Systems Development for Computational Science
CS107/AC207 Fall 2022

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Pair-Programming 6

Automatic differentiation, Forward mode

Issued:	October 7, 2022
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In this pair-programming session you will work on forward mode automatic differentiation. *There will be no coding part for this exercise.*

You should work on the exercises in groups of 3 to 4 students. Your team members can submit the same file. Please indicate your names in a header in the files. See the tutorials on the class website for an example pair-programming workflow.[1] Do not forget to commit and push your work when you are done. Ensure that you are on your *default branch* for this and not, possibly, on your homework branch.

Exercise 1: Forward Mode and Computational Graph

Deliverables:

1. `exercise_1.md` including a Markdown table for the forward primal and tangent traces and the solution for the derivative evaluations at the specified points in an itemized list. *You may write your solution in a Jupyter notebook for this exercise if you prefer the superior math markup. Use the file* `exercise_1.ipynb` *in that case.*
2. `graph_1.png`

You will work with the following function for this exercise

$$f(x_1, x_2) = e^{-(\sin x_1 - \cos x_2)^2}. \tag{1}$$

Draw the computational graph for the function and save it in the file `graph_1.png`. Note that this graph will have 2 inputs since the input vector is $x = [x_1, x_2]^\intercal$. In addition to the computational graph, compute the *forward primal trace* and the *forward tangent trace* of the function given in equation 1. Write your results using a table in `exercise_1.(md|ipynb)`.

Use the trace table and evaluate the following quantities:

$$f\left(\frac{\pi}{2}, \frac{\pi}{3}\right), \qquad \frac{\partial f}{\partial x_1}\left(\frac{\pi}{2}, \frac{\pi}{3}\right), \qquad \frac{\partial f}{\partial x_2}\left(\frac{\pi}{2}, \frac{\pi}{3}\right).$$

Primal trace	Tangent trace	Pass $p^{(j=1)}$	Pass $p^{(j=2)}$
$v_{-1} = x_1 = \dots$	$D_p v_{-1} = p_1$	$D_p v_{-1} = \dots$	$D_p v_{-1} = \dots$
$v_0 = x_2 = \dots$	$D_p v_0 = p_2$	$D_p v_0 = \dots$	$D_p v_0 = \dots$
$v_1 = v_{-1} v_0 = \dots$	$D_p v_1 = v_0 D_p v_{-1} + v_{-1} D_p v_0$	$D_p v_1 = \dots$	$D_p v_1 = \dots$

TABLE 1: Example table for the computation of the forward primal and tangent traces including $j = 2$ passes to compute the directional derivative with j different seed vectors. The ellipses denote *actual* values to be computed. Note that a seed vector pointing in some direction j has two components in this example and is given by $p^{(j)} = [p_1, p_2]^\intercal$.

You may use a similar format as shown in table 1 that follows the notation used in the lecture. Note that the function used in this table does not correspond to equation 1. The forward primal trace can be written symbolically and additionally evaluated at some point $x = [x_1, x_2]^\intercal$. The forward tangent trace is written symbolically because its actual value depends on the chosen seed vector $p = [p_1, p_2]^\intercal$. Table 1 uses two additional columns that evaluate the forward tangent trace for a specific seed vector. Identifying the correct direction the seed vector is pointing to is part of this exercise.

The computational graph for this problem is shown in figure 1. The forward primal and

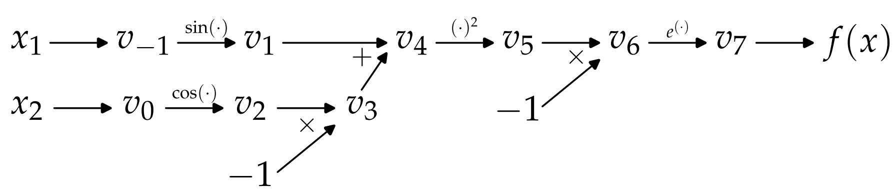

FIGURE 1: Computational graph for the function in equation 1. Some variations are possible.

forward tangent traces can be found in table 2. To evaluate the partial derivative in the di-

