Automatic Differentiation

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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

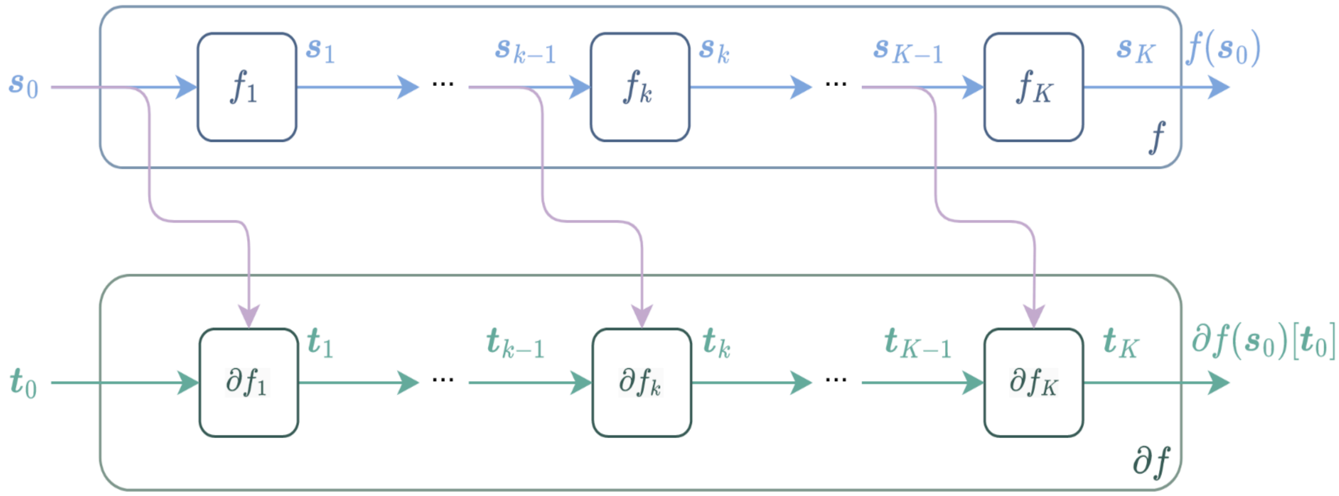


Figure 8.1

Implementation

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

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

```
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)

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

f_1 (generic function with 1 method)

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

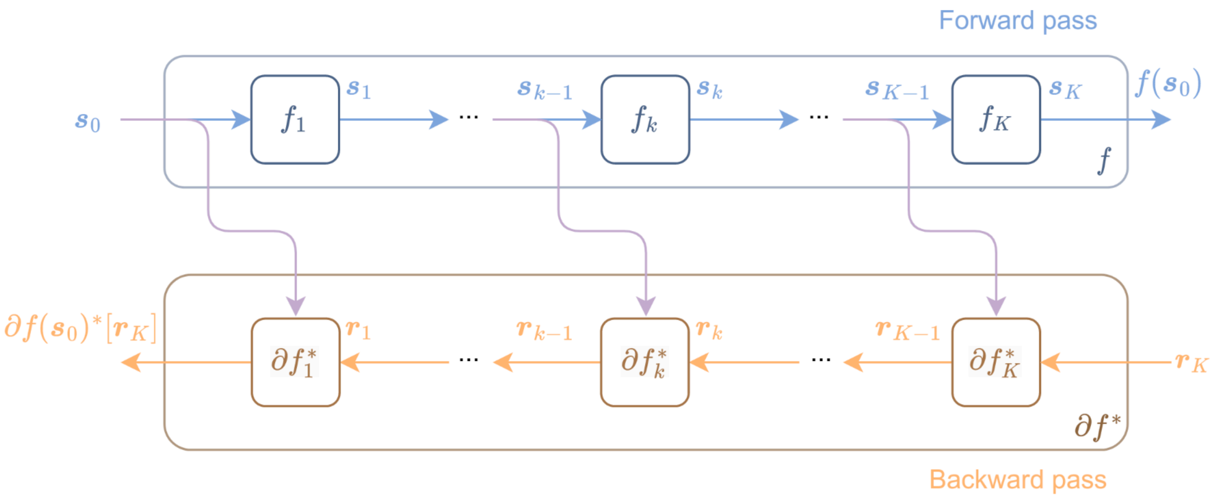
f_2 (generic function with 1 method)

```
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

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

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

Forward

$$t_3 = \frac{\partial s_3}{\partial s_1} t_1 + \frac{\partial s_3}{\partial s_2} t_2$$

- Given s_1, s_2, computes $\frac{\partial s_3}{\partial s_1}(s_1, s_2)$ and $\frac{\partial s_3}{\partial s_2}(s_1, s_2)$
- Given t_1 and t_2, computes $\partial f_3/\partial x$

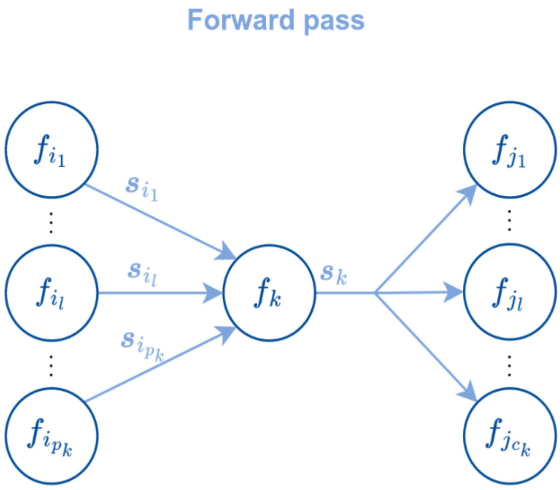
Reverse

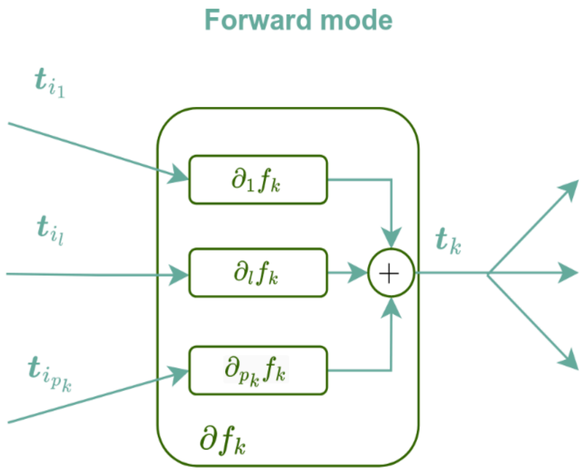
- Given s_1, s_2, computes $\frac{\partial s_3}{\partial s_1}(s_1, s_2)$ and $\frac{\partial s_3}{\partial s_2}(s_1, s_2)$
- Given $r_3 = \partial s_K/\partial s_3$
  - **Add** $r_3 \cdot (\partial s_3/\partial s_1)$ to r_1
  - **Add** $r_3 \cdot (\partial s_3/\partial s_2)$ to r_2

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

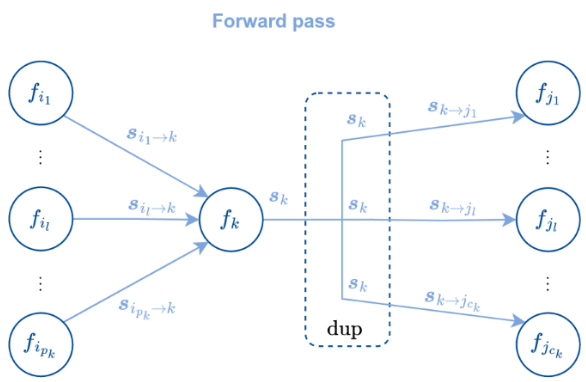
▶ **Apply the automatic differentiation to $s_3 = f_3(s_1, s_2) = s_1 + s_2$, with $s_1 = f_1(x) = x$ and $s_2 = f_2(x) = x^2$**

