Automatic differentiation

Refs:

1. https://github.com/karpathy/micrograd/tree/master/micrograd
2. https://github.com/mattjj/autodidact
3. https://github.com/mattjj/autodidact/blob/master/autograd/numpy/numpy_vjps.p
4. https://auto-ed.readthedocs.io/en/latest/mod2.html#ii-more-theory
5. https://github.com/lindseysbrown/Auto-eD/blob/master/docs/mod2.rst?plain=1

Latex macros

Chain rule

Scalar single-variable chain rule

Recall the limit definition of derivative of a function,

$$g'(x) = \lim_{h \to 0} \frac{g(x+h) - g(x)}{h}.$$

From the limit definition you can find the value of $g(x+h)$ as

$$\lim_{h \to 0} g(x+h) = \lim_{h \to 0} g(x) + g'(x)h.$$

You can use this rule to find the chain rule of finding the chaining of two functions together,

$$\begin{aligned}
\frac{\partial f(g(x))}{\partial x} &= \lim_{h \to 0} \frac{f(g(x+h)) - f(g(x))}{h} \\
&= \lim_{h \to 0} \frac{f(g(x) + g'(x)h) - f(g(x))}{h} \\
&= \lim_{h \to 0} \frac{f(g(x)) + f'(g(x))g'(x)h - f(g(x))}{h} \\
&= f'(g(x))g'(x)
\end{aligned}$$

Scalar two-variable chain rule

Vector Jacobian Products

$$f(\underline{x}, \underline{y}) = \underline{x}^T \underline{y} \quad , \quad \text{Given } \frac{\partial l}{\partial f} \quad l(f(\underline{x}, \underline{y}))$$

Find $\frac{\partial l}{\partial \underline{x}}$, $\frac{\partial l}{\partial \underline{y}}$ in terms of $\underline{x}$, $\underline{y}$ and $\frac{\partial l}{\partial f}$

$$\frac{\partial l}{\partial f} \frac{\partial f}{\partial \underline{x}} \qquad \frac{\partial l}{\partial f} \frac{\partial f}{\partial \underline{y}}$$

$$\frac{\partial}{\partial \underline{x}} \underline{b}^T \underline{x} = \underline{b}^T$$

$$\frac{\partial l}{\partial \underline{x}} = \frac{\partial l}{\partial f} y^T \qquad \frac{\partial l}{\partial \underline{y}} = \frac{\partial l}{\partial f} \underline{x}^T$$

Matrix-vector multiplication

$$\underline{f}(A, \underline{x}) = A\underline{x} \quad , \quad \text{Given } \frac{\partial l}{\partial \underline{f}}$$

Find $\frac{\partial l}{\partial A}$, $\frac{\partial l}{\partial \underline{x}}$

we have not defined derivative wrt matrices

$$\frac{\partial l}{\partial A} = \begin{bmatrix} \frac{\partial l}{\partial a_{11}} & \cdots & \frac{\partial l}{\partial a_{1n}} \\ \vdots & & \\ \frac{\partial l}{\partial a_{m1}} & \cdots & \frac{\partial l}{\partial a_{mn}} \end{bmatrix}_{m \times n}$$

$$A = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \\ a_{m1} & \cdots & a_{mn} \end{bmatrix}$$

vectorization function / flattening function

$$vec(A) = \begin{bmatrix} a_{11} \\ a_{12} \\ \vdots \\ a_{1n} \\ a_{21} \\ a_{22} \\ \vdots \\ a_{mn} \end{bmatrix}$$

row-wise vectorization

$$\frac{\partial l}{\partial\, vec(A)} \xrightarrow{vec^{-1}} \frac{\partial l}{\partial A}$$

$$\underline{f}(A, \underline{x}) = A\underline{x} = \begin{bmatrix} \leftarrow \underline{a}_1^T \rightarrow \\ \leftarrow \underline{a}_2^T \rightarrow \\ \vdots \\ \leftarrow \underline{a}_m^T \rightarrow \end{bmatrix} \begin{bmatrix} \uparrow \\ \underline{x} \\ \downarrow \end{bmatrix}$$

$$\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{bmatrix} = \begin{bmatrix} \underline{a}_1^T \underline{x} \\ \underline{a}_2^T \underline{x} \\ \vdots \\ \underline{a}_m^T \underline{x} \end{bmatrix}$$

$$\frac{\partial l}{\partial \underline{f}} = \left[\frac{\partial l}{\partial f_1}, \cdots \frac{\partial l}{\partial f_m}\right]$$

$$\frac{\partial \ell}{\partial \underline{x}} = \frac{\partial \ell}{\partial \underline{f}} \frac{\partial \underline{f}}{\partial \underline{x}} = \frac{\partial \ell}{\partial \underline{f}} \frac{\partial}{\partial \underline{x}} (A \underline{x}) = \frac{\partial \ell}{\partial \underline{f}} A$$

$$\frac{\partial \ell}{\partial \underline{a}_1} = \frac{\partial \ell}{\partial \underline{f}} \frac{\partial \underline{f}}{\partial \underline{a}_1} = \left[\frac{\partial \ell}{\partial f_1}, \frac{\partial \ell}{\partial f_2} \cdots \frac{\partial \ell}{\partial f_m}\right] \begin{bmatrix} \frac{\partial f_1}{\partial \underline{a}_1} \\ \frac{\partial f_2}{\partial \underline{a}_1} \to 0 \\ \vdots \\ \frac{\partial f_m}{\partial \underline{a}_1} \to 0 \end{bmatrix}$$

$$= \frac{\partial \ell}{\partial f_1} \frac{\partial f_1}{\partial \underline{a}_1}$$

$$= \frac{\partial \ell}{\partial f_1} \frac{\partial}{\partial \underline{a}_1} (\underline{a}_1^T \underline{x}) = \frac{\partial \ell}{\partial f_1} \underline{x}^T$$

$$\frac{\partial \ell}{\partial \underline{a}_i} = \frac{\partial \ell}{\partial f_i} \underline{x}^T$$

$$\frac{\partial \ell}{\partial A} = \begin{bmatrix} \longleftarrow \frac{\partial \ell}{\partial \underline{a}_1} \longrightarrow \\ \\ \\ \end{bmatrix}$$

$$= \begin{bmatrix} \longleftarrow \frac{\partial \ell}{\partial f_1} \underline{x}^T \longrightarrow \\ \longleftarrow \frac{\partial \ell}{\partial f_2} \underline{x}^T \longrightarrow \\ \vdots \\ \frac{\partial \ell}{\partial f_m} \underline{x}^T \end{bmatrix}_{m \times n} = \underbrace{\begin{bmatrix} \frac{\partial \ell}{\partial f_1} \\ \frac{\partial \ell}{\partial f_2} \\ \vdots \\ \frac{\partial \ell}{\partial f_m} \end{bmatrix}_{m \times 1} \underline{x}^T_{1 \times n}}_{\text{outer product}}$$

$$\underline{x}\,\underline{y}^T$$

$$\frac{\partial \ell}{\partial A} = \left(\frac{\partial \ell}{\partial \underline{f}}\right)^T \underline{x}^T$$

$$\underline{x}^T \underline{y}$$

inner product
dot product

The main tool:

$$\underbrace{\frac{\partial l}{\partial \underline{f}}}_{\text{row vector}} \frac{\partial \underline{f}}{\partial \underline{x}} = \frac{\partial l}{\partial f_1}\frac{\partial f_1}{\partial \underline{x}} + \frac{\partial l}{\partial f_2}\frac{\partial f_2}{\partial \underline{x}} + \cdots + \frac{\partial l}{\partial f_m}\frac{\partial f_m}{\partial \underline{x}}$$

$$\frac{\partial l}{\partial \underline{f}} \frac{\partial \underline{f}}{\partial A} = \frac{\partial l}{\partial f_1}\frac{\partial f_1}{\partial A} + \frac{\partial l}{\partial f_2}\frac{\partial f_2}{\partial A} + \cdots + \frac{\partial l}{\partial f_m}\frac{\partial f_m}{\partial A}$$

$$\frac{\partial f_1}{\partial A} = \begin{bmatrix} \boxed{\frac{\partial f_1}{\partial a_{11}} \cdots \frac{\partial f_1}{\partial a_{1n}}} \\ \vdots \\ \frac{\partial f_1}{\partial a_{m1}} \cdots \frac{\partial f_1}{\partial a_{mn}} \end{bmatrix} = \begin{bmatrix} \leftarrow \underline{x}^T \rightarrow \\ \leftarrow \underline{0}^T \rightarrow \\ \leftarrow \underline{0}^T \rightarrow \\ \vdots \\ \leftarrow \underline{0}^T \rightarrow \end{bmatrix}$$

$$\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{bmatrix} = \begin{bmatrix} \underline{a}_1^T \underline{x} \\ \underline{a}_2^T \underline{x} \\ \vdots \\ \underline{a}_m^T \underline{x} \end{bmatrix}$$