Primal trace	Tangent trace	Pass $p^{(j=1)}$	Pass $p^{(j=2)}$
$v_{-1} = x_1 = \frac{\pi}{2}$	$D_p v_{-1} = p_1$	$D_p v_{-1} = 1$	$D_p v_{-1} = 0$
$v_0 = x_2 = \frac{\pi}{3}$	$D_p v_0 = p_2$	$D_p v_0 = 0$	$D_p v_0 = 1$
$v_1 = \sin v_{-1} = 1$	$D_p v_1 = \cos(v_{-1}) D_p v_{-1}$	$D_p v_1 = 0$	$D_p v_1 = 0$
$v_2 = \cos v_0 = \frac{1}{2}$	$D_p v_2 = -\sin(v_0) D_p v_0$	$D_p v_2 = 0$	$D_p v_2 = -\frac{\sqrt{3}}{2}$
$v_3 = -v_2 = -\frac{1}{2}$	$D_p v_3 = -D_p v_2$	$D_p v_3 = 0$	$D_p v_3 = \frac{\sqrt{3}}{2}$
$v_4 = v_1 + v_3 = \frac{1}{2}$	$D_p v_4 = D_p v_1 + D_p v_3$	$D_p v_4 = 0$	$D_p v_4 = \frac{\sqrt{3}}{2}$
$v_5 = v_4^2 = \frac{1}{4}$	$D_p v_5 = 2 v_4 D_p v_4$	$D_p v_5 = 0$	$D_p v_5 = \frac{\sqrt{3}}{2}$
$v_6 = -v_5 = -\frac{1}{4}$	$D_p v_6 = -D_p v_5$	$D_p v_6 = 0$	$D_p v_6 = -\frac{\sqrt{3}}{2}$
$v_7 = e^{v_6} = e^{-\frac{1}{4}}$	$D_p v_7 = e^{v_6} D_p v_6$	$D_p v_7 = 0$	$D_p v_7 = -e^{-\frac{1}{4}} \frac{\sqrt{3}}{2}$

TABLE 2: Forward primal and tangent traces for the function in equation 1, evaluated at $x = [\frac{\pi}{2}, \frac{\pi}{3}]^\intercal$.

[1] https://harvard-iacs.github.io/2022-CS107/pages/tutorials.html#tutorial-pp

rection of coordinate x_1, the seed vector has to be $p^{(1)} = [1,0]^\intercal$ and for the partial derivative in direction of x_2 it has to be $p^{(2)} = [0,1]^\intercal$. From the last row in table 1 we find $f(x) = v_7$, $\frac{\partial f}{\partial x_1}\Big|_x = D_p v_7$ for the seed vector $p^{(1)}$ and $\frac{\partial f}{\partial x_2}\Big|_x = D_p v_7$ for the seed vector $p^{(2)}$.

Exercise 2: (Optional) Evaluation Trace of a Vector Function

Deliverables:

1. `exercise_2.md` including a Markdown table for the forward primal and tangent traces and the solution for the derivative evaluations at the specified points in an itemized list. *You may write your solution in a Jupyter notebook for this exercise if you prefer the superior math markup. Use the file* `exercise_2.ipynb` *in that case.*

Note: this exercise is optional for submission. It is recommended you try to solve it or come back to it when you are working on the project. Your automatic differentiation code must be able to do forward mode with vector functions that take high dimensional inputs eventually. That is $f\colon \mathbb{R}^m \mapsto \mathbb{R}^n$ for $m, n > 1$.

Let

$$f(x_1, x_2) = \begin{bmatrix} x_1^2 + x_2^2 \\ e^{x_1 + x_2} \end{bmatrix}. \tag{2}$$

Write the evaluation trace for this vector function and its derivatives. Evaluate the vector function and its gradient $\nabla f(x)$ at the point $x = [1,1]^\intercal$. Note that the gradient of this vector function is

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}. \tag{3}$$

The forward primal and forward tangent traces can be found in table 3. From the table we find that

$$f(1,1) = \begin{bmatrix} 2 \\ e^2 \end{bmatrix} \tag{4}$$

Primal trace	Tangent trace	Pass $p^{(j=1)}$	Pass $p^{(j=2)}$
$v_{-1} = x_1 = 1$	$D_p v_{-1} = p_1$	$D_p v_{-1} = 1$	$D_p v_{-1} = 0$
$v_0 = x_2 = 1$	$D_p v_0 = p_2$	$D_p v_0 = 0$	$D_p v_0 = 1$
$v_1 = v_{-1}^2 = 1$	$D_p v_1 = 2v_{-1} D_p v_{-1}$	$D_p v_1 = 2$	$D_p v_1 = 0$
$v_2 = v_0^2 = 1$	$D_p v_2 = 2v_0 D_p v_0$	$D_p v_2 = 0$	$D_p v_2 = 2$
$v_3 = v_{-1} + v_0 = 2$	$D_p v_3 = D_p v_{-1} + D_p v_0$	$D_p v_3 = 1$	$D_p v_3 = 1$
$v_4 = v_1 + v_2 = 2$	$D_p v_4 = D_p v_1 + D_p v_2$	$D_p v_4 = 2$	$D_p v_4 = 2$
$v_5 = e^{v_3} = e^2$	$D_p v_5 = e^{v_3} D_p v_3$	$D_p v_5 = e^2$	$D_p v_5 = e^2$

TABLE 3: Forward primal and tangent traces for the vector function in equation 2, evaluated at $x = [1,1]^\intercal$.

and its gradient is

$$\nabla f(1,1) = \begin{bmatrix} 2 & 2 \\ e^2 & e^2 \end{bmatrix}. \tag{5}$$