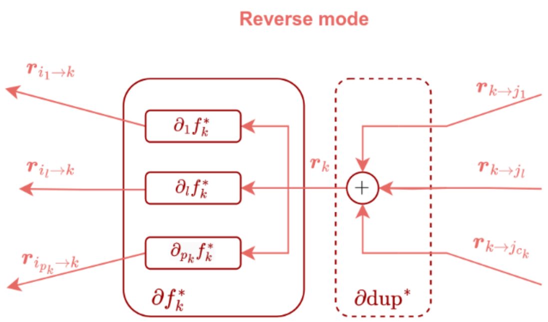
Forward tangents





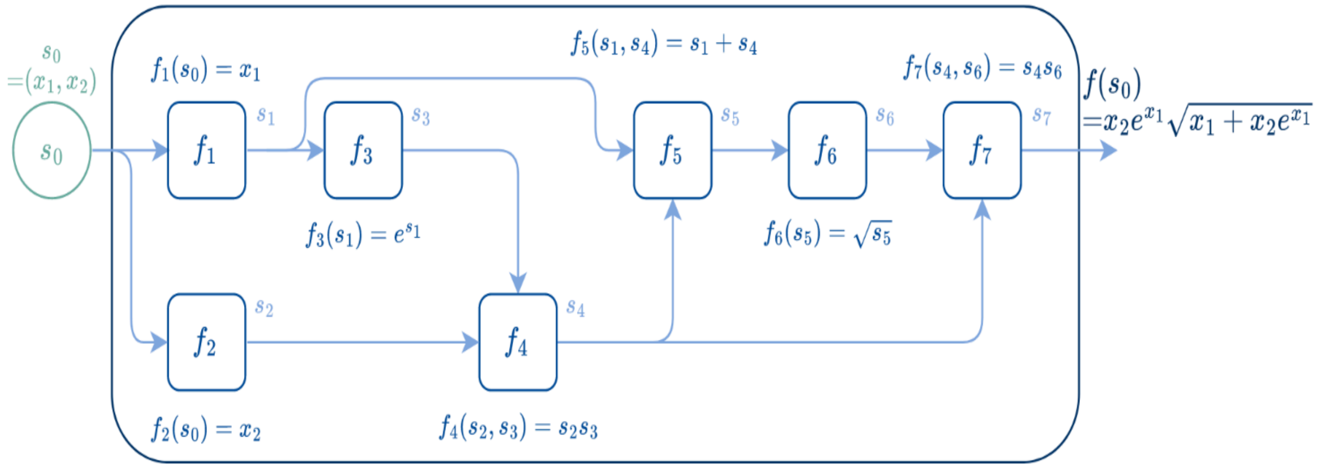
Reverse tangents





▶ **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

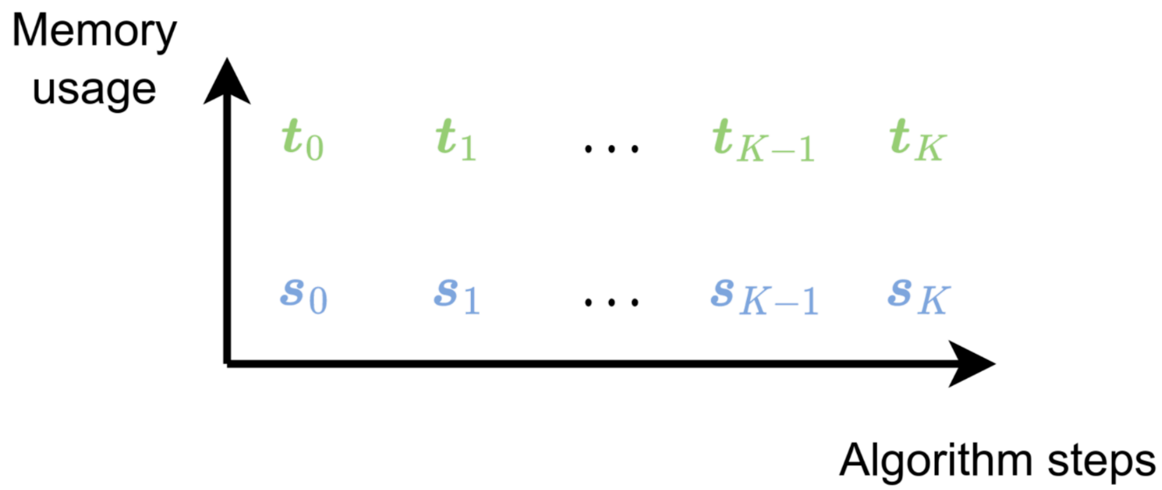
- Forward mode of $f(x)$ with dual numbers `Dual.(x, v)` computes Jacobian-Vector Product (JVP) $J_f(x) \cdot v$
- Reverse mode of $f(x)$ computes Vector-Jacobian Product (VJP) $v^\top J_f(x)$ or in other words $J_v(x)^\top v$

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

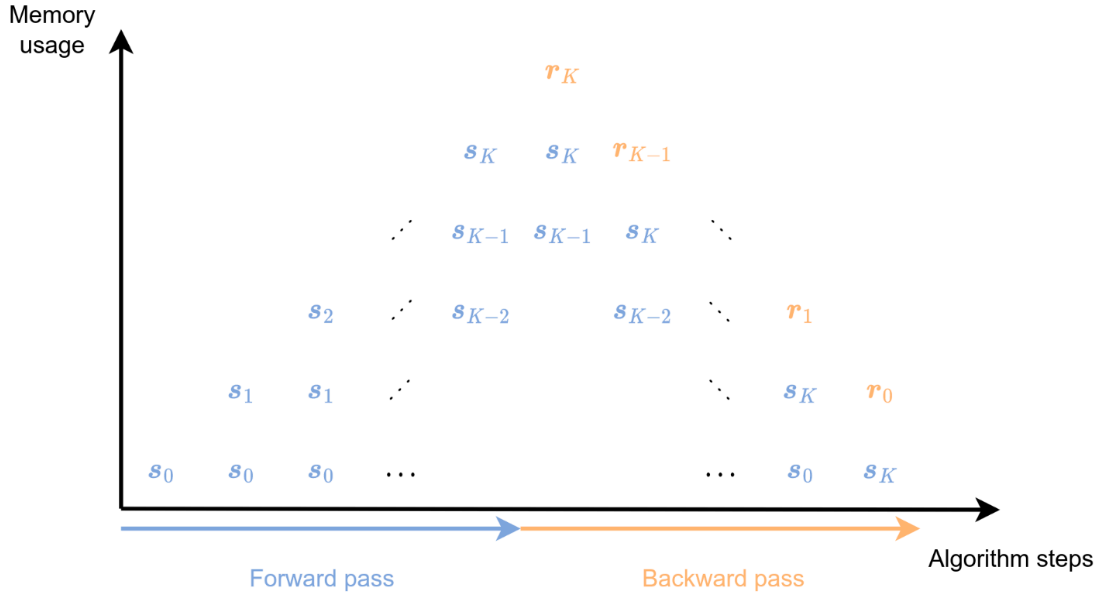
▶ **When is each mode faster than the other one to compute the full Jacobian ?**

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

Memory usage of forward mode

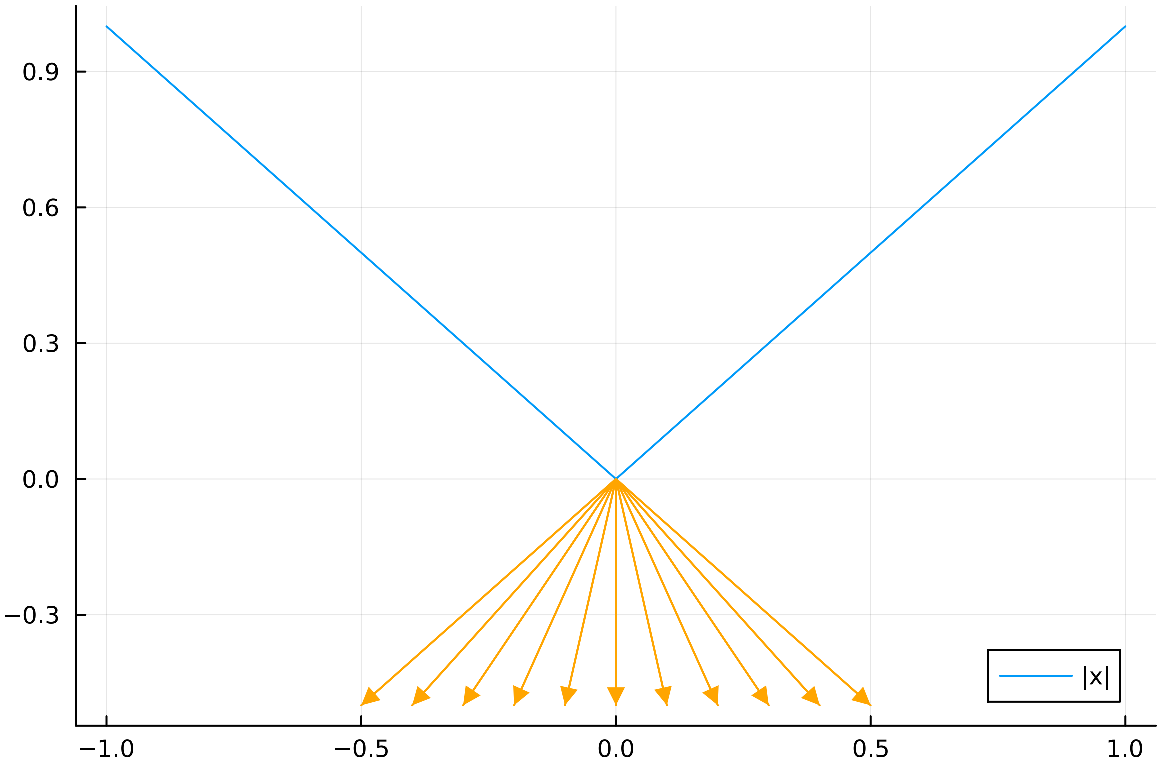


Memory usage of reverse mode



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.

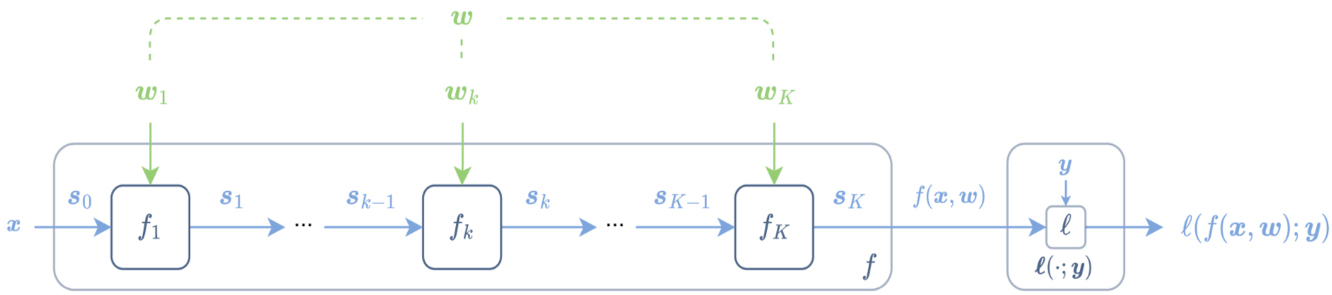
Right-to-left

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

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

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

▶ **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

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

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.)

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

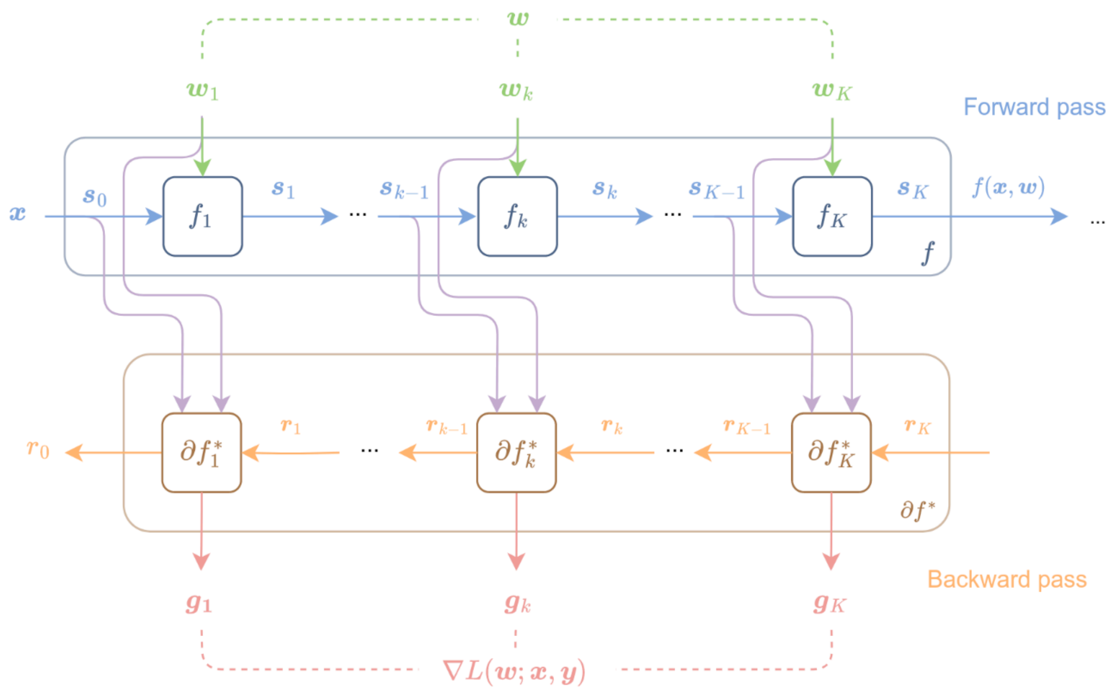
Broadcasting (Scalar product way)

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

▶ **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 ?**

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
```

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

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