Scalar - Matrix multiplication

$$F(\alpha, X) = \alpha X \qquad X \in \mathbb{R}^{m\times n}$$
$$\alpha \in \mathbb{R},\ F \in \mathbb{R}^{m\times n}$$

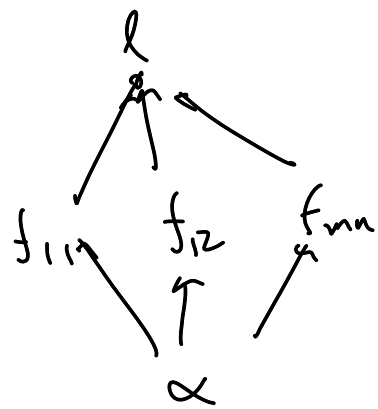
Find $\frac{\partial l}{\partial \alpha}$, $\frac{\partial l}{\partial X}$. Given $\frac{\partial l}{\partial F}$

$$\ell(F(\alpha, X)) \qquad F = \begin{bmatrix} f_{11} & f_{12} & \cdots & f_{1n} \\ \vdots & \vdots & & \vdots \\ f_{m1} & f_{m2} & \cdots & f_{mn} \end{bmatrix}$$

$$\frac{\partial \ell}{\partial \alpha} \neq \frac{\partial \ell}{\partial F} \frac{\partial F}{\partial \alpha}$$

$$\frac{\partial \ell}{\partial \alpha} = \frac{\partial \ell}{\partial f_{11}} \frac{\partial f_{11}}{\partial \alpha} + \frac{\partial \ell}{\partial f_{12}} \frac{\partial f_{12}}{\partial \alpha} + \cdots + \frac{\partial \ell}{\partial f_{mn}} \frac{\partial f_{mn}}{\partial \alpha}$$

$$\frac{\partial \ell}{\partial \alpha} = \sum_i \sum_j \underbrace{\frac{\partial \ell}{\partial f_{ij}}}_{\uparrow \text{ given}} \underbrace{\frac{\partial f_{ij}}{\partial \alpha}}_{\text{find ?}}$$



$$\frac{\partial f_{ij}}{\partial \alpha} = \frac{\partial}{\partial \alpha} (\alpha X)_{ij} = \frac{\partial}{\partial \alpha} (\alpha x_{ij}) = x_{ij}$$

$$\frac{\partial \ell}{\partial \alpha} = \sum_i \sum_j \frac{\partial \ell}{\partial f_{ij}} x_{ij} \qquad X = \begin{bmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & & \vdots \\ x_{m1} & \cdots & x_{mn} \end{bmatrix}$$

$$\frac{\partial \ell}{\partial \alpha} = \left[\frac{\partial \ell}{\partial \mathrm{vec}(F)} \right]_{1 \times mn} \Big[\mathrm{vec}(X) \Big]_{mn \times 1} \qquad \in \mathbb{R}$$

$$\frac{\partial \ell}{\partial X} = \begin{bmatrix} \frac{\partial \ell}{\partial x_{11}} & \cdots & \frac{\partial \ell}{\partial x_{1n}} \\ \vdots & & \\ \frac{\partial \ell}{\partial x_{m1}} & \cdots & \frac{\partial \ell}{\partial x_{mn}} \end{bmatrix}$$

$$\frac{\partial l}{\partial x_{ij}} = \sum_p \sum_q \frac{\partial l}{\partial f_{pq}} \frac{\partial f_{pq}}{\partial x_{ij}}$$

$$f_{pq} = \alpha x_{pq} \qquad F = \alpha X$$

$\frac{\partial l}{\partial x_{ij}} = \frac{\partial l}{\partial f_{ij}} \alpha$	$i = p$ and $q = j$	$\frac{\partial f_{pq}}{\partial x_{ij}} = \alpha$
	$i \neq p$ OR $q \neq j$	$\frac{\partial f_{pq}}{\partial x_{ij}} = 0$

$$\frac{\partial l}{\partial X} = \begin{bmatrix} \frac{\partial l}{\partial x_{11}} & \cdots & \frac{\partial l}{\partial x_{1n}} \\ \vdots & & \\ \frac{\partial l}{\partial x_{m1}} & \cdots & \frac{\partial l}{\partial x_{mn}} \end{bmatrix} = \begin{bmatrix} \frac{\partial l}{\partial f_{11}} & \cdots & \frac{\partial l}{\partial f_{1n}} \\ \vdots & & \\ \frac{\partial l}{\partial f_{m1}} & \cdots & \frac{\partial l}{\partial f_{mn}} \end{bmatrix} \alpha$$

$$\Rightarrow \frac{\partial l}{\partial X} = \frac{\partial l}{\partial F} \alpha \quad , \quad \frac{\partial l}{\partial \alpha} = \frac{\partial l}{\partial \, vec(F)} \, vec(X)$$

$$F(\alpha, X) = \alpha X$$

$$\underbrace{vec(F(\alpha, X))}_{g} = \alpha \underbrace{vec(X)}_{\underline{y}}$$

$$\underline{g}(\alpha, \underline{y}) = \alpha \underline{y} \Rightarrow \frac{\partial l}{\partial \alpha} = \frac{\partial l}{\partial \underline{g}} \underline{y}$$

$$= \frac{\partial \ell}{\partial \underline{y}} = \frac{\partial \ell}{\partial \underline{g}} (\alpha I) = \frac{\partial \ell}{\partial \underline{g}} \alpha$$

Matrix - matrix multiplication

$$F(A, B) = A_{m\times n} B_{n\times p}$$

$$\begin{bmatrix} - \underline{f}_1^T - \\ - \underline{f}_2^T - \\ \vdots \\ - \underline{f}_m^T - \end{bmatrix} = \begin{bmatrix} - \underline{a}_1^T - \\ - a_2^T - \\ \vdots \\ - a_m^T - \end{bmatrix} \begin{bmatrix} | & | & & | \\ \underline{b}_1 & \underline{b}_2 & \cdots & \underline{b}_p \\ | & | & & | \end{bmatrix}$$

$$= \begin{bmatrix} \underline{a}_1^T \underline{b}_1 & \underline{a}_1^T \underline{b}_2 & \cdots & \underline{a}_1^T \underline{b}_p \\ & \vdots & & \\ & & & \end{bmatrix}$$

$$\begin{bmatrix} - f_1^T - \\ - f_2^T - \\ \\ - f_m^T - \end{bmatrix} = \begin{bmatrix} - \underline{a}_1^T B - \\ - \underline{a}_2^T B - \\ \\ - a_m^T B - \end{bmatrix}$$

$$\underline{f}_i^T = \underline{a}_i^T B \Rightarrow \underline{f}_i = B \underline{a}_i$$

$$\mathrm{vec}(F(A, B)) = \begin{bmatrix} \underline{f}_1 \\ \underline{f}_2 \\ \vdots \\ \underline{f}_m \end{bmatrix}_{mp\times 1} = \begin{bmatrix} B \underline{a}_1 \\ B \underline{a}_2 \\ \vdots \\ B \underline{a}_m \end{bmatrix}$$

$$\frac{\partial l}{\partial B} = \frac{\partial l}{\partial \underline{f}_1}\boxed{\frac{\partial \underline{f}_1}{\partial B}} + \frac{\partial l}{\partial \underline{f}_2}\frac{\partial \underline{f}_2}{\partial B} + \cdots + \frac{\partial l}{\partial \underline{f}_m}\frac{\partial \underline{f}_m}{\partial B}$$

?

come back to this

$$\frac{\partial l}{\partial \underline{a}_1} = \frac{\partial l}{\partial \underline{f}_1}\underbrace{\frac{\partial \underline{f}_1}{\partial \underline{a}_1}}_{B} + \underbrace{\frac{\partial l}{\partial \underline{f}_2}\frac{\partial \underline{f}_2}{\partial \underline{a}_1}}_{0} + \cdots + \underbrace{\frac{\partial l}{\partial \underline{f}_m}\frac{\partial \underline{f}_m}{\partial \underline{a}_m}}_{0}$$

$$\frac{\partial l}{\partial \underline{a}_1} = \frac{\partial l}{\partial f_1} B$$

$$\frac{\partial l}{\partial vec(A)} = \frac{\partial l}{\partial vec(F)} B$$

Consider a function of two variables $f(u(x), v(x))$. Find its derivative,

$$\begin{aligned}\frac{\partial f(u(x), v(x))}{\partial x} &= \lim_{h \to 0} \frac{f(u(x+h), v(x+h)) - f(u(x), v(x))}{h} \\ &= \lim_{h \to 0} \frac{f(u(x) + u'(x)h, v(x) + v'(x)h) - f(u(x), v(x))}{h}\end{aligned}$$

Now $f(u + \delta u, v + \delta v)$ should not be expanded in one step but in two steps. First keep $v + \delta v$ as it is, and expand with respect to $u + \delta u$

$$\lim_{\delta v, \delta u \to 0} f(u + \delta u, v + \delta v) = \lim_{\delta v, \delta u \to 0} f(u, v + \delta v) + f_u'(u, v + \delta v)\delta u,$$

and then do the same with $v + \delta v$,

$$\lim_{\delta v, \delta u \to 0} f(u + \delta u, v + \delta v) = \lim_{\delta v, \delta u \to 0} f(u, v) + f_v'(u, v)\delta v + f_u'(u, v + \delta v)\delta u,$$

We use $\lim_{\delta v, \delta u \to 0} f_u'(u, v + \delta v)\delta u = \lim_{\delta v, \delta u \to 0} f_u'(u, v)\delta u + f_{uv}''(u, v)(\delta v)(\delta u) = \lim_{\delta u \to 0} f_u'(u, v)\delta u$ to get,

$$\lim_{\delta v, \delta u \to 0} f(u + \delta u, v + \delta v) = \lim_{\delta v, \delta u \to 0} f(u, v) + f_v'(u, v)\delta v + f_u'(u, v)\delta u.$$

Going back to the chain rule,

$$\begin{aligned}\frac{\partial f(u(x), v(x))}{\partial x} &= \lim_{h \to 0} \frac{f(u(x) + u'(x)h, v(x) + v'(x)h) - f(u(x), v(x))}{h} \\ &= \lim_{h \to 0} \frac{f(u(x), v(x)) + f_v'(u(x), v(x))v'(x)h + f_u'(u(x), v(x))u'(x)h - f(u(x), v(x))}{h} \\ &= \lim_{h \to 0} \frac{f_v'(u(x), v(x))v'(x)h + f_u'(u(x), v(x))u'(x)h}{h} \\ &= f_v'(u(x), v(x))v'(x) + f_u'(u(x), v(x))u'(x)\end{aligned}$$

Scalar valued vector function chain rule

Consider two functions $f(\mathbf{g}) : \mathrm{R}^m \to \mathrm{R}$, $\mathbf{g}(x) : \mathrm{R} \to \mathrm{R}^m$ that can be composed together $f(\mathbf{g}(x))$. We want to find the derivative of composition $f \circ g$ by chain rule.

Recall that the derivative (Jacobian) of $f(\mathbf{g})$ is a row vector,

$$\frac{\partial f(\mathbf{g})}{\partial \mathbf{g}} = \begin{bmatrix} \frac{\partial f}{\partial g_1} & \frac{\partial f}{\partial g_2} & \dots & \frac{\partial f}{\partial g_m} \end{bmatrix}.$$

And the derivative (Jacobian) of $\mathbf{g}(x)$ is a column vector,

$$\frac{\partial \mathbf{g}(x)}{\partial x} = \begin{bmatrix} \frac{\partial g_1}{\partial x} \\ \frac{\partial g_2}{\partial x} \\ \vdots \\ \frac{\partial g_m}{\partial x} \end{bmatrix}.$$

Note that a vector function is a multi-variate scalar function

$$f(\mathbf{g}(x)) = f(g_1(x), g_2(x), \ldots, g_m(x)).$$

We can apply the multi-variate scalar function chain rule,

$$\begin{aligned} \frac{\partial}{\partial x} f(\mathbf{g}(x)) &= f'_{g_1}(g_1(x), \ldots, g_m(x)) g'_1(x) + \cdots + f'_{g_m}(g_1(x), \ldots, g_m(x)) g'_m(x) \\ &= f'_{g_1}(\mathbf{g}(x)) g'_1(x) + \cdots + f'_{g_m}(\mathbf{g}(x)) g'_m(x). \end{aligned}$$

The derivatives of $\mathbf{g}$ can be separated from derivatives of f as vector multiplication,

$$\frac{\partial}{\partial x} f(\mathbf{g}(x)) = \begin{bmatrix} f'_{g_1}(\mathbf{g}(x)) & \cdots & f'_{g_m}(\mathbf{g}(x)) \end{bmatrix} \begin{bmatrix} g'_1(x) \\ \vdots \\ g'_m(x) \end{bmatrix}.$$

Hence the chain rule for vector derivatives works out for our definition of vector derivatives,

$$\frac{\partial}{\partial \mathbf{x}} f(\mathbf{g}(x)) = \frac{\partial f(\mathbf{g}(x))}{\partial \mathbf{g}} \frac{\partial \mathbf{g}(x)}{\partial x}.$$

Note that the order of multiplication matters, specifically

$$\frac{\partial}{\partial \mathbf{x}} f(\mathbf{g}(x)) \neq \frac{\partial \mathbf{g}(x)}{\partial x} \frac{\partial f(\mathbf{g}(x))}{\partial \mathbf{g}}.$$

This is a consequence of row-vector convention. If we chose a column-vector convention the result will be completely different.

General chain rule

Let the function be $\mathbf{f}(\mathbf{g}) : \mathrm{R}^m \rightarrow \mathrm{R}^n$ and $\mathbf{g}(\mathbf{x}) : \mathrm{R}^p \rightarrow \mathrm{R}^m$, then the derivative (Jacobian) of their composition $\mathbf{f} \circ \mathbf{g}$ is

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{f}(\mathbf{g}(\mathbf{x})) = \frac{\partial \mathbf{f}(\mathbf{g}(\mathbf{x}))}{\partial \mathbf{g}} \frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x}}$$

Computational complexity of Forward vs Reverse mode differentiation

Consider three functions, $\mathbf{h}(\mathbf{x}) : \mathrm{R}^m \rightarrow \mathrm{R}^n$, $\mathbf{g}(\mathbf{h}) : \mathrm{R}^n \rightarrow \mathrm{R}^p$ and $\mathbf{f}(\mathbf{g}) : \mathrm{R}^p \rightarrow \mathrm{R}^q$ chained together for composition $\mathbf{f}(\mathbf{g}(\mathbf{h}(\mathbf{x}))) : \mathrm{R}^m \rightarrow \mathrm{R}^q$. To find the derivative (Jacobian) the composite function, we use chain rule:

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{f}(\mathbf{g}(\mathbf{h}(\mathbf{x}))) = \frac{\partial \mathbf{f}}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{x}}$$

Computational complexity of matrix multiplication

Let's say you multiply two matrices $A \in \mathrm{R}^{m \times n}$ and $B \in \mathrm{R}^{n \times p}$, total number of additions and multiplications (floating point operations) can be calculated by

$$C = AB = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_m^\top \end{bmatrix} \begin{bmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_p \end{bmatrix},$$

where $\mathbf{a}_i^\top$ are the row-vectors of matrix A and $\mathbf{b}_i$ are the column vectors of matrix B. Then matrix C is written as

$$C = \begin{bmatrix} \mathbf{a}_1^\top \mathbf{b}_1 & \mathbf{a}_1^\top \mathbf{b}_2 & \dots & \mathbf{a}_1^\top \mathbf{b}_p \\ \mathbf{a}_2^\top \mathbf{b}_1 & \mathbf{a}_2^\top \mathbf{b}_2 & \dots & \mathbf{a}_2^\top \mathbf{b}_p \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_m^\top \mathbf{b}_1 & \mathbf{a}_m^\top \mathbf{b}_2 & \dots & \mathbf{a}_m^\top \mathbf{b}_p \end{bmatrix}$$

We note that C matrix has pm elments and each element requires computing dot product of size n vectors,

$$\mathbf{a}_i^\top \mathbf{b}_j = a_{i1} b_{j1} + a_{i2} b_{j2} + \cdots + a_{in} b_{in}.$$

Each dot product requires n multiplications and $n - 1$ additions. Hence matrix multiplication which has pm dot products requires $pm(n + n - 1)$ (floating point) operations.

Matrix multiplication has a computation complexity of $O(pmn)$ for matrices of size $m \times n$ and $n \times p$.

Computational complexity of forward-mode differentiation

In forward diff, we compute computaional complexity from input side to the output side.

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{f}(\mathbf{g}(\mathbf{h}(\mathbf{x}))) = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{g}} \left(\frac{\partial \mathbf{g}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{x}} \right) \right)$$

The first two matrix multiplications $X_{p \times n} = \left(\frac{\partial \mathbf{g}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{x}} \right)$ are of the size $p \times m$ and $m \times n$, resulting in $O(pmn)$ complexity.

The second two matrix multiplications $\left(\frac{\partial \mathbf{f}}{\partial \mathbf{g}} X_{p \times n} \right)$ are of the size $q \times p$ and $p \times n$, resulting in $O(qpn)$ complexity.

The total computational complexity of forward differentiation is $O(qpn + pmn) = O((qp + pm)n)$.

For a longer chain of functions of Jacobians of shape $q_i \times p_i$ with $(p_i = q_{i-1})$.

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{f}_n(\ldots \mathbf{f}_2(\mathbf{f}_1(\mathbf{x}))) = \frac{\partial \mathbf{f}_n}{\partial \mathbf{f}_{n-1}}_{q_n \times p_n} \cdots \frac{\partial \mathbf{f}_2}{\partial \mathbf{f}_1}_{q_1 \times p_1} \frac{\partial \mathbf{f}_1}{\partial \mathbf{x}}_{q_0 \times p_0}$$

We get a computational complexity that looks like $O((\sum_{i=1}^{n} q_i p_i) p_0)$. Note that the size of input p_0 is the only common factor for the entire chain.

Computational complexity of reverse-mode diff

In reverse-mode diff, we compute computaional complexity from input side to the output side.

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{f}(\mathbf{g}(\mathbf{h}(\mathbf{x}))) = \left(\left(\frac{\partial \mathbf{f}}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{h}} \right) \frac{\partial \mathbf{h}}{\partial \mathbf{x}} \right)$$

The first two matrix multiplications $X_{q \times p} = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{h}} \right)$ are of the size $q \times p$ and $p \times m$, resulting in $O(qpm)$ complexity.

The second two matrix multiplications $\left(X_{q \times p} \frac{\partial \mathbf{h}}{\partial \mathbf{x}}\right)$ are of the size $q \times p$ and $p \times n$, resulting in $O(qpn)$ complexity.

The total computational complexity of forward differentiation is $O(qpm + qmn) = O(q(pm + mn))$.

For a longer chain of functions of Jacobians of shape $q_i \times p_i$ with $(p_i = q_{i-1})$.

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{f}_n(\ldots \mathbf{f}_2(\mathbf{f}_1(\mathbf{x}))) = \frac{\partial \mathbf{f}_n}{\partial \mathbf{f}_{n-1}}_{q_n \times p_n} \cdots \frac{\partial \mathbf{f}_2}{\partial \mathbf{f}_1}_{q_1 \times p_1} \frac{\partial \mathbf{f}_1}{\partial \mathbf{x}}_{q_0 \times p_0}$$

We get a computational complexity that looks like $O(q_n(\sum_{i=0}^{n-1} q_i p_i))$. Note that the size of output q_n is the only common factor for the entire chain.

Reverse-mode differentiation is called backpropagation

Reverse-mode differentiation is called backpropagation in neural networks. It is more popular because most of the times you compute the derivatives of the loss function which is a scalar function with output dimension as only 1. This makes reverse-mode differentiation clearly superior for loss function gradient.

Implementation of forward/reverse mode differentiation in Pytorch

Reverse mode

Let's compute the derivatives of

$$f(x_1, x_2) = x_1 x_2 + sin(x_1)$$

In [24]:

```
import torch as t


x1 = t.Tensor([2]) # Initialize a tensor
x1.requires_grad_(True) # enable gradient tracking
x2 = t.Tensor([7])
x2.requires_grad_(True)
f = x1 * x2 + x1.sin() # Create computation graph
print("Before backward:", x1.grad, x2.grad) # print df/dx1 and df/dx2

f.backward(t.Tensor([1])) # Intialize backward computation with dg/df = 1

print("After backward:", x1.grad, x2.grad) # print df/dx1 and df/dx2
```

```
Before backward: None None
After backward: tensor([6.5839]) tensor([2.])
```

Forward mode

In [25]:
```
import torch as t
import torch.autograd.forward_ad as fwAD
x1 = t.Tensor([2]) # Initialize a tensor
x2 = t.Tensor([7]) # Initialize a tensor
with fwAD.dual_level():
    x1_pd = fwAD.make_dual(x1, t.Tensor([1])) # Intialize dx1/dz = 1
    x2_pd = fwAD.make_dual(x2, t.Tensor([0])) # Intialize dx2/dz = 0

    f = x1_pd * x2_pd + x1_pd.sin() # compute the function
    dfdx1 = fwAD.unpack_dual(f).tangent
    print(dfdx1)


    x1_pd = fwAD.make_dual(x1, t.Tensor([0])) # Intialize dx1/dz = 0
    x2_pd = fwAD.make_dual(x2, t.Tensor([1])) # Intialize dx2/dz = 1

    f = x1_pd * x2_pd + x1_pd.sin() # compute the function
    dfdx2 = fwAD.unpack_dual(f).tangent
    print(dfdx2)
```

```
tensor([6.5839])
tensor([2.])
```

Vector Jacobian product (vjp) for reverse-mode differentiation

Typical output of a neural network is a loss function. Loss function is always a scalar. Most neural network libraries implement reverse-mode differentiation only for a scalar output.

Hence, the first Jacobian on the output side of chain rule is a row-vector.

$$\frac{\partial}{\partial \mathbf{x}} l(\mathbf{f}(\mathbf{g}(\mathbf{x}))) = \frac{\partial l}{\partial \mathbf{f}} \frac{\partial \mathbf{f}}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{x}},$$

$\mathbf{g}(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}^p$, $\mathbf{f}(\mathbf{g}) : \mathbb{R}^p \to \mathbb{R}^q$ and $l(\mathbf{f}) : \mathbb{R}^q \to \mathbb{R}$.

When you are writing a programmatic derivative function for reverse mode differentation, the function does two things:

1. Compute the local Jacobian of the function for example $\frac{\partial \mathbf{f}}{\partial \mathbf{g}}$.
2. Left multiply the Jacobian with a row-vector of accumulated derivative so far. For example, $\frac{\partial l}{\partial \mathbf{f}} \frac{\partial \mathbf{f}}{\partial \mathbf{g}}$.

The template of the function is like this:

```
def g(arg1, arg2):
    # Compute g
    return g
```

```python
def g_vjp(arg1, arg2, dl_dg):
    # Compute vector Jacobian product with respect to each oargument
    return dl_arg1, dl_arg2
```

If you are given a function $\mathbf{g}(\mathbf{x})$, and you want to implement `vjp` function for it. It is often easier to imagine a sclar loss function $l(\mathbf{g}(\mathbf{x}))$ whose accumulated gradient $\frac{\partial l}{\partial \mathbf{g}}$ is given as an input argument. The function `vjp` returns the derivative of the loss function with respect to the inputs,

$$\frac{\partial}{\partial \mathbf{x}} l(\mathbf{g}(\mathbf{x})) = \frac{\partial l}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{x}},$$

which looks like a vector Jacobian product, but you are free to not compute the Jacobian separately. Sometimes it is computationally harder to compute the jacobian separately then multiply it by the vector.

Jacobian vector product (jvp) for forward-mode differentiation

It is also common to implment foward mode differentiation with only a scalar input assumption, say t.

Say $\mathbf{h}(\mathbf{x}) : \mathbb{R}^m \to \mathbb{R}^n$, $\mathbf{g}(\mathbf{h}) : \mathbb{R}^n \to \mathbb{R}^p$ and $\mathbf{f}(\mathbf{g}) : \mathbb{R}^p \to \mathbb{R}^q$

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{f}(\mathbf{g}(\mathbf{h}(\mathbf{x}))) = \frac{\partial \mathbf{f}}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{x}}$$

You can assume $\mathbf{x}$ to be function of scalar $t \in \mathbb{R}$, $\mathbf{x}(t)$. Then the chain rule is

$$\frac{\partial}{\partial t} \mathbf{f}(\mathbf{g}(\mathbf{h}(\mathbf{x}(t)))) = \frac{\partial \mathbf{f}}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial t}$$

You can compute the derivative with respect to one element of $\mathbf{x}$ at a time by setting that element's derivative to be 1 and the rest to be zero. For example, if you want to compute the $\frac{\partial \mathbf{f}}{\partial x_2}$ then set

$$\frac{\partial \mathbf{x}}{\partial t} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

.

For forward pass you typically implement a function called `jvp` which stands for Jacobian vector product:

1. The Jacobian is the local derivative. For example $\frac{\partial \mathbf{h}}{\partial \mathbf{x}}$
2. Multiplication of the jacobian with an incoming accumulated gradient which is a column-vector. For example, $\frac{\partial \mathbf{x}}{\partial t}$.

The template of the function is like this:

```python
def g(arg1, arg2):
    # Compute g
    return g

def g_jvp(arg1, arg2, darg1_dt, darg2_dt):
    # Compute Jacobian vector product with respect to t
    return dg_dt
```

If you are given a function $\mathbf{g}(\mathbf{x})$, and you want to implement `jvp` function for it. It is often easier to imagine a sclar input variable $\mathbf{g}(\mathbf{x}(t))$ whose accumulated gradient $\frac{\partial \mathbf{x}}{\partial t}$ are given as an input argument. The function `jvp` returns the derivative of the output with respect to the scalar input t,

$$\frac{\partial}{\partial t}\mathbf{g}(\mathbf{x}(t)) = \frac{\partial \mathbf{g}}{\partial \mathbf{x}}\frac{\partial \mathbf{x}}{\partial t},$$

which looks like a Jacobian vector product, but you are free to not compute the Jacobian separately. Sometimes it is computationally harder to compute the jacobian separately then multiply it by the vector.

Implementing numpy backpropagation for various operations

In [1]:
```python
# Refs:
# 1. https://github.com/karpathy/micrograd/tree/master/micrograd
# 2. https://github.com/mattjj/autodidact
# 3. https://github.com/mattjj/autodidact/blob/master/autograd/numpy/numpy_v
from collections import namedtuple
import numpy as np


def unbroadcast(target, g, axis=0):
    """Remove broadcasted dimensions by summing along them.
    When computing gradients of a broadcasted value, this is the right thing
    do when computing the total derivative and accounting for cloning.
    """
    while np.ndim(g) > np.ndim(target):
        g = g.sum(axis=axis)
    for axis, size in enumerate(target.shape):
        if size == 1:
            g = g.sum(axis=axis, keepdims=True)
```

```
    if np.iscomplexobj(g) and not np.iscomplex(target):
        g = g.real()
    return g

Op = namedtuple('Op', ['apply',
                       'vjp',
                       'name',
                       'nargs'])
```

Vector Jacobian Product for addition

$$\mathbf{f}(\mathbf{a}, \mathbf{b}) = \mathbf{a} + \mathbf{b}$$

where $\mathbf{a}, \mathbf{b}, \mathbf{f} \in \mathrm{R}^n$

Let $l(\mathbf{f}(\mathbf{a}, \mathbf{b})) \in \mathrm{R}$ be the eventual scalar output. We find $\frac{\partial l}{\partial \mathbf{a}}$ and $\frac{\partial l}{\partial \mathbf{b}}$ for Vector Jacobian product.

$$\frac{\partial}{\partial \mathbf{a}} l(\mathbf{f}(\mathbf{a}, \mathbf{b})) = \frac{\partial l}{\partial \mathbf{f}} \frac{\partial}{\partial \mathbf{a}}(\mathbf{a} + \mathbf{b}) = \frac{\partial l}{\partial \mathbf{f}}(\mathbf{I}_{n \times n} + 0_{n \times n}) = \frac{\partial l}{\partial \mathbf{f}}$$

Similarly,

$$\frac{\partial}{\partial \mathbf{b}} l(\mathbf{f}(\mathbf{a}, \mathbf{b})) = \frac{\partial l}{\partial \mathbf{f}}$$

In [2]:

```
def add_vjp(dldf, a, b):
    dlda = unbroadcast(a, dldf)
    dldb = unbroadcast(b, dldf)
    return dlda, dldb

add = Op(
    apply=np.add,
    vjp=add_vjp,
    name='+',
    nargs=2)
```

VJP for element-wise multiplication

$$f(\alpha, \beta) = \alpha\beta$$

where $\alpha, \beta, f \in \mathrm{R}$

Let $l(f(\alpha, \beta)) \in \mathrm{R}$ be the eventual scalar output. We find $\frac{\partial l}{\partial \alpha}$ and $\frac{\partial l}{\partial \beta}$ for Vector Jacobian product.

$$\frac{\partial}{\partial \alpha} l(f(\alpha, \beta)) = \frac{\partial l}{\partial f} \frac{\partial}{\partial \alpha}(\alpha\beta) = \frac{\partial l}{\partial f}\beta$$

$$\frac{\partial}{\partial \beta} l(f(\alpha, \beta)) = \frac{\partial l}{\partial f} \frac{\partial}{\partial \beta}(\alpha\beta) = \frac{\partial l}{\partial f}\alpha$$

In [3]:
```python
def mul_vjp(dldf, a, b):
    dlda = unbroadcast(a, dldf * b)
    dldb = unbroadcast(b, dldf * a)
    return dlda, dldb

mul = Op(
    apply=np.multiply,
    vjp=mul_vjp,
    name='*',
    nargs=2)
```

VJP for matrix-matrix, matrix-vector and vector-vector multiplication

Case 1: VJP for vector-vector multiplication

$$f(\mathbf{a}, \mathbf{b}) = \mathbf{a}^\top \mathbf{b}$$

where $f \in \mathrm{R}$, and $\mathbf{b}, \mathbf{a} \in \mathrm{R}^n$

Let $l(f(\mathbf{a}, \mathbf{b})) \in \mathrm{R}$ be the eventual scalar output. We find $\frac{\partial l}{\partial \mathbf{a}}$ and $\frac{\partial l}{\partial \mathbf{b}}$ for Vector Jacobian product.

$$\frac{\partial}{\partial \mathbf{a}} l(f(\mathbf{a}, \mathbf{b})) = \frac{\partial l}{\partial f} \frac{\partial}{\partial \mathbf{a}}(\mathbf{a}^\top \mathbf{b}) = \frac{\partial l}{\partial f}\mathbf{b}^\top$$

Similarly,

$$\frac{\partial}{\partial \mathbf{b}} l(f(\mathbf{a}, \mathbf{b})) = \frac{\partial l}{\partial f}\mathbf{a}^\top$$

Case 2: VJP for matrix-vector multiplication

Let

$$\mathbf{f}(\mathbf{A}, \mathbf{b}) = \mathbf{A}\mathbf{b}$$

where $\mathbf{f} \in \mathrm{R}^m$, $\mathbf{b} \in \mathrm{R}^n$, and $\mathbf{A} \in \mathrm{R}^{m \times n}$

Let $l(\mathbf{f}(\mathbf{A}, \mathbf{b})) \in \mathrm{R}$ be the eventual scalar output. We want to findfind $\frac{\partial l}{\partial \mathbf{A}}$ and $\frac{\partial l}{\partial \mathbf{b}}$ for Vector Jacobian product.

Let

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_m^\top \end{bmatrix}$$

, where each $\mathbf{a}_i^\top \in \mathrm{R}^{1\times n}$ and $a_{ij} \in \mathrm{R}$.

Define matrix derivative of scalar to be:

$$\frac{\partial l}{\partial \mathbf{A}} = \begin{bmatrix} \frac{\partial l}{\partial a_{11}} & \frac{\partial l}{\partial a_{12}} & \cdots & \frac{\partial l}{\partial a_{1n}} \\ \frac{\partial l}{\partial a_{21}} & \frac{\partial l}{\partial a_{22}} & \cdots & \frac{\partial l}{\partial a_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial l}{\partial a_{m1}} & \frac{\partial l}{\partial a_{m2}} & \cdots & \frac{\partial l}{\partial a_{mn}} \end{bmatrix} = \begin{bmatrix} \frac{\partial l}{\partial \mathbf{a}_1} \\ \frac{\partial l}{\partial \mathbf{a}_2} \\ \vdots \\ \frac{\partial l}{\partial \mathbf{a}_m} \end{bmatrix}$$

$$\frac{\partial}{\partial \mathbf{A}} l(\mathbf{f}(\mathbf{a}, \mathbf{b})) = \frac{\partial l}{\partial \mathbf{f}} \frac{\partial}{\partial \mathbf{A}} (\mathbf{A}\mathbf{b})$$

.

Note that

$$\mathbf{A}\mathbf{b} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_m^\top \end{bmatrix} \mathbf{b} = \begin{bmatrix} \mathbf{a}_1^\top \mathbf{b} \\ \mathbf{a}_2^\top \mathbf{b} \\ \vdots \\ \mathbf{a}_m^\top \mathbf{b} \end{bmatrix}$$

Since $\mathbf{a}_i^\top \mathbf{b}$ is a scalar, it is easier to find its derivative with respect to the matrix $\mathbf{A}$.

$$\frac{\partial}{\partial \mathbf{A}} \mathbf{a}_i^\top \mathbf{b} = \begin{bmatrix} \frac{\partial \mathbf{a}_i^\top \mathbf{b}}{\partial \mathbf{a}_1} \\ \frac{\partial \mathbf{a}_i^\top \mathbf{b}}{\partial \mathbf{a}_2} \\ \vdots \\ \frac{\partial \mathbf{a}_i^\top \mathbf{b}}{\partial \mathbf{a}_i} \\ \vdots \\ \frac{\partial \mathbf{a}_i^\top \mathbf{b}}{\partial \mathbf{a}_m} \end{bmatrix} = \begin{bmatrix} \mathbf{0}_n^\top \\ \mathbf{0}_n^\top \\ \vdots \\ \mathbf{b}^\top \\ \vdots \\ \mathbf{0}_n^\top \end{bmatrix} \in \mathrm{R}^{m \times n}$$

Let

$$\frac{\partial l}{\partial \mathbf{f}} = \begin{bmatrix} \frac{\partial l}{\partial f_1} & \frac{\partial l}{\partial f_2} & \cdots & \frac{\partial l}{\partial f_m} \end{bmatrix}$$

Then

$$\frac{\partial l}{\partial \mathbf{f}} \frac{\partial}{\partial \mathbf{A}} \mathbf{a}_i^\top \mathbf{b} = \begin{bmatrix} \frac{\partial l}{\partial f_1} & \frac{\partial l}{\partial f_2} & \cdots & \frac{\partial l}{\partial f_m} \end{bmatrix} \begin{bmatrix} \mathbf{0}_n^\top \\ \mathbf{0}_n^\top \\ \vdots \\ \mathbf{b}^\top \\ \vdots \\ \mathbf{0}_n^\top \end{bmatrix} = \frac{\partial l}{\partial f_i} \mathbf{b}^\top \in \mathrm{R}^{1 \times n}$$

Returning to our original quest for

$$\frac{\partial}{\partial \mathbf{A}} l(\mathbf{f}(\mathbf{A}, \mathbf{b})) = \frac{\partial l}{\partial \mathbf{f}} \frac{\partial}{\partial \mathbf{A}} \mathbf{A}\mathbf{b} = \frac{\partial l}{\partial \mathbf{f}} \frac{\partial}{\partial \mathbf{A}} \begin{bmatrix} \mathbf{a}_1^\top \mathbf{b} \\ \mathbf{a}_2^\top \mathbf{b} \\ \vdots \\ \mathbf{a}_m^\top \mathbf{b} \end{bmatrix} = \begin{bmatrix} \frac{\partial l}{\partial \mathbf{f}} \frac{\partial}{\partial \mathbf{A}} \mathbf{a}_1^\top \mathbf{b} \\ \frac{\partial l}{\partial \mathbf{f}} \frac{\partial}{\partial \mathbf{A}} \mathbf{a}_2^\top \mathbf{b} \\ \vdots \\ \frac{\partial l}{\partial \mathbf{f}} \frac{\partial}{\partial \mathbf{A}} \mathbf{a}_m^\top \mathbf{b} \end{bmatrix} = \begin{bmatrix} \frac{\partial l}{\partial f_1} \mathbf{b}^\top \\ \frac{\partial l}{\partial f_2} \mathbf{b}^\top \\ \vdots \\ \frac{\partial l}{\partial f_m} \mathbf{b}^\top \end{bmatrix}$$

Note that

$$\begin{bmatrix} \frac{\partial l}{\partial f_1} \mathbf{b}^\top \\ \frac{\partial l}{\partial f_2} \mathbf{b}^\top \\ \vdots \\ \frac{\partial l}{\partial f_m} \mathbf{b}^\top \end{bmatrix} = \begin{bmatrix} \frac{\partial l}{\partial f_1} \\ \frac{\partial l}{\partial f_2} \\ \cdots \\ \frac{\partial l}{\partial f_m} \end{bmatrix} \mathbf{b}^\top = \left(\frac{\partial l}{\partial \mathbf{f}} \right)^\top \mathbf{b}^\top$$

We can group the terms inside a single transpose.

Which results in

$$\frac{\partial}{\partial \mathbf{A}} l(\mathbf{f}(\mathbf{A}, \mathbf{b})) = \left(\mathbf{b} \frac{\partial l}{\partial \mathbf{f}} \right)^\top$$

The derivative with respect to $\mathbf{b}$ is simpler:

$$\frac{\partial}{\partial \mathbf{b}} l(\mathbf{f}(\mathbf{A}, \mathbf{b})) = \frac{\partial l}{\partial \mathbf{f}} \frac{\partial}{\partial \mathbf{b}} (\mathbf{A}\mathbf{b}) = \frac{\partial l}{\partial \mathbf{f}} \mathbf{A}$$

Case 3: VJP for matrix-matrix multiplication

Let

$$\mathbf{F}(\mathbf{A}, \mathbf{B}) = \mathbf{A}\mathbf{B}$$

where $\mathbf{F} \in \mathrm{R}^{m \times p}$, $\mathbf{B} \in \mathrm{R}^{n \times p}$, and $\mathbf{A} \in \mathrm{R}^{m \times n}$

Let $l(\mathbf{F}(\mathbf{A}, \mathbf{B})) \in \mathbb{R}$ be the eventual scalar output. We want to find $\frac{\partial l}{\partial \mathbf{A}}$ and $\frac{\partial l}{\partial \mathbf{B}}$ for Vector Jacobian product.

Note that a matrix-matrix multiplication can be written in terms horizontal stacking of matrix-vector multiplications. Specifically, write $\mathbf{F}$ and $\mathbf{B}$ in terms of their column vectors:

$$\mathbf{B} = \begin{bmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_p \end{bmatrix}$$

$$\mathbf{F} = \begin{bmatrix} \mathbf{f}_1 & \mathbf{f}_2 & \cdots & \mathbf{f}_p \end{bmatrix}.$$

Then for all i

$$\mathbf{f}_i = \mathbf{A}\mathbf{b}_i$$

From the VJP of matrix-vector multiplication, we can write

$$\frac{\partial l}{\partial \mathbf{f}_i} \frac{\partial}{\partial \mathbf{A}} \mathbf{f}_i = \frac{\partial l}{\partial \mathbf{f}_i} \frac{\partial}{\partial \mathbf{A}} (\mathbf{A}\mathbf{b}_i) = \left(\mathbf{b}_i \frac{\partial l}{\partial \mathbf{f}_i} \right)^\top \in \mathbb{R}^{m \times n}$$

and for all $i \neq j$

$$\frac{\partial l}{\partial \mathbf{f}_j} \frac{\partial}{\partial \mathbf{A}} (\mathbf{A}\mathbf{b}_i) = \mathbf{0}_{m \times n}$$

Instead of writing $l(\mathbf{F})$, we can also write $l(\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_p)$, then by chain rule of functions with multiple arguments, we have,

$$\frac{\partial}{\partial \mathbf{A}} l(\mathbf{F}(\mathbf{A}, \mathbf{B})) = \frac{\partial}{\partial \mathbf{A}} l(\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_p) = \frac{\partial l}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_1}{\partial \mathbf{A}} + \frac{\partial l}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_2}{\partial \mathbf{A}} + \cdots + \frac{\partial l}{\partial \mathbf{f}_p} \frac{\partial \mathbf{f}_p}{\partial \mathbf{A}}$$

$$\frac{\partial}{\partial \mathbf{A}} l(\mathbf{F}(\mathbf{A}, \mathbf{B})) = \left(\mathbf{b}_1 \frac{\partial l}{\partial \mathbf{f}_1} \right)^\top + \left(\mathbf{b}_2 \frac{\partial l}{\partial \mathbf{f}_2} \right)^\top + \cdots + \left(\mathbf{b}_p \frac{\partial l}{\partial \mathbf{f}_p} \right)^\top = \left(\mathbf{b}_1 \frac{\partial l}{\partial \mathbf{f}_1} + \mathbf{b}_2 \frac{\partial l}{\partial \mathbf{f}_2} + \cdots + \mathbf{b}_p \frac{\partial l}{\partial \mathbf{f}_p} \right)^\top$$

It turns out that some of outer products can be compactly written as matrix-matrix multiplication:

$$\mathbf{b}_1 \frac{\partial l}{\partial \mathbf{f}_1} + \mathbf{b}_2 \frac{\partial l}{\partial \mathbf{f}_2} + \cdots + \mathbf{b}_p \frac{\partial l}{\partial \mathbf{f}_p} = \begin{bmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_p \end{bmatrix} \begin{bmatrix} \frac{\partial l}{\partial \mathbf{f}_1} \\ \frac{\partial l}{\partial \mathbf{f}_2} \\ \vdots \\ \frac{\partial l}{\partial \mathbf{f}_p} \end{bmatrix} = \mathbf{B} \left(\frac{\partial l}{\partial \mathbf{F}} \right)^\top$$

Hence,

$$\frac{\partial}{\partial \mathbf{A}} l(\mathbf{F}(\mathbf{A}, \mathbf{B})) = \frac{\partial l}{\partial \mathbf{F}} \mathbf{B}^\top$$

The vector Jacobian product for $\mathbf{B}$ can be found by applying the above rule to $\mathbf{F}_2(\mathbf{A}, \mathbf{C}) = \mathbf{F}^\top(\mathbf{A}, \mathbf{B}) = \mathbf{B}^\top \mathbf{A}^\top = \mathbf{C} \mathbf{A}^\top$ where $\mathbf{C} = \mathbf{B}^\top$ and $\mathbf{F}_2 = \mathbf{F}^\top$.

$$\frac{\partial}{\partial \mathbf{C}} l(\mathbf{F}_2(\mathbf{A}, \mathbf{C})) = \frac{\partial l}{\partial \mathbf{F}_2} \mathbf{A}$$

Take transpose of both sides

$$\frac{\partial}{\partial \mathbf{C}^\top} l(\mathbf{F}_2^\top(\mathbf{A}, \mathbf{C})) = \mathbf{A}^\top \frac{\partial l}{\partial \mathbf{F}_2^\top}$$

Put back, $\mathbf{C} = \mathbf{B}^\top$ and $\mathbf{F}_2 = \mathbf{F}^\top$,

$$\frac{\partial}{\partial \mathbf{B}} l(\mathbf{F}(\mathbf{A}, \mathbf{B})) = \mathbf{A}^\top \frac{\partial l}{\partial \mathbf{F}}$$

In [4]:
```
def matmul_vjp(dldF, A, B):
    G = dldF
    if G.ndim == 0:
        # Case 1: vector-vector multiplication
        assert A.ndim == 1 and B.ndim == 1
        dldA = G*B
        dldB = G*A
        return (unbroadcast(A, dldA),
                unbroadcast(B, dldB))

    assert not (A.ndim == 1 and B.ndim == 1)

    # 1. If both arguments are 2-D they are multiplied like conventional mat
    # 2. If either argument is N-D, N > 2, it is treated as a stack of matri
    # residing in the last two indexes and broadcast accordingly.
    if A.ndim >= 2 and B.ndim >= 2:
        dldA = G @ B.swapaxes(-2, -1)
        dldB = A.swapaxes(-2, -1) @ G
```

```python
    if A.ndim == 1:
        # 3. If the first argument is 1-D, it is promoted to a matrix by pre
        #    1 to its dimensions. After matrix multiplication the prepended
        A_ = A[np.newaxis, :]
        G_ = G[np.newaxis, :]
        dldA = G @ B.swapaxes(-2, -1)
        dldB = A_.swapaxes(-2, -1) @ G_ # outer product
    elif B.ndim == 1:
        # 4. If the second argument is 1-D, it is promoted to a matrix by ap
        #    a 1 to its dimensions. After matrix multiplication the appended
        B_ = B[:, np.newaxis]
        G_ = G[:, np.newaxis]
        dldA = G_ @ B_.swapaxes(-2, -1) # outer product
        dldB = A.swapaxes(-2, -1) @ G
    return (unbroadcast(A, dldA),
            unbroadcast(B, dldB))


matmul = Op(
    apply=np.matmul,
    vjp=matmul_vjp,
    name='@',
    nargs=2)
```

In [5]:
```python
def exp_vjp(dldf, x):
    dldx = dldf * np.exp(x)
    return (unbroadcast(x, dldx),)
exp = Op(
    apply=np.exp,
    vjp=exp_vjp,
    name='exp',
    nargs=1)
```

In [6]:
```python
def log_vjp(dldf, x):
    dldx = dldf / x
    return (unbroadcast(x, dldx),)
log = Op(
    apply=np.log,
    vjp=log_vjp,
    name='log',
    nargs=1)
```

In [7]:
```python
def sum_vjp(dldf, x, axis=None, **kwargs):
    if axis is not None:
        dldx = np.expand_dims(dldf, axis=axis) * np.ones_like(x)
    else:
        dldx = dldf * np.ones_like(x)
    return (unbroadcast(x, dldx),)

sum_ = Op(
    apply=np.sum,
    vjp=sum_vjp,
    name='sum',
    nargs=1)
```

In [18]:

```python
def maximum_vjp(dldf, a, b):
    dlda = dldf * np.where(a > b, 1, 0)
    dldb = dldf * np.where(a > b, 0, 1)
    return unbroadcast(a, dlda), unbroadcast(b, dldb)

maximum = Op(
    apply=np.maximum,
    vjp=maximum_vjp,
    name='maximum',
    nargs=2)
```

In [19]:

```python
NoOp = Op(apply=None, name='', vjp=None, nargs=0)
class Tensor:
    __array_priority__ = 100
    def __init__(self, value, grad=None, parents=(), op=NoOp, kwargs={}, rec
        self.value = np.asarray(value)
        self.grad = grad
        self.parents = parents
        self.op = op
        self.kwargs = kwargs
        self.requires_grad = requires_grad

    shape = property(lambda self: self.value.shape)
    ndim  = property(lambda self: self.value.ndim)
    size  = property(lambda self: self.value.size)
    dtype = property(lambda self: self.value.dtype)

    def __add__(self, other):
        cls = type(self)
        other = other if isinstance(other, cls) else cls(other)
        return cls(add.apply(self.value, other.value),
                   parents=(self, other),
                   op=add)
    __radd__ = __add__

    def __mul__(self, other):
        cls = type(self)
        other = other if isinstance(other, cls) else cls(other)
        return cls(mul.apply(self.value, other.value),
                   parents=(self, other),
                   op=mul)
    __rmul__ = __mul__

    def __matmul__(self, other):
        cls = type(self)
        other = other if isinstance(other, cls) else cls(other)
        return cls(matmul.apply(self.value, other.value),
                  parents=(self, other),
                  op=matmul)

    def exp(self):
        cls = type(self)
        return cls(exp.apply(self.value),
                parents=(self,),
                op=exp)
```

```
    def log(self):
        cls = type(self)
        return cls(log.apply(self.value),
                parents=(self, ),
                op=log)

    def __pow__(self, other):
        cls = type(self)
        other = other if isinstance(other, cls) else cls(other)
        return (self.log() * other).exp()

    def __div__(self, other):
        return self * (other**(-1))

    def __sub__(self, other):
        return self + (other * (-1))

    def __neg__(self):
        return self*(-1)

    def sum(self, axis=None):
        cls = type(self)
        return cls(sum_.apply(self.value, axis=axis),
                   parents=(self,),
                   op=sum_,
                   kwargs=dict(axis=axis))

    def maximum(self, other):
        cls = type(self)
        other = other if isinstance(other, cls) else cls(other)
        return cls(maximum.apply(self.value, other.value),
                   parents=(self, other),
                   op=maximum)

    def __repr__(self):
        cls = type(self)
        return f"{cls.__name__}(value={self.value}, op={self.op.name})" if s
        #return f"{cls.__name__}(value={self.value}, parents={self.parents},

    def backward(self, grad):
        self.grad = grad if self.grad is None else (self.grad+grad)
        if self.requires_grad and self.parents:
            p_vals = [p.value for p in self.parents]
            assert len(p_vals) == self.op.nargs
            p_grads = self.op.vjp(grad, *p_vals, **self.kwargs)
            for p, g in zip(self.parents, p_grads):
                p.backward(g)
```

In [20]:

```
Tensor([1, 2]).sum()
```

Out[20]:

```
Tensor(value=3, op=sum)
```

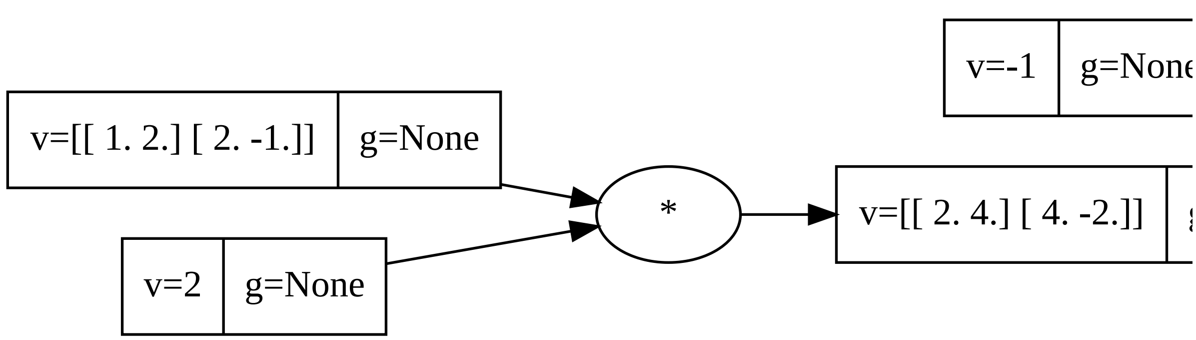
In [68]:

```
try:
    from graphviz import Digraph
```

```python
except ImportError as e:
    import subprocess
    subprocess.call("pip install --user graphviz".split())

def trace(root):
    nodes, edges = set(), set()
    def build(v):
        if v not in nodes:
            nodes.add(v)
            for p in v.parents:
                edges.add((p, v))
                build(p)
    build(root)
    return nodes, edges

def draw_dot(root, format='svg', rankdir='LR'):
    """
    format: png | svg | ...
    rankdir: TB (top to bottom graph) | LR (left to right)
    """
    assert rankdir in ['LR', 'TB']
    nodes, edges = trace(root)
    dot = Digraph(format=format, graph_attr={'rankdir': rankdir}) #, node_at

    for n in nodes:
        vstr = np.array2string(np.asarray(n.value), precision=4)
        gradstr= np.array2string(np.asarray(n.grad), precision=4)
        dot.node(name=str(id(n)), label = f"{{v={vstr} | g={gradstr}}}", sha
        if n.parents:
            dot.node(name=str(id(n)) + n.op.name, label=n.op.name)
            dot.edge(str(id(n)) + n.op.name, str(id(n)))

    for n1, n2 in edges:
        dot.edge(str(id(n1)), str(id(n2)) + n2.op.name)

    return dot
```

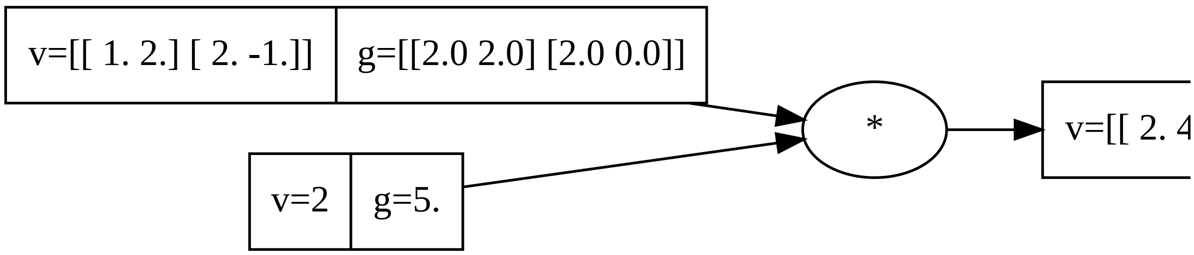
In [69]:
```python
# a very simple example
x = Tensor([[1.0, 2.0],
            [2.0, -1.0]])
y = (x * 2 - 1).maximum(0).sum(axis=-1)
draw_dot(y)
```

Out[69]:



In [70]:
```python
y.backward(np.ones_like(y))
draw_dot(y)
```

Out[70]:

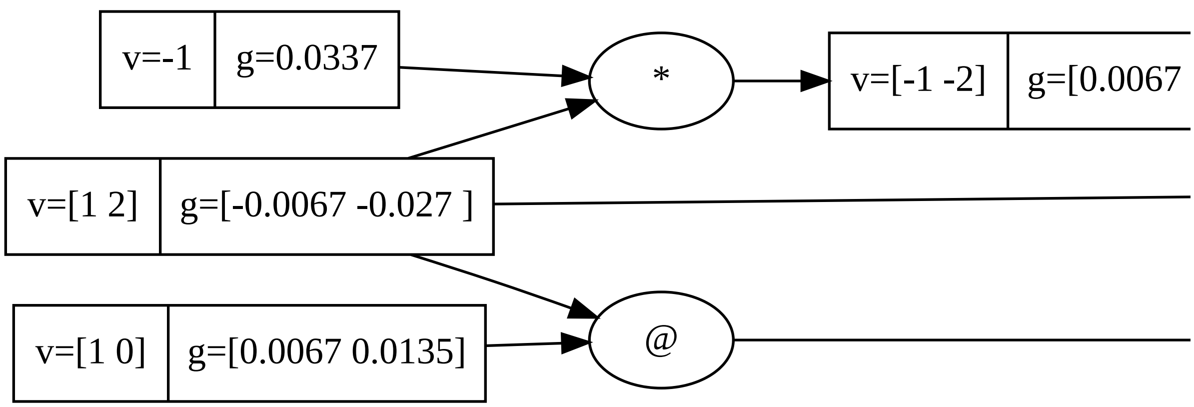


In [73]:
```python
def f_np(x):
    b = [1, 0]
    return (x @ b)*np.exp((-x*x).sum(axis=-1))

def f_T(x):
    b = [1, 0]
    return (x @ b)*(-x*x).sum(axis=-1).exp()

def grad_f(x):
    xT = Tensor(x)
    y = f_T(xT)
    y.backward(np.ones_like(y.value))
    return xT.grad
```

In [74]:
```python
xT = Tensor([1, 2])
out = f_T(xT)
out.backward(1)
print(xT.grad)
draw_dot(out)
```

```
[-0.00673795 -0.02695179]
```

Out[74]:



In [57]:
```python
def numerical_jacobian(f, x, h=1e-10):
    n = x.shape[-1]
    eye = np.eye(n)
    x_plus_dx = x + h * eye # n x n
    num_jac = (f(x_plus_dx) - f(x)) / h # limit definition of the formula #
```

```
    if num_jac.ndim >= 2:
        num_jac = num_jac.swapaxes(-1, -2) # m x n
    return num_jac

# Compare our grad_f with numerical gradient
def check_numerical_jacobian(f, jac_f,  nD=2, **kwargs):
    x = np.random.rand(nD)
    print(x)
    num_jac = numerical_jacobian(f, x, **kwargs)
    print(num_jac)
    print(jac_f(x))
    return np.allclose(num_jac, jac_f(x), atol=1e-06, rtol=1e-4) # m x n

## Throw error if grad_f is wrong
assert check_numerical_jacobian(f_np, grad_f)
```

```
[0.4717993  0.90549333]
[ 0.19560853 -0.30124125]
[ 0.19560835 -0.30124165]
```

Customizing backward step (vector-Jacobian product) in PyTorch

Consider the derivative of Sigmoid activation function

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

$$\frac{\partial}{\partial x}\sigma(x) = -\frac{1}{(1 + \exp(-x))^2}(-\exp(-x))$$

The above derivative is computed by chain rule. However, there is much simpler expression that can avoid unnecessary computations,

$$\frac{\partial}{\partial x}\sigma(x) = \frac{1}{1 + \exp(-x)}\frac{\exp(-x)}{1 + \exp(-x)}$$

$$\frac{\partial}{\partial x}\sigma(x) = \frac{1}{1 + \exp(-x)}\left(1 - \frac{1}{1 + \exp(-x)}\right)$$

$$\frac{\partial}{\partial x}\sigma(x) = \sigma(x)(1 - \sigma(x))$$

In [47]:

```
# https://pytorch.org/tutorials/beginner/basics/autogradqs_tutorial.html
# https://pytorch.org/docs/stable/notes/autograd.html
import torch as t

class SigmoidCustom(t.autograd.Function):
    @staticmethod
    def forward(ctx, x):
        # Because we are saving one of the inputs use `save_for_backward`
        # Save non-tensors and non-inputs/non-outputs directly on ctx
```

```python
        sigmoid_x = 1/(1+(-x).exp())
        ctx.save_for_backward(x, sigmoid_x)
        return sigmoid_x

    @staticmethod
    def backward(ctx, grad_out):
        # A function support double backward automatically if autograd
        # is able to record the computations performed in backward
        x, sigmoid_x = ctx.saved_tensors
        jacobian = sigmoid_x * (1-sigmoid_x)
        return grad_out * jacobian # vector jacobian product

def sigmoid_c(x):
    return SigmoidCustom.apply(x)
```

In [55]:

```python
%%timeit
x = t.tensor([100.], requires_grad=True)
def s(x):
    return 1/(1+(-x).exp())
out = s(s(s(x)))
out.backward(t.tensor([1.]))
x.grad
```

```
191 µs ± 2.97 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

In [56]:

```python
%%timeit
x = t.tensor([100.], requires_grad=True)
out = sigmoid_c(sigmoid_c(sigmoid_c(x)))
out.backward(t.tensor([1.]))
x.grad
```

```
191 µs ± 2.94 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

In [ ]: