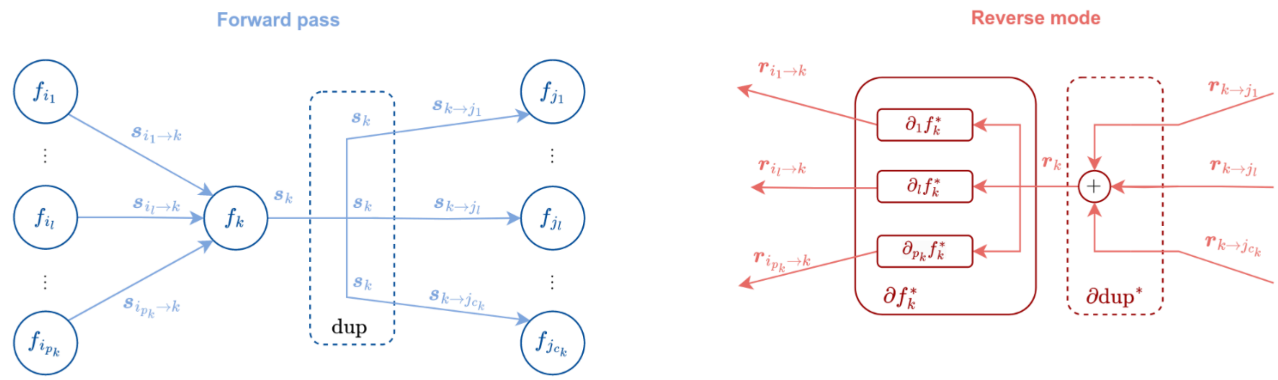
When using automatic differentiation, don't forget that we must always evaluate the derivatives. For the following example we choose to evaluate it in $x = 3$

▶ **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

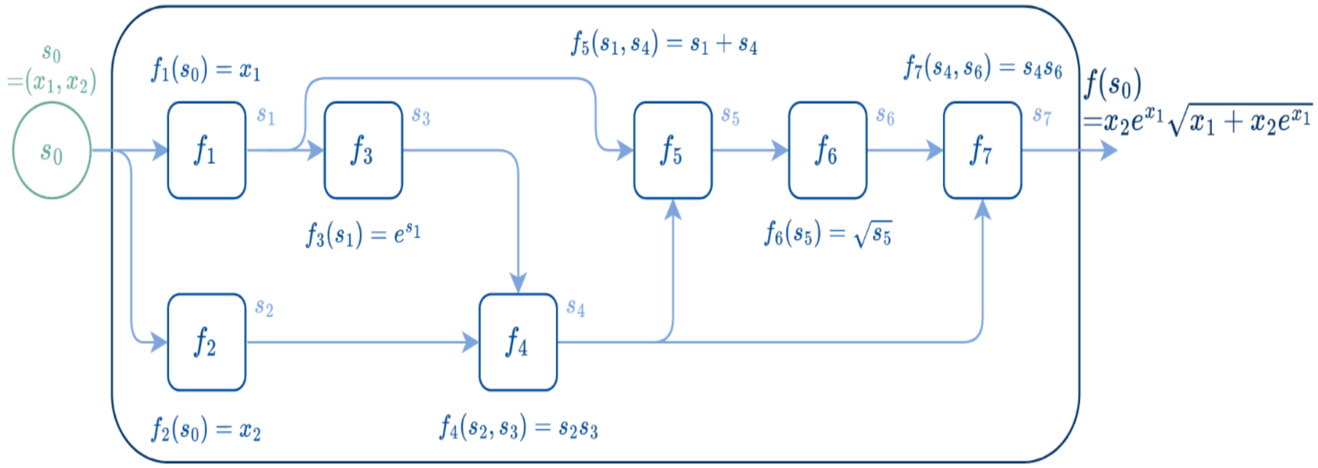


Reverse tangents



▶ **Why is $\partial\mathrm{dup}^*$ 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

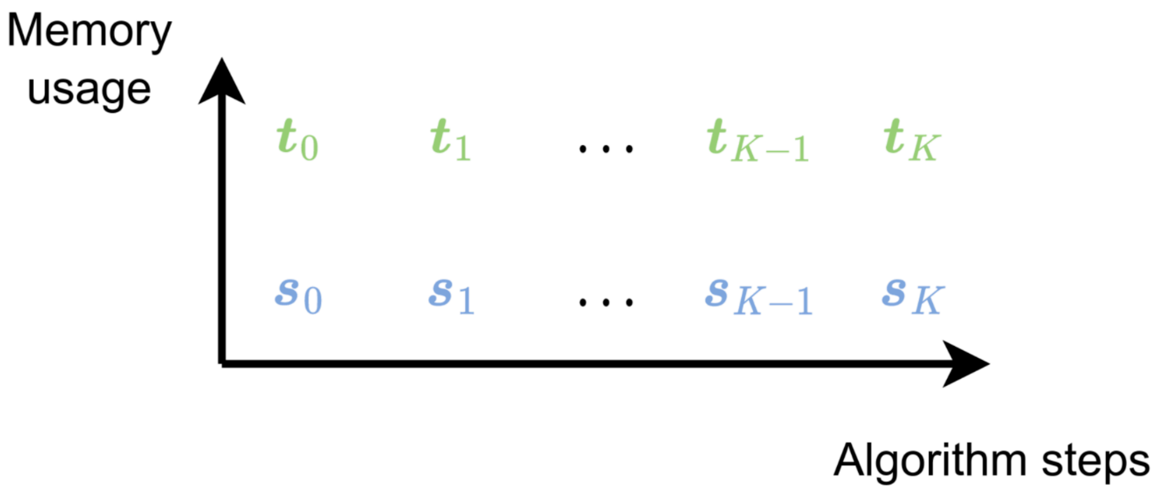
- Forward mode of $f(x)$ with dual numbers `Dual.(x, v)` computes Jacobian-Vector Product (JVP) $J_f(x) \cdot v$
- Reverse mode of $f(x)$ computes Vector-Jacobian Product (VJP) $v^\top J_f(x)$ or in other words $J_v(x)^\top v$

▶ **How can we compute the full Jacobian ?**

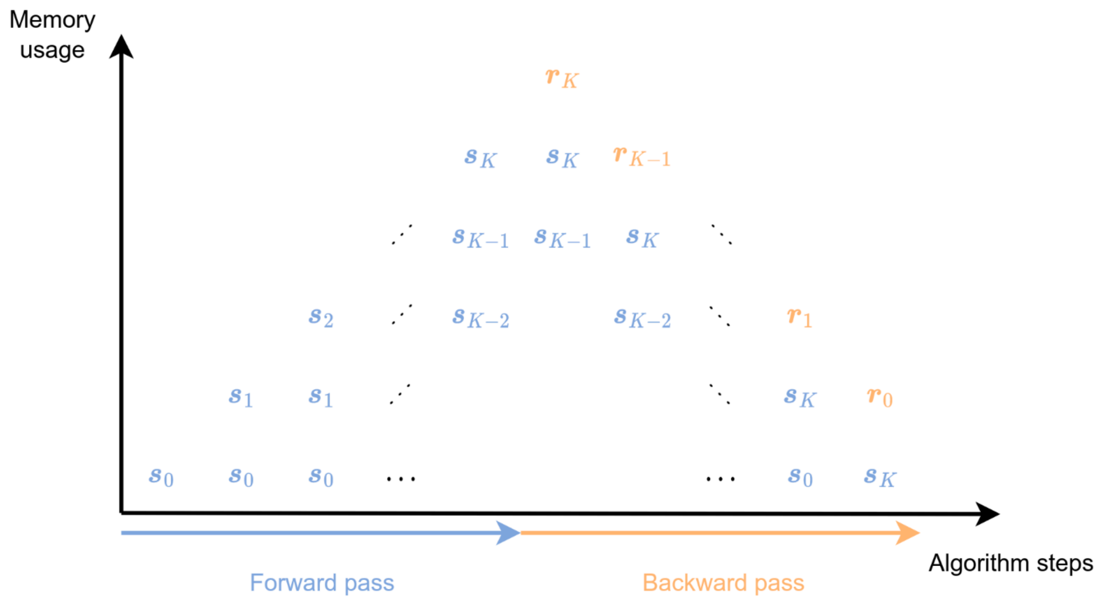
▶ **When is each mode faster than the other one to compute the full Jacobian ?**

▶ **When is the speed of numerical differentation comparable to autodiff ?**

Memory usage of forward mode

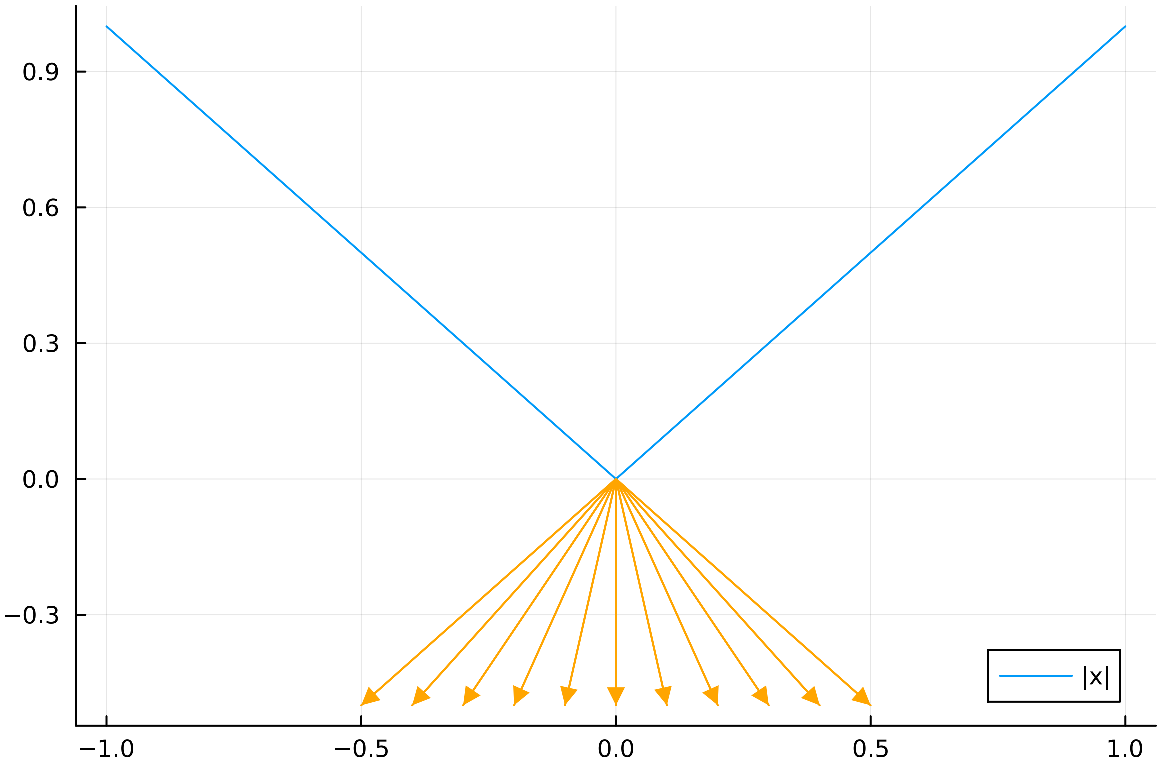


Memory usage of reverse mode



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)
```

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

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

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

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

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

Dual(0, 1)

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

Dual(0, -1)

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

Neural network

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

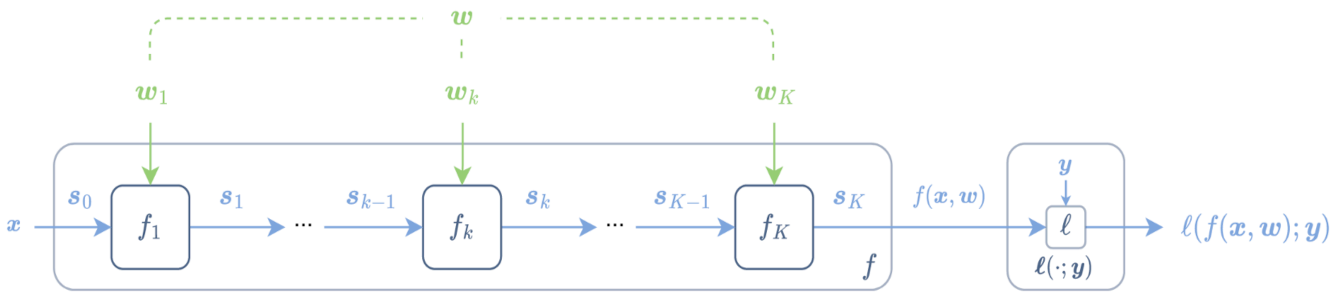
Right-to-left

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

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

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

▶ **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

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

For the scalar product

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

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.)

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

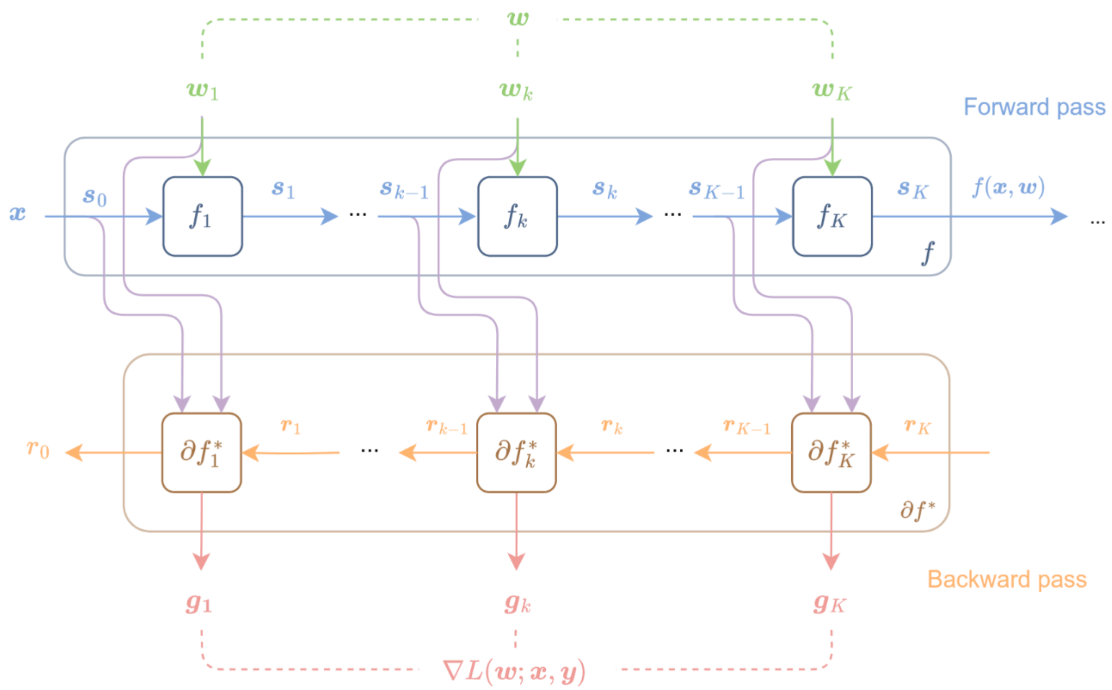
Broadcasting (Scalar product way)

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

▶ **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: $(f_n \circ f_{n-1} \circ \cdots \circ f_2 \circ f_1)(w)$. 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    =>    13×178 Matrix{Float64}
         targets     =>    1×178 Matrix{Int64}
         dataframe   =>    nothing
```

```julia
wine = MLDatasets.Wine(; as_df = false)
```

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

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

```
X = 13×178 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
```

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

```
y =
1×178 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  1.0  1.0
```

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

Neural network

h = 16

W =
[16×13 Matrix{Float32}: , 1×16
 0.236027 0.308693 0.585844 0.705263 … 0.829723 0.212261 0.76601 0.40

```
W = [rand(Float32, h, size(X, 1)), rand(Float32, size(y, 1), h)]
```

66.36216f0

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

Forward mode

forward_pass (generic function with 1 method)

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

forward_diff (generic function with 1 method)

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

forward_diff (generic function with 2 methods)

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

```
16×13 Matrix{Float32}:
 1.04964     0.0655278   0.171851   -0.771603    …  -0.079571     0.641803   0.838214
 1.46885    -0.651935   -0.0590148  -1.62874         1.55764      1.63905    1.59999
 1.33611     0.764662    0.629348   -0.87326        -0.180618     1.22412    1.54006
 0.153573   -0.0687102   0.180797    0.00633693     -0.0124792    0.0661557  0.212615
 0.210337    0.0182636   0.0920603  -0.0302179       0.00600257  -0.0175566  0.177999
 0.0338393   0.199906    0.41397     0.0233268   …   0.119807     0.0780009  0.135605
 0.701931    0.434825    0.514749   -0.209099       -0.263038     0.46571    0.790662
 ⋮                                               ⋱   ⋮
 0.793485   -0.534683    0.209974   -0.818405    …   0.702516     1.01624    0.899772
 0.319025    0.375648    0.869738    0.341923        0.00940278  -0.0936657  0.339416
 2.18812     1.07933     0.634837   -0.865755       -0.715943    -0.502493   2.05445
 0.706795   -0.894235    0.0722831  -1.30391         1.45139      1.46889    1.38438
 0.148724   -0.0463969   0.6828      0.186771        0.587335     0.911601   0.475006
 0.0188028  -0.136066    0.0356962  -0.0784971   …   0.123632     0.157679   0.147255
```

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

```
0.030430 seconds (6.24 k allocations: 12.209 MiB, 52.53% gc time)
```

Reverse mode

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

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

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

```
16×13 Matrix{Float32}:
 1.04964     0.0655278   0.171851   -0.771604    …  -0.079571     0.641803   0.838214
 1.46885    -0.651935   -0.0590148  -1.62874         1.55764      1.63905    1.59999
 1.33611     0.764661    0.629348   -0.87326        -0.180618     1.22412    1.54006
 0.153573   -0.0687102   0.180797    0.00633692     -0.0124792    0.0661557  0.212615
 0.210337    0.0182636   0.0920603  -0.0302179       0.00600257  -0.0175566  0.177999
 0.0338394   0.199906    0.413969    0.0233268   …   0.119807     0.0780009  0.135605
 0.701931    0.434825    0.514749   -0.209099       -0.263038     0.46571    0.790662
 ⋮                                               ⋱   ⋮
 0.793485   -0.534683    0.209974   -0.818405    …   0.702516     1.01624    0.899772
 0.319025    0.375648    0.869738    0.341923        0.00940276  -0.0936657  0.339416
 2.18812     1.07933     0.634837   -0.865755       -0.715943    -0.502493   2.05445
 0.706795   -0.894235    0.0722831  -1.30391         1.45139      1.46889    1.38438
 0.148724   -0.0463968   0.6828      0.186771        0.587335     0.911601   0.475006
 0.0188028  -0.136066    0.0356962  -0.0784971   …   0.123632     0.157679   0.147255
```

```julia
@time reverse_diff(W, X, y)
```

```
0.000064 seconds (25 allocations: 60.039 KiB)
```

🚀 GPU acceleration ⚡

```julia
if CUDA.functional()
    X_gpu = CUDA.CuArray(X)
    y_gpu = CUDA.CuArray(y)
    W_gpu = CUDA.CuArray.(W)
    @time reverse_diff(W_gpu, X_gpu, y_gpu)
end
```

▶ **Why is the GPU version slower than the CPU version ?**

Second-order

Consider a function $f : \mathbb{R}^n \to \mathbb{R}$, 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:

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

The Hessian of the Lagrangian $\mathcal{L}(x, \lambda) = f(x) - \lambda_1 g_1(x) - \cdots - \lambda_m g_m(x)$ 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 $f_k : \mathbb{R}^{d_{k-1}} \to \mathbb{R}^{d_k}$. $\partial f_k \triangleq \partial f_k(s_{k-1}) \in \mathbb{R}^{d_k \times d_{k-1}}$, $\partial^2 f_k \triangleq \partial^2 f_k(s_{k-1}) \in \mathbb{R}^{d_k \times d_{k-1} \times d_{k-1}}$ 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 $u \in \mathbb{R}^{d_k}$, by the product $(u \cdot \partial^2 f_k) \in \mathbb{R}^{d_{k-1} \times d_{k-1}}$, we denote the contraction of the the 1st dimension.

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

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

Chain rule

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

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

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

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

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

▶ **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 $s_1 = \mathrm{Dual}(f_1(x), \frac{\partial f_1}{\partial x_j})$

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

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

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

▶ **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 $s_1 = \mathrm{Dual}(f_1(x), \frac{\partial f_1}{\partial x_i})$

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 $s_2 = f_2(s_1)$ → Jacobian $\partial s_2/\partial s_1 = J_2$
2. Local Jacobian $J_2 = \partial f_2(s_1)$ → The Jacobian is the 3D array $\partial J_2/\partial s_1 = \partial^2 f_2$
3. Backward pass computes $r_1 = r_2 \cdot \partial f_2(s_1)$ → 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

```
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)